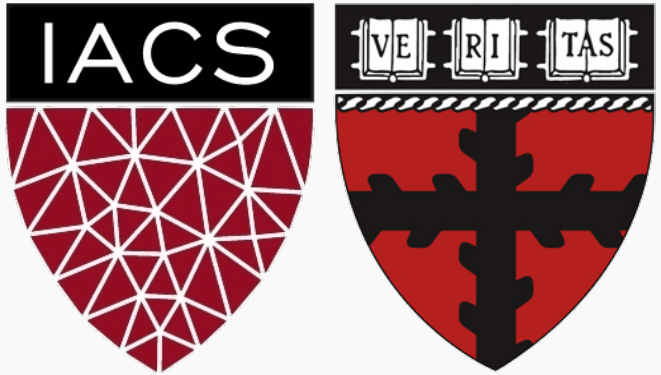
Multi-Linear Regression

CS109A Introduction to Data Science

Pavlos Protopapas, Natesh Pillai



Lecture Outline

Announcements

Q&A

Part A:

Multi-linear regression

Part B:

Polynomial Regression

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Part A:

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Announcements

- Videos should be available now!
- Deadline for quiz/ex for Monday's lectures are now on the following Friday @9:30am
- Deadline for quiz/ex for Wednesday's lectures remain the same: the following Monday @9:30am
- Homework 1 is due tonight @11:59.99999999999999pm
- Homework 2 will be released on today somewhere on planet earth

Lecture Outline

Announcements

Q&A

Part A:

Multi-linear regression

Part B:

Polynomial Regression

How would we choose between a kNN and a linear model to predict our response variable?

Can kNN be used when there are multiple predictor variables?

Does kNN work on binary outcomes?

What would you do if multiple k values are equally good for kNN regression?

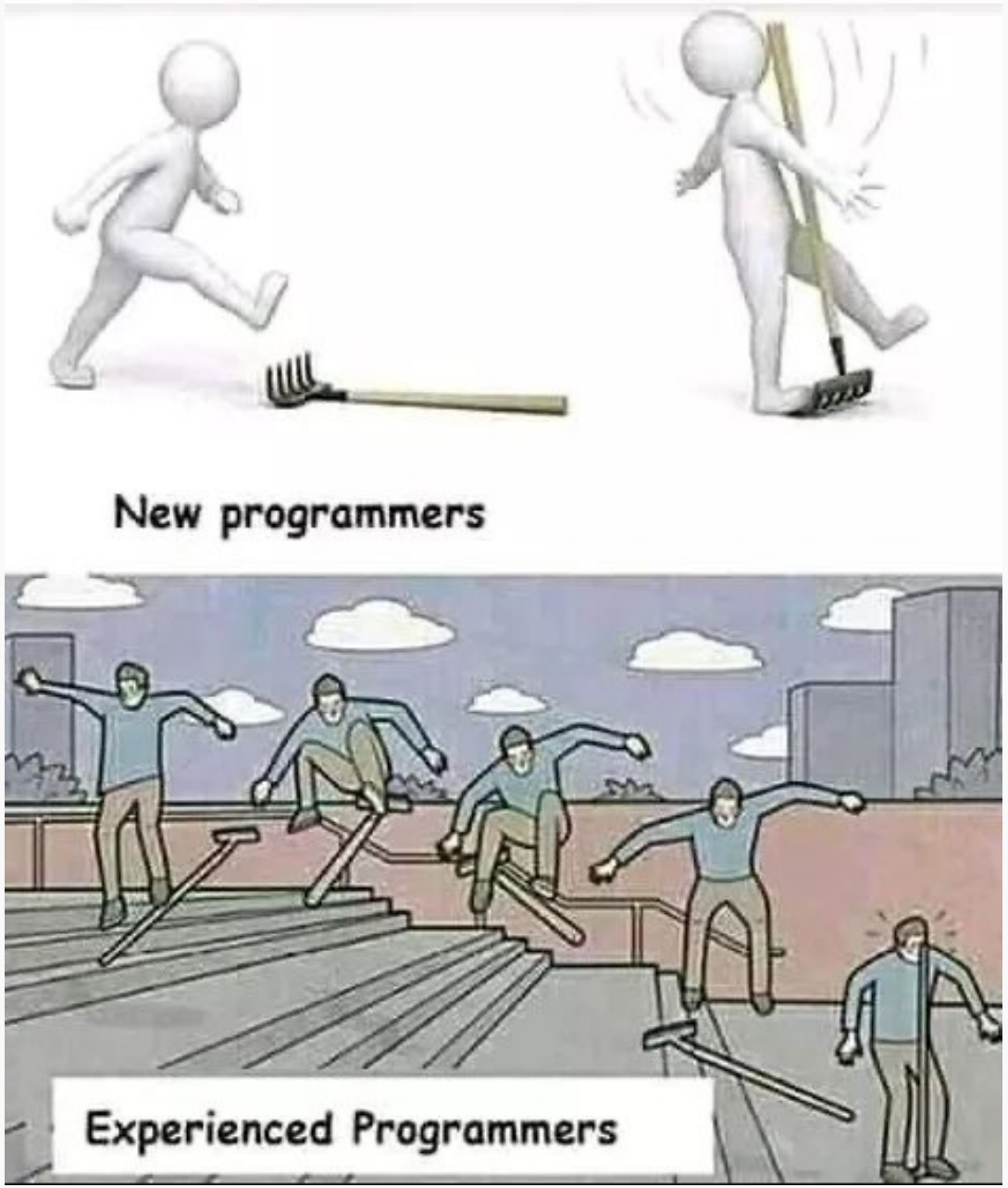
Does gradient descent guarantee the same solution as the analytical one?

Can we have some more scenarios on when mean absolute error is useful as a loss function?

How do we make sure that we are not taking a biased subset ?

What should the train-test split be?

What is the difference between inference and prediction?


New programmers
Experienced Programmers

Lecture Outline

Announcements

Q&A

Part A:

Multi-linear regression

Part B:

Polynomial Regression

Multiple Linear Regression

If you have to guess someone's height, would you rather be told

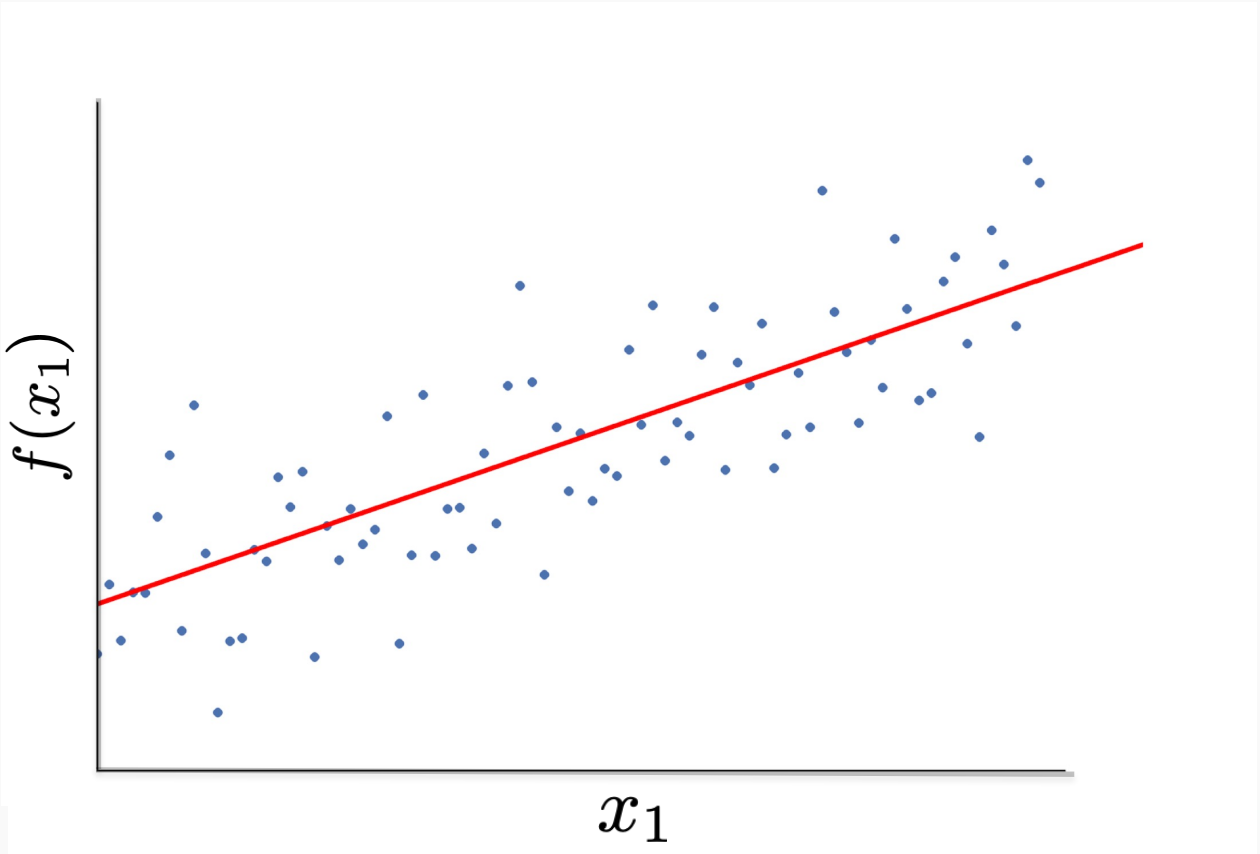
- Their weight, only
- Their weight and sex
- Their weight, sex, and income
- Their weight, sex, income, and favorite number

Of course, you'd always want as much data about a person as possible. Even though height and favorite number may not be strongly related, at worst you could just ignore the information on favorite number.

We want our models to be able to take in lots of data as they make their predictions.

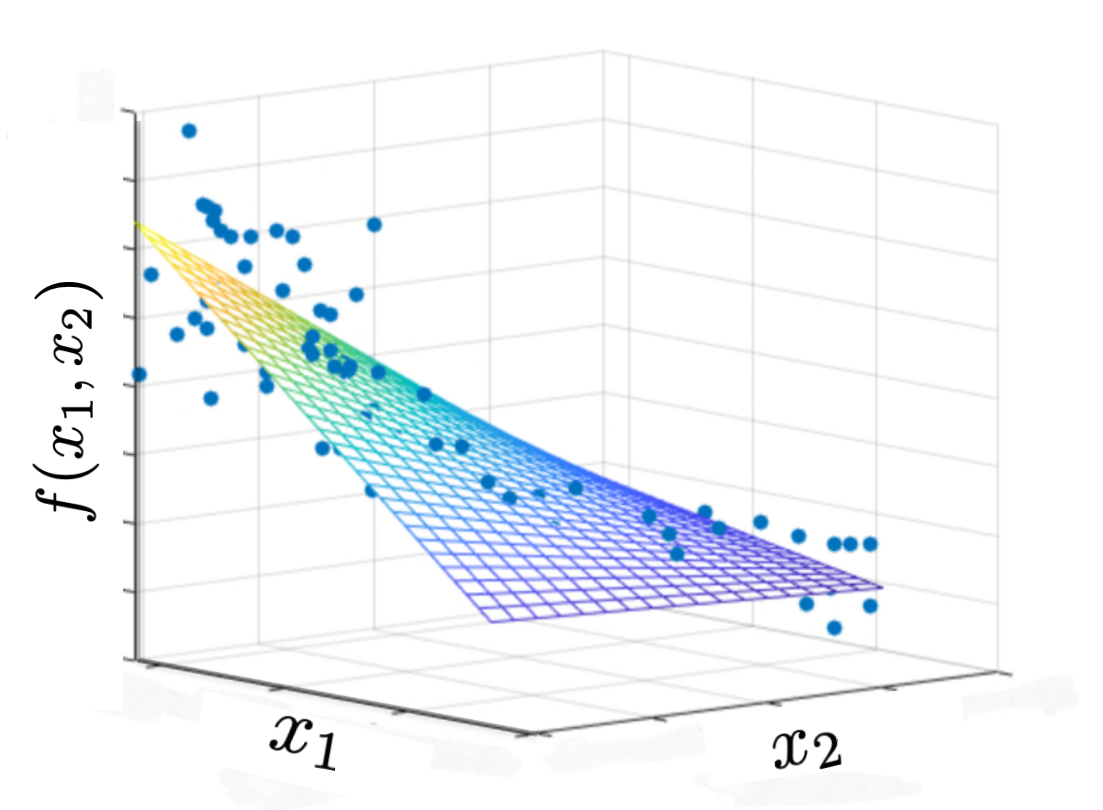
Linear Regression in 2D

$$\hat{f}(x_1) = \hat{\beta}_0 + \hat{\beta}_1 x_1$$



Linear Regression in 3D

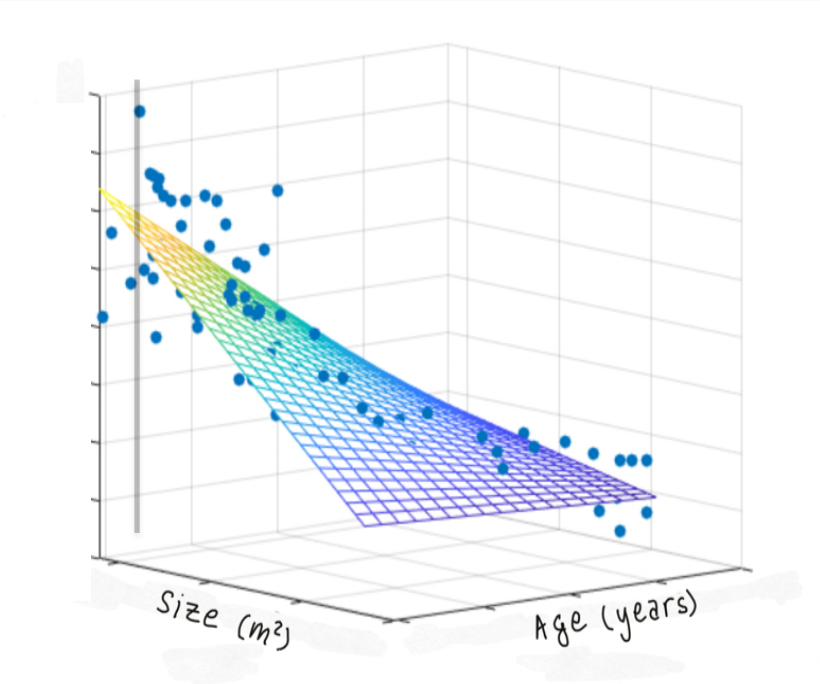
$$\hat{f}(x_1, x_2) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2$$



Multilinear Models

In practice, it is unlikely that any response variable Y depends solely on one predictor x. Rather, we expect that is a function of multiple predictors $f(X_1, \dots, X_J)$. Using the notation we introduced last lecture,

$$Y = y_1, \dots, y_n, \qquad X = X_1, \dots, X_J \qquad \text{and} \qquad X_j = x_{1j}, \dots, x_{ij}, \dots, x_{nj}$$



In this case, we can still assume a simple form for f -a multilinear form:

$$f(X_1, \dots, X_J) = \beta_0 + \beta_1 X_1 + \cdots + \beta_J X_J$$

Hence, $\hat{f}$, has the form:

$$\hat{f}(X_1, \dots, X_J) = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_J X_J$$

Response vs. Predictor Variables

This is called X: a.k.a.

The Design Matrix

n observations

TV
230.1
44.5
17.2
151.5
180.8

x_1

y:
The response variable

sales
22.1
10.4
9.3
18.5
12.9

Response vs. Predictor Variables

This is called X: a.k.a.
The Design Matrix

y:
The response variable

n observations

TV	radio	newspaper
230.1	37.8	69.2
44.5	39.3	45.1
17.2	45.9	69.3
151.5	41.3	58.5
180.8	10.8	58.4

x_1 x_2 x_3

sales
22.1
10.4
9.3
18.5
12.9

Multilinear Model, example

For our data

$$Sales = \beta_0 + \beta_1 \times TV + \beta_2 \times Radio + \beta_3 \times Newspaper$$

In linear algebra notation

$$\boldsymbol{Y} = \begin{pmatrix} Sales_1 \\ \vdots \\ Sales_n \end{pmatrix}, \boldsymbol{X} = \begin{pmatrix} 1 & TV_1 & Radio_1 & News_1 \\ \vdots & \vdots & \vdots & \\ 1 & TV_n. & Radio_n & News_n \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_3 \end{pmatrix}$$

$$\begin{pmatrix} Sales_1 \end{pmatrix} = \begin{pmatrix} 1 & TV_1 & Radio_1 & News_1 \end{pmatrix} \times \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_3 \end{pmatrix}$$

Multilinear Model, example

$$\begin{pmatrix} Sales_1 \end{pmatrix} = \begin{pmatrix} 1 & TV_1 & Radio_1 & News_1 \end{pmatrix} \times \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_3 \end{pmatrix}$$

$$Sales = \beta_0 + \beta_1 \times TV + \beta_2 \times Radio + \beta_3 \times Newspaper$$

$$Y = X\beta$$

Multiple Linear Regression

For simplicity we consider only two predictors and ignore β_0

Given a set of observations,

$$\{(x_{11}, x_{12}, y_1), (x_{21}, x_{22}, y_2), \dots (x_{n1}, x_{n2}, y_n)\}$$

the data and the model can be expressed in vector notation,

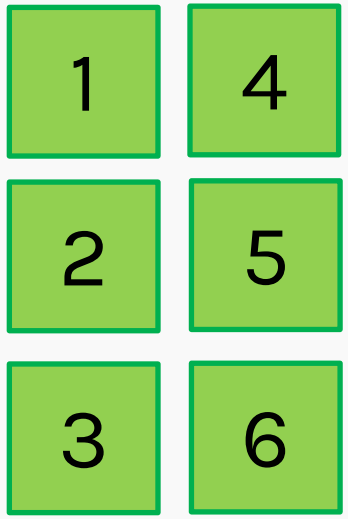
$$Y = X\beta$$

where,

$$Y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \end{pmatrix} \qquad X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \dots & \dots \end{pmatrix} \qquad \beta = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$$

RECAP: Transpose of a matrix

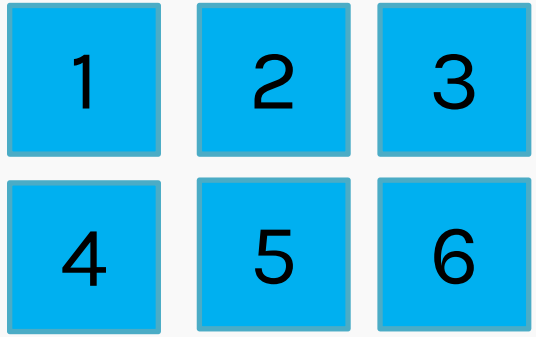
$$X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \dots & \dots \end{pmatrix}$$



(n,2)

In transpose, rows become columns and columns become rows.

$$X^T = \begin{pmatrix} x_{11} & x_{21} & \dots \\ x_{12} & x_{13} & \dots \end{pmatrix}$$



(2,n)

You can perform transpose over numpy objects by calling **np.transpose()** or **ndarray.T**

RECAP: Inverse of a matrix

When we multiply a number by its reciprocal we get 1.

$$n * \frac{1}{n} = 1$$

When we multiply a matrix by its inverse, we get the Identity Matrix

$$\boldsymbol{A\,A^{-1} = I}$$

```
In [16]: x = np.array([[1,2],[3,4]])
    ...:
    ...: #Inverse array x
    ...: invX = np.linalg.inv(x)
    ...: print(invX)
    ...:
    ...: #Verifying
    ...: print(np.dot(x, invX))
[[-2.   1. ]
 [ 1.5 -0.5]]
[[1.00000000e+00 1.11022302e-16]
 [0.00000000e+00 1.00000000e+00]]
```

numpy.linalg.inv() is used to calculate the inverse of a matrix (if it exists!)

Resource for Linear Algebra basics

Multiple Linear Regression

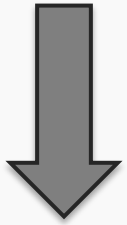
The model takes a simple algebraic form: $Y = X\beta$

We will again choose the **MSE** as our loss function, which can be expressed in vector notation as

$$MSE(\beta) = \frac{1}{n}\|Y - X\beta\|^2$$

$$MSE(\beta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - x_{i1}\beta_1 - x_{i2}\beta_2)^2$$

$$MSE(\beta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - x_{i1}\beta_1 - x_{i2}\beta_2)^2$$



$$MSE(\beta) = (y_1 - x_{11}\beta_1 - x_{12}\beta_2)^2 + (y_2 - x_{21}\beta_1 - x_{22}\beta_2)^2 + \ \ldots$$

$$MSE(\beta) = (y_1 - x_{11}\beta_1 - x_{12}\beta_2)^2 + (y_2 - x_{21}\beta_1 - x_{22}\beta_2)^2 + \ldots$$

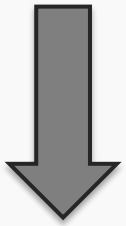
$$\frac{\partial L}{\partial \beta_1} = -2x_{11}(y_1 - x_{11}\beta_1 - x_{12}\beta_2) - 2x_{21}(y_2 - x_{21}\beta_1 - x_{22}\beta_2) - \ldots$$

$$\frac{\partial L}{\partial \beta_2} = -2x_{12}(y_1 - x_{11}\beta_1 - x_{12}\beta_2) - 2x_{22}(y_2 - x_{21}\beta_1 - x_{22}\beta_2) - \ldots$$

$$\begin{pmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \end{pmatrix} = \begin{pmatrix} -2x_{11}(y_1 - x_{11}\beta_1 - x_{12}\beta_2) & -2x_{21}(y_2 - x_{21}\beta_1 - x_{22}\beta_2) - \ \dots \\ -2x_{12}(y_1 - x_{11}\beta_1 - x_{12}\beta_2) & -2x_{22}(y_2 - x_{21}\beta_1 - x_{22}\beta_2) - \ \dots \end{pmatrix}$$

$$\begin{pmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \end{pmatrix} = -2 \begin{pmatrix} x_{11} & x_{21} & \dots \\ x_{12} & x_{22} & \dots \end{pmatrix} \begin{pmatrix} (y_1 - x_{11}\beta_1 - x_{12}\beta_2) \\ (y_2 - x_{21}\beta_1 - x_{22}\beta_2) \\ \dots \end{pmatrix}$$

$$\begin{pmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \end{pmatrix} = -2 \begin{pmatrix} x_{11} & x_{21} & \dots \\ x_{12} & x_{22} & \dots \end{pmatrix} \begin{pmatrix} (y_1 - x_{11}\beta_1 - x_{12}\beta_2) \\ (y_2 - x_{21}\beta_1 - x_{22}\beta_2) \\ \dots \end{pmatrix}$$



$$\begin{pmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \end{pmatrix} = -2 \begin{pmatrix} x_{11} & x_{21} & \dots \\ x_{12} & x_{22} & \dots \end{pmatrix} \left[\begin{pmatrix} y_1 \\ y_2 \\ \dots \end{pmatrix} - \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \dots & \dots \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \right]$$

$$\begin{pmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \end{pmatrix} = -2 \begin{pmatrix} x_{11} & x_{21} & \cdots \\ x_{12} & x_{22} & \cdots \end{pmatrix} \left[\begin{pmatrix} y_1 \\ y_2 \\ \cdots \end{pmatrix} - \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \cdots & \cdots \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \right]$$

$$\left(\frac{\partial L}{\partial \boldsymbol{\beta}}\right) = -2X^T(Y - X\boldsymbol{\beta})$$

For optimization, we set the values of the partial derivative to zero, i.e., $\left(\frac{\partial L}{\partial \boldsymbol{\beta}}\right) = 0$

$$\begin{pmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \end{pmatrix} = -2 \begin{pmatrix} x_{11} & x_{21} & \cdots \\ x_{12} & x_{22} & \cdots \end{pmatrix} \left[\begin{pmatrix} y_1 \\ y_2 \\ \cdots \end{pmatrix} - \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \cdots & \cdots \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \right]$$

$$\left(\frac{\partial L}{\partial \boldsymbol{\beta}}\right) = 0 \quad \Rightarrow \quad -2X^T(Y - X\boldsymbol{\beta}) = 0$$

$$\Rightarrow \quad X^T(Y - X\boldsymbol{\beta}) = 0$$

Optimization

$$X^T(Y - X\boldsymbol{\beta}) = 0$$

Which gives us,

$$X^T X\boldsymbol{\beta} = X^T Y$$

Multiplying on both sides with $(X^T X)^{-1}$

$$(X^T X)^{-1} X^T X\boldsymbol{\beta} = (X^T X)^{-1} X^T Y$$

$$\Rightarrow \boldsymbol{\beta} = (X^T X)^{-1} X^T Y$$

RECAP: Multiple Linear Regression

The model takes a simple algebraic form: $\mathbf{Y} = \mathbf{X}\beta + \epsilon$

We will again choose the **MSE** as our loss function, which can be expressed in vector notation as

$$\mathrm{MSE}(\beta) = \frac{1}{\mathrm{n}}\|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|^2$$

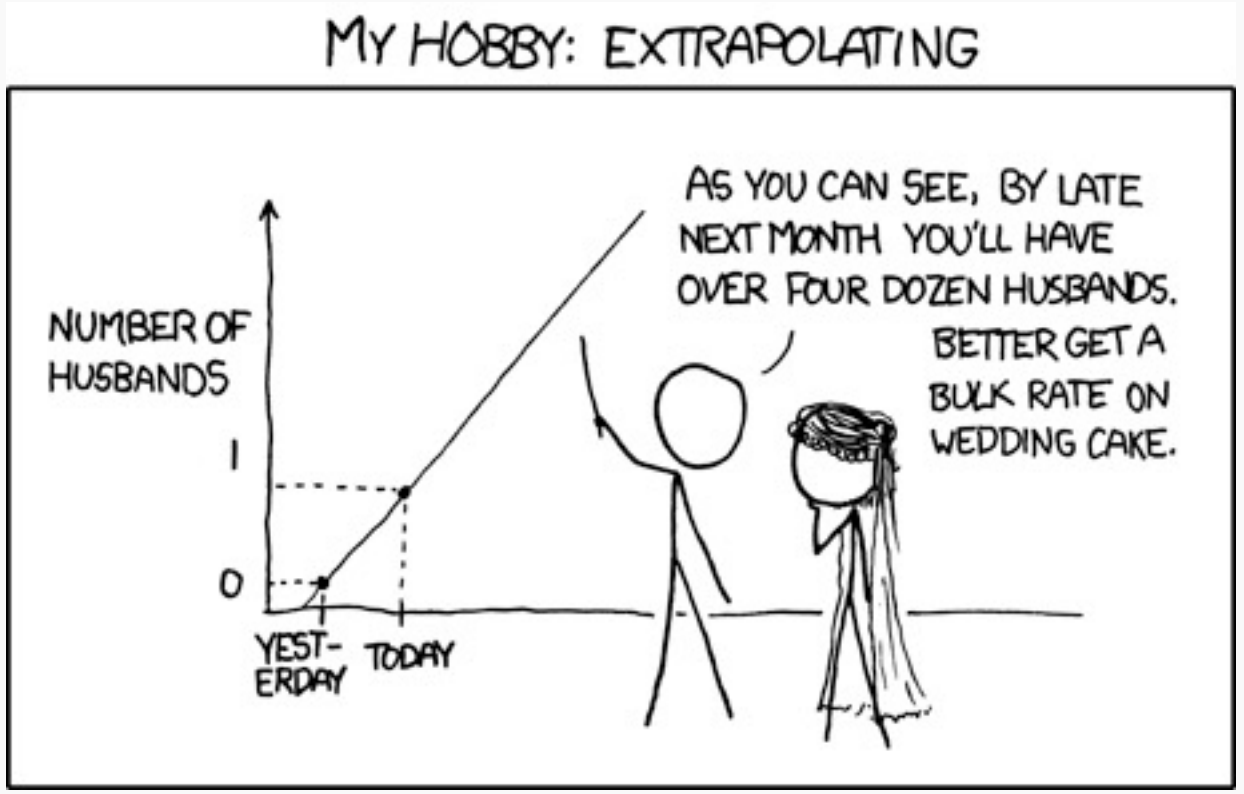
Minimizing the MSE using vector calculus yields,

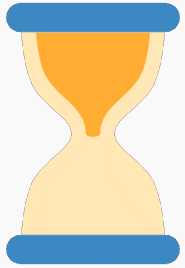
$$\widehat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}}\ \mathrm{MSE}(\boldsymbol{\beta}).$$

Multiple Linear Regression

$$\widehat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}}\ \mathrm{MSE}(\boldsymbol{\beta}).$$

```
>>> import numpy as np
>>> X = …
>>> y = …
>>> X_sq = X.T @ X
>>> X_inv = np.linalg.inv(X.T @ X)
>>> beta_hat = X_inv @ (X.T @ y)
```

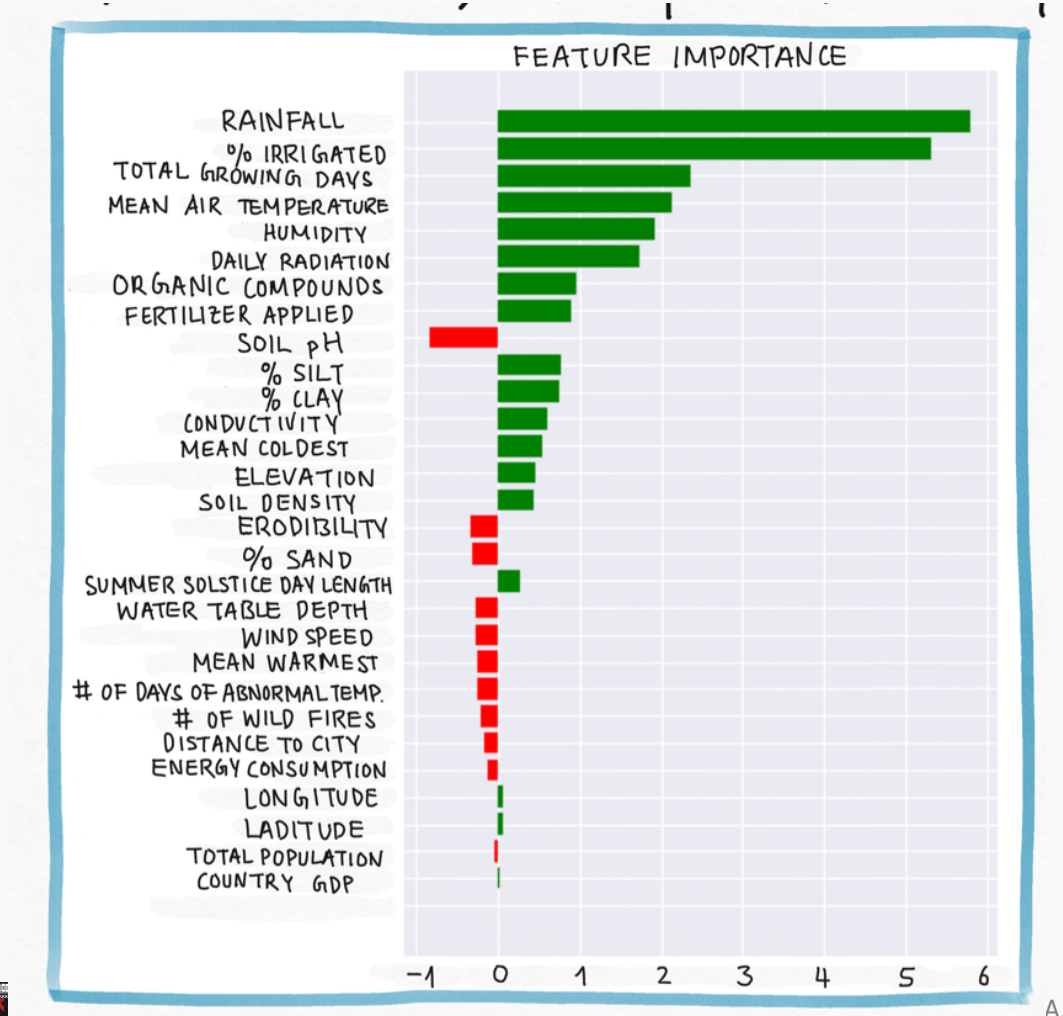




Digestion Time

Interpreting multi-linear regression

For linear models, it is easy to interpret the model parameters.



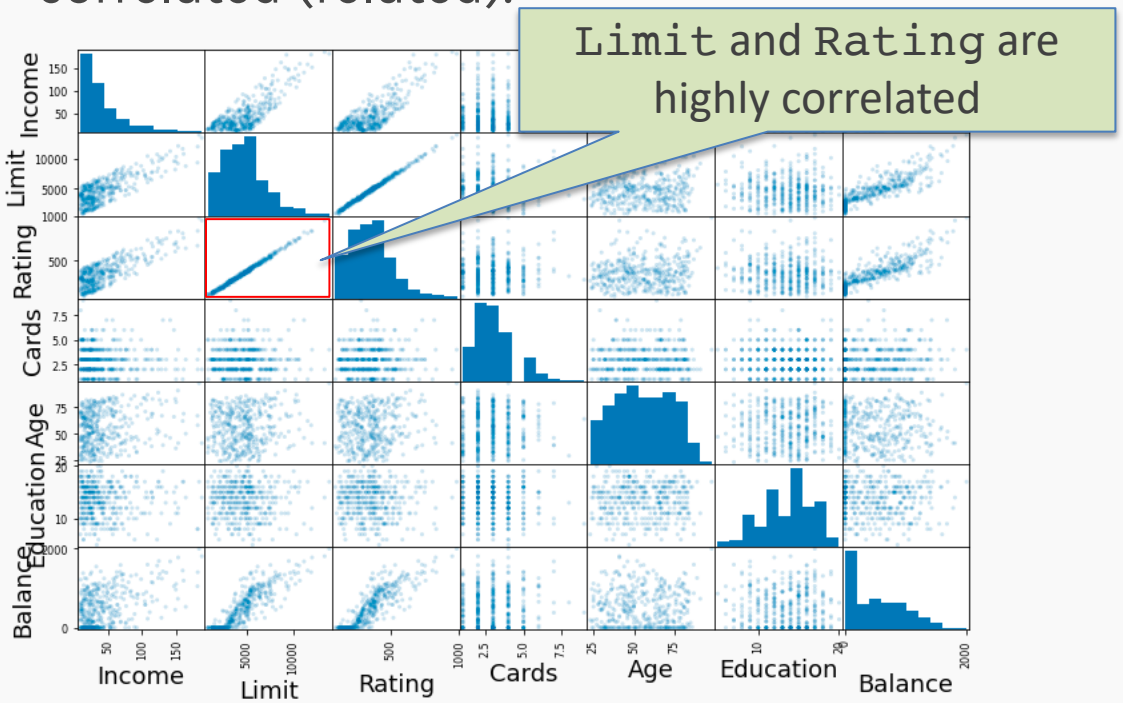
When we have a large number of predictors: $X_1, \ldots, X_J$, there will be a large number of model parameters, $\beta_1, \beta_2, \ldots, \beta_J$.

Looking at the values of β's is impractical, so we visualize these values in a feature importance graph.

The feature importance graph shows which predictors has the most impact on the model's prediction.

Collinearity

Collinearity and multicollinearity refers to the case in which two or more predictors are correlated (related).



	Columns	Coefficients
0	Income	-7.802001
1	Limit	0.193077
2	Rating	1.102269
3	Cards	17.923274
4	Age	-0.634677
5	Education	-1.115028
6	Gender	10.406651
7	Student	426.469192
8	Married	-7.019100

	Columns	Coefficients
0	Income	-7.770915
1	Rating	3.976119
2	Cards	4.031215
3	Age	-0.669308
4	Education	-0.375954
5	Gender	10.368840
6	Student	417.417484
7	Married	-13.265344

The regression coefficients are not uniquely determined. In turn it hurts the interpretability of the model as then the regression coefficients are not unique and have influences from other features.

Both `limit` and `rating` have positive coefficients, but it is hard to understand if the balance is higher because of the `rating` or is it because of the `limit`? If we remove `limit` then we achieve almost the same model performance, but the coefficients change.

Collinearity

Collinearity refers to the case in which two or more predictors are correlated (related).

We will re-visit collinearity in the next lecture when we address **overfitting**, but for now we want to examine how does collinearity affects our confidence on the coefficients and consequently on the importance of those coefficients.

Qualitative Predictors

So far, we have assumed that all variables are quantitative. But in practice, often some predictors are **qualitative**.

Example: The *credit data set* contains information about balance, age, cards, education, income, limit , and rating for a number of potential customers.

Income	Limit	Rating	Cards	Age	Education	Sex	Student	Married	Ethnicity	Balance
14.890	3606	283	2	34	11	Male	No	Yes	Caucasian	333
106.02	6645	483	3	82	15	Female	Yes	Yes	Asian	903
104.59	7075	514	4	71	11	Male	No	No	Asian	580
148.92	9504	681	3	36	11	Female	No	No	Asian	964
55.882	4897	357	2	68	16	Male	No	Yes	Caucasian	331

Qualitative Predictors

If the predictor takes only two values, then we create an **indicator** or **dummy variable** that takes on two possible numerical values.

For example, for the sex, we create a new variable:

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

We then use this variable as a predictor in the regression equation.

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

Qualitative Predictors

Question: What is interpretation of β_0 and β_1?

Qualitative Predictors

Question: What is interpretation of β_0 and β_1?

- β_0 is the average credit card balance among males,
- $\beta_0 + \beta_1$ is the average credit card balance among females,
- and β_1 the average difference in credit card balance between females and males.

Example: Calculate β_0 and β_1 for the Credit data.

You should find $\beta_0 \sim \$509, \beta_1 \sim \$19$

More than two levels: One hot encoding

Often, the qualitative predictor takes more than two values (e.g. ethnicity in the credit data).

In this situation, a single dummy variable cannot represent all possible values.

We create additional dummy variable as:

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

$$x_{i,2} = \begin{cases} 1 & \text{if } i\,\text{th person is Caucasian} \\ 0 & \text{if } i\,\text{th person is not Caucasian} \end{cases}$$

More than two levels: One hot encoding

We then use these variables as predictors, the regression equation becomes:

$$y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} = \begin{cases} \beta_0 + \beta_1 & \text{if } i \text{ th person is Asian} \\ \beta_0 + \beta_2 & \text{if } i \text{ th person is Caucasian} \\ \beta_0 & \text{if } i \text{ th person is AfricanAmerican} \end{cases}$$

Question: What is the interpretation of $\beta_0, \beta_1, \beta_2$?

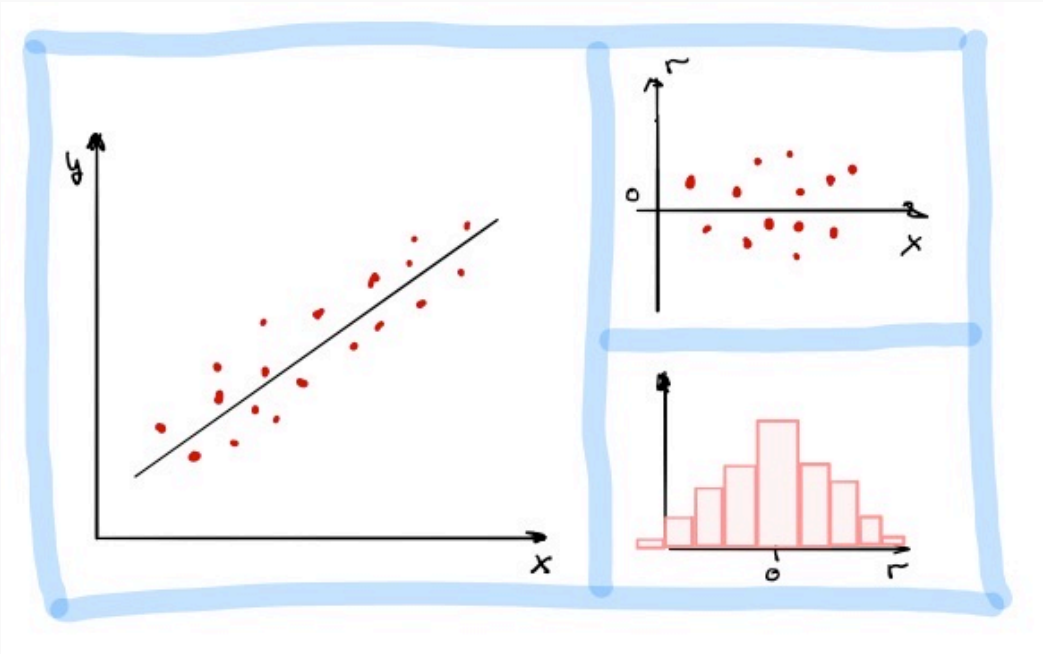
Beyond linearity

So far, we assumed:

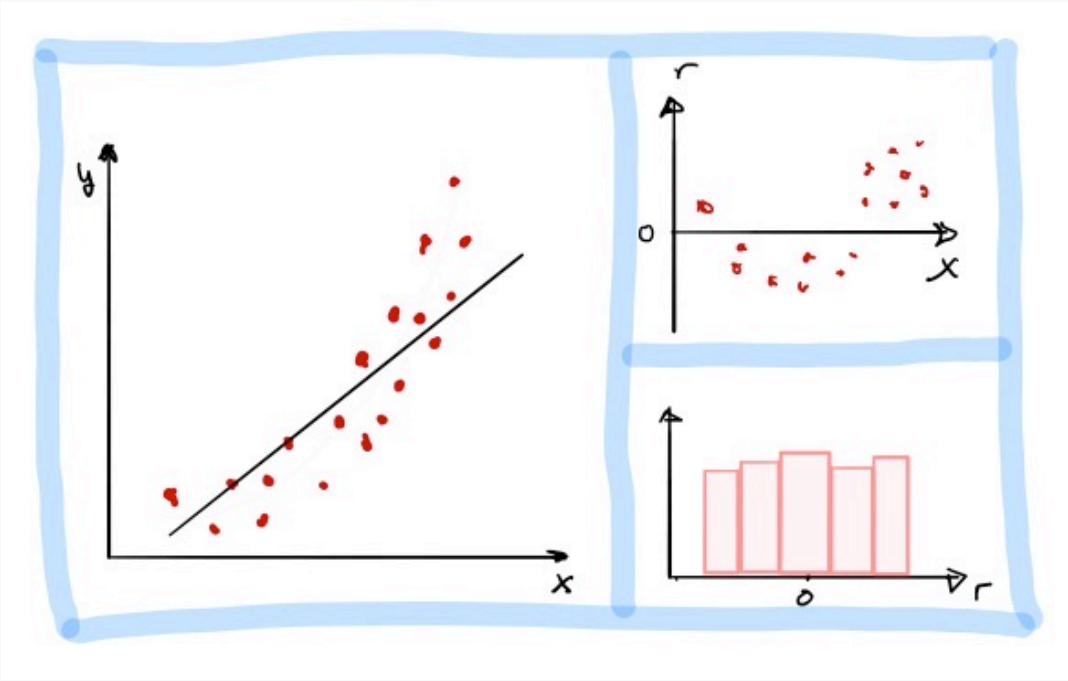
- linear relationship between X and Y
- the residuals $r_i = y_i - \hat{y}_i$ were uncorrelated (taking the average of the square residuals to calculate the MSE implicitly assumed uncorrelated residuals)

These assumptions need to be verified using the data. This is often done by **visually inspecting the residuals.**

Residual Analysis



Linear assumption is correct. There is no obvious relationship between residuals and x. Histogram of residuals is symmetric and normally distributed.



Linear assumption is incorrect. There is an obvious relationship between residuals and x. Histogram of residuals is symmetric but **not** normally distributed.

Note: For multi-regression, we plot the residuals vs predicted y, $\hat{y}$, since there are too many x's and that could wash out the relationship.

Beyond linearity: **synergy effect** or **interaction effect**

We also assume that the average effect on *sales* of a one-unit increase in *TV,* is always β_1 regardless of the amount spent on *radio* or *newspaper*.

Synergy effect or **interaction effect** states that when an increase on the *radio budget* affects the effectiveness of the *TV* spending on *sales*.

To account for it, we simply add a term as:

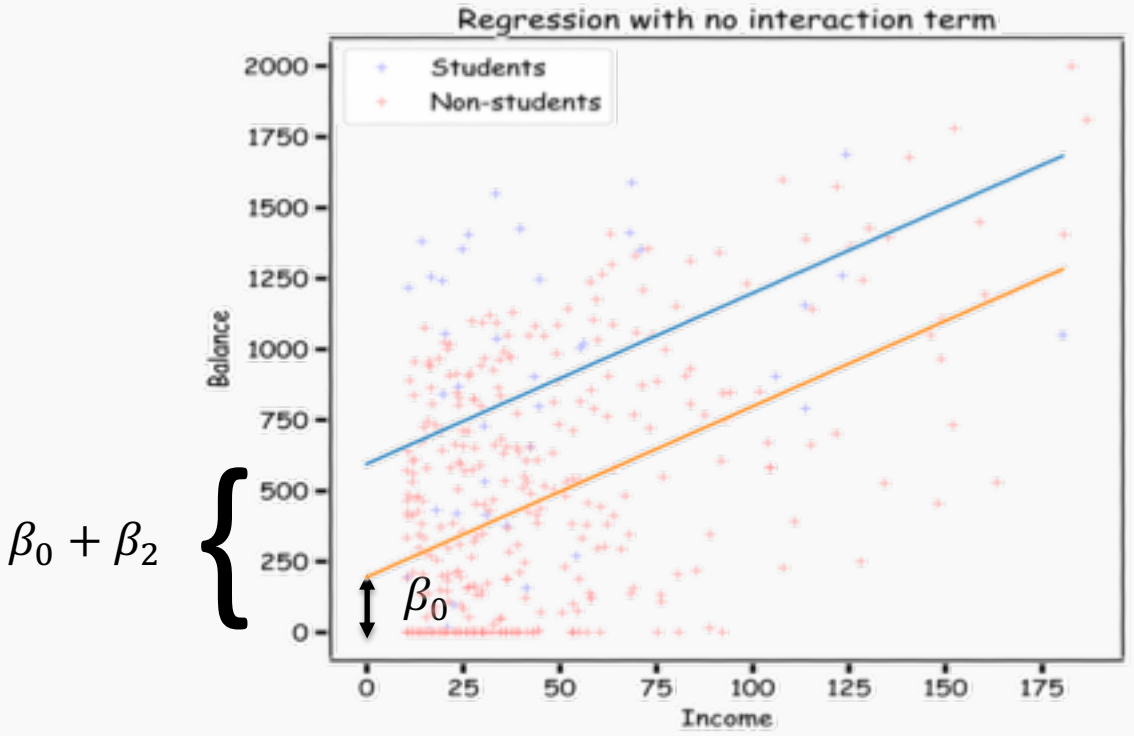
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \boxed{\beta_3 X_1 X_2}$$

What does it mean? No interaction term

$$balance = \beta_0 + \beta_1 \times income + \beta_2 \times student$$

$$student = \begin{cases} 0 & balance = \beta_0 + \beta_1 \times income \\ 1 & balance = \beta_0 + \beta_1 \times income + \beta_2 \end{cases} \rightarrow balance = \overbrace{(\beta_0 + \beta_2)}^{\text{intercept}} + \beta_1 \times income$$

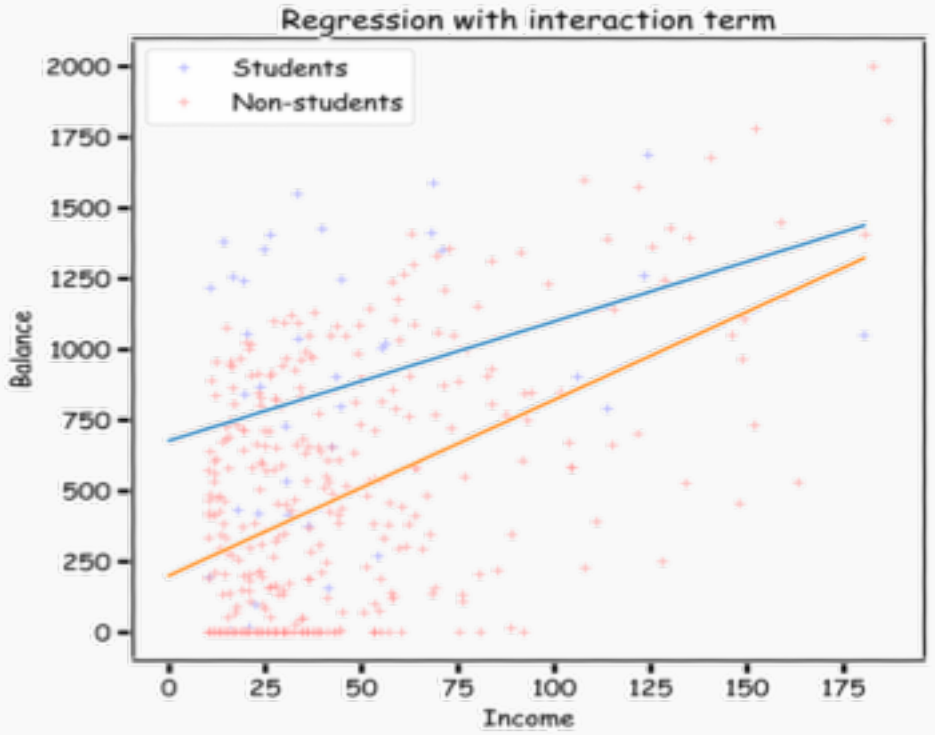


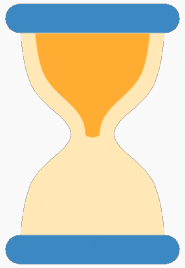
What does it mean? With interaction term

$$balance = \beta_0 + \beta_1 \times income + \beta_2 \times student + \beta_3 \times income \times student$$

$$student = \begin{cases} 0 & balance = \beta_0 + \beta_1 \times income \\ 1 & balance = \beta_0 + \beta_1 \times income + \beta_2 + \beta_3 \times income \end{cases}$$

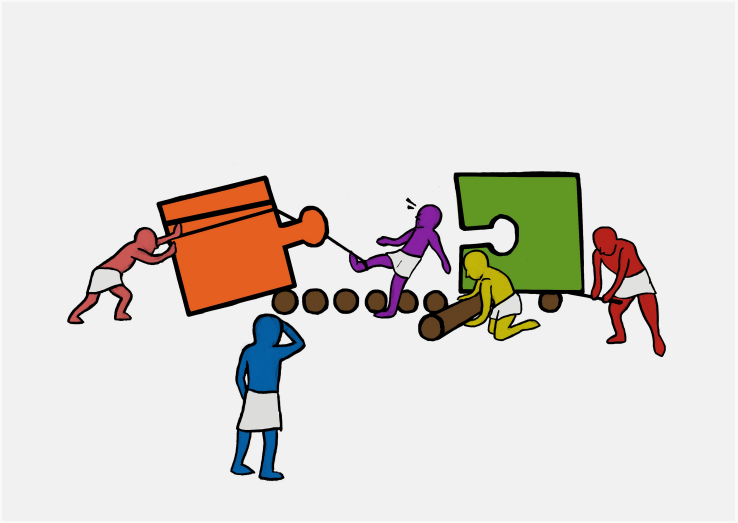
$$\rightarrow balance = \underbrace{(\beta_0 + \beta_2)}_{\text{intercept}} + \underbrace{(\beta_1 + \beta_3)}_{\text{slope}} \times income$$





Digestion Time

Too many predictors, collinearity and too many interaction terms leads to **OVERFITTING!**



```
+------------------------------+--------------------+
|          Predictors          |        MSE         |
+------------------------------+--------------------+
|            ['TV']            | 10.18618193453022  |
|          ['Radio']           | 24.23723303713214  |
|        ['Newspaper']         | 32.13714634300907  |
|       ['TV', 'Radio']        | 4.391429763581883  |
|     ['TV', 'Newspaper']      | 8.687682675690592  |
|    ['Radio', 'Newspaper']    | 24.78339548293816  |
| ['TV', 'Radio', 'Newspaper'] | 4.402118291449686  |
+------------------------------+--------------------+
```

👨🏽 Exercise: Simple Multi-linear Regression

The aim of this exercise is to understand how to use multi regression. Here we will observe the difference in MSE for each model as the predictors change.

	TV	Radio	Newspaper	Sales
0	230.1	37.8	69.2	22.1
1	44.5	39.3	45.1	10.4
2	17.2	45.9	69.3	9.3
3	151.5	41.3	58.5	18.5
4	180.8	10.8	58.4	12.9

Instructions:

- Read the file Advertisement.csv as a dataframe.
- For each instance of the predictor combination, form a model. For example, if you have 2 predictors, A and B, you will end up getting 3 models - one with only A, one with only B, and one with both A and B.
- Split the data into train and test sets.
- Compute the MSE of each model.
- Print the Predictor - MSE value pair.

Hints: