

Machine Learning | Enginyeria Informàtica

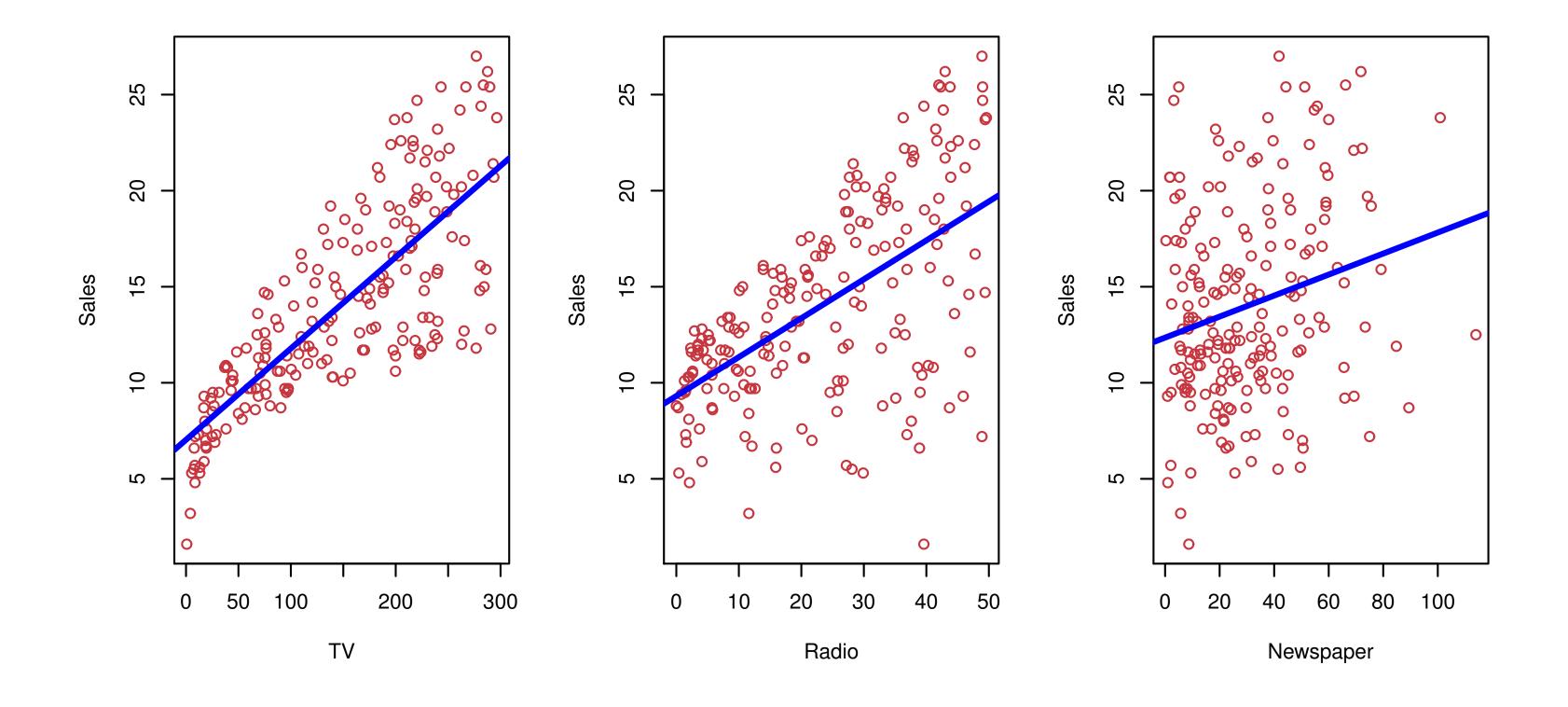
Santi Seguí I **2024-2025** 

- Linear Regression
- Regularized Linear Models
  - Ridge Regression
  - Lasso Regression
  - Elastic Net
  - Early Stopping
- Knn for Regression



- Linear regression is a **simple** approach to supervised learning.
- It assumes linear dependence of Y on  $X_1, X_2, ..., X_p$ .
- True linear regression function are "never" linear!
- Although it may seem overly simplistic, linear regression is **extremely useful** both conceptually and practically.







### Linear regression for advertising data

- Is there a relationship between advertising budget and sales?
- How strong is the relationship between advertising budget and sales?
- Which media contribute to sales?
- How accurately can we predict future sales?
- Is the relationship linear?
- Is there synergy among the advertising media?



- Widely used due to its **simplicity** but also because its interpretability.
- However, when features are correlations predictions can cause problems:
  - The variance of all coefficients tends to increase dramatically
  - Interpretations becomes harzarouds- When  $X_j$  changes, everything else changes.
- Causes of causality must be avoided for observational data.



#### Simple Linear regression using a single predictor X

We assume a model:

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

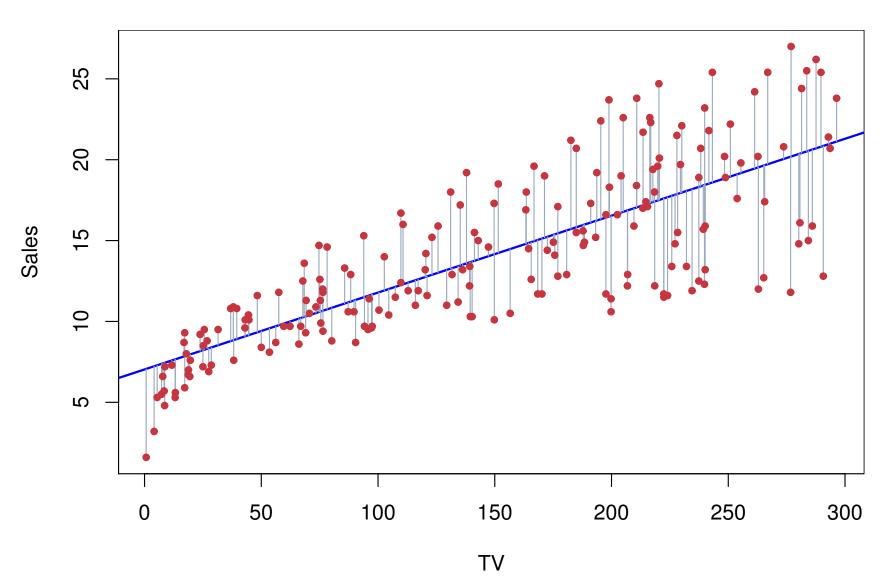
where  $\beta_0$  and  $\beta_1$  are two unknown constants that represents the **intercept** and **slop**, also known as **parameters** or **coefficients**, and  $\epsilon$  is the error term.

ullet Given some estimates  $\hat{eta}_0$  and  $\hat{eta}_1$  for the model coefficients, we predict the 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.

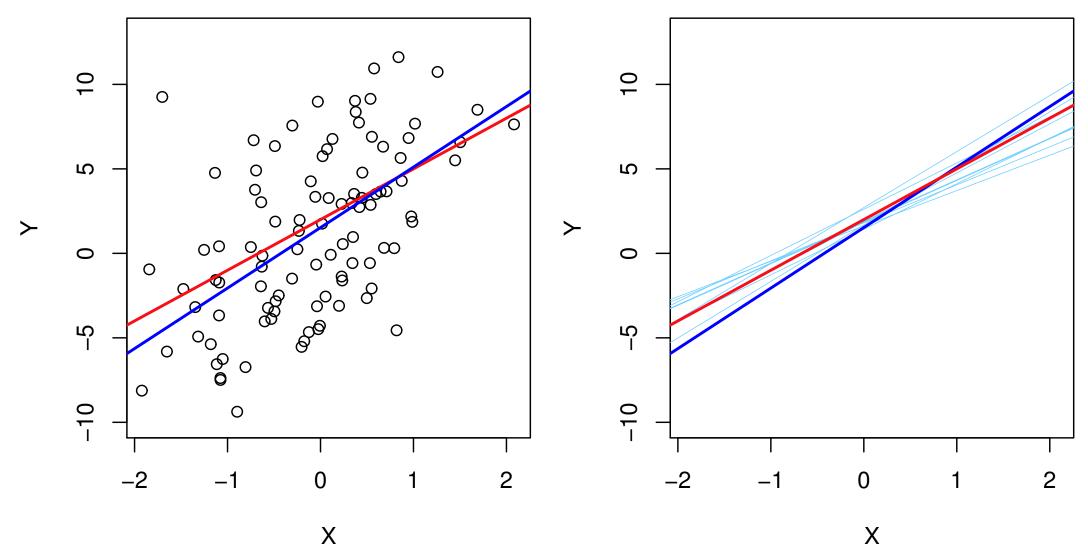
# Example: Advertising data



The **least square** 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.



### Example: Synthetic data



• Simulated data set. Left: the **red** line represents the true relationship f(X) = 2 + 3X, called population line and the **blue** line is the least squares line. Right: The red and blue line represents again the population line and least squares line, while light blue are ten least squares lines computed with a separate random set of observations.



#### Assessing the Accuracy of the Coefficient Estimates

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

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

where  $\sigma^2 = Var(\epsilon)$ 

• These standard errors 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. It has the form

$$\hat{\beta}_1 \pm 2 \cdot SE(\hat{\beta}_1)$$

### Confidence Interval

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

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

• will contain the true value of  $\beta_1$  (under a scenario where we got repeated samples like the present sample)

• For the advertising data, the 95% confidence interval for  $\beta_1$  is [0.042,0.053]

# 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.
  - $H_1$ : There is some relationship between X and Y.
- Mathematically, this corresponds to testing

$$H_0: \beta_1 = 0$$

versus 
$$H_A: \beta_1 \neq 0$$

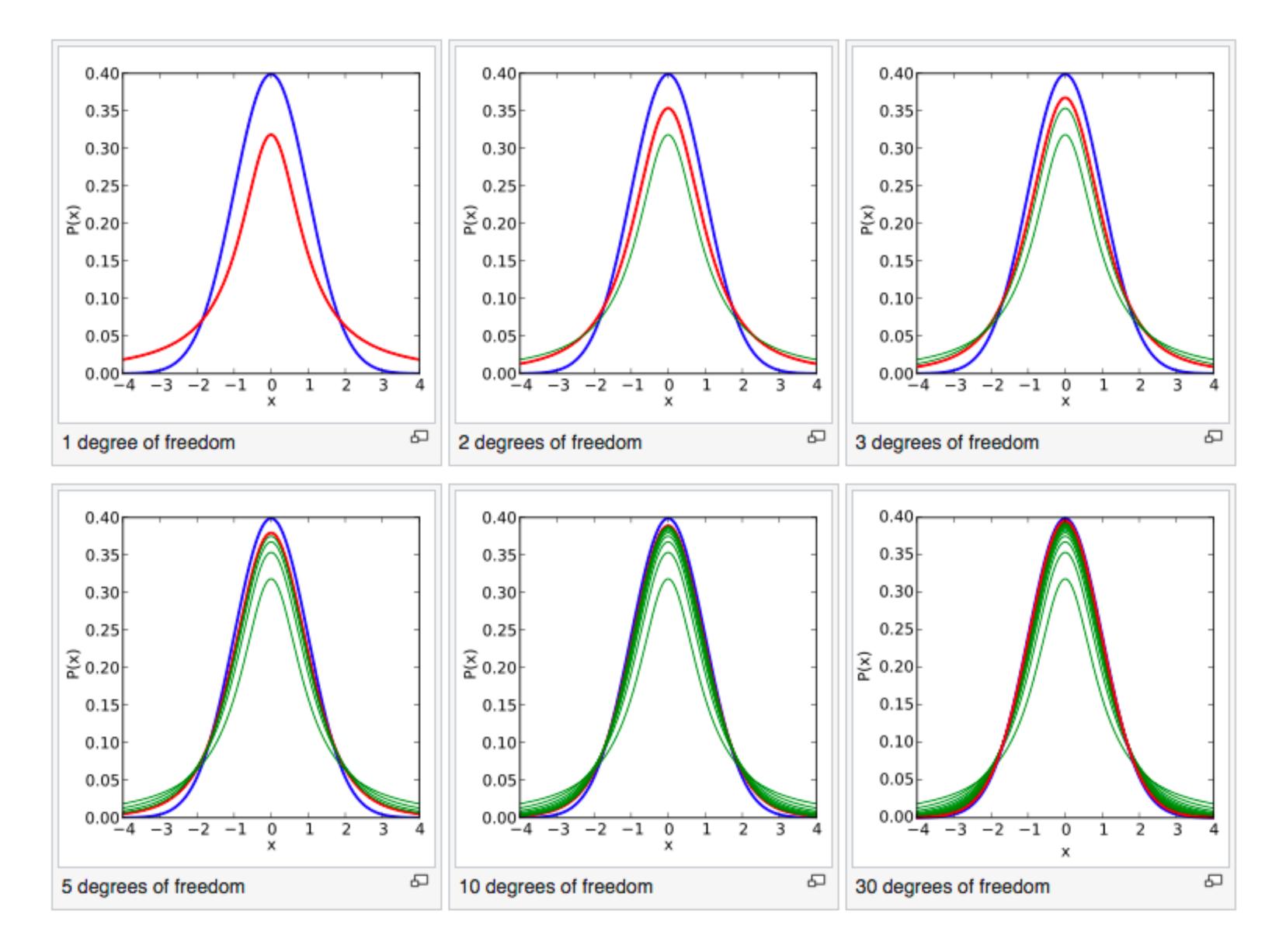
• If  $H_0$  is true then the model <u>reduces</u> to  $Y = \beta_0 + \epsilon$ , and X is not associated with Y.

# Hypothesis Testing

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

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





### P-value

A small p-value indicates that it is **unlikely** to observe such a substantial association between the predictor and response.

If the null hypothesis if the p-value is small enough. Typically p-value cutoffs for rejecting the null hypothesis are 5 or 1 %.



- Parameter Estimation:
  - Given estimates  $\hat{B}_1, \hat{B}_2, \dots, \hat{B}_p$ , we can make predictions using the formula:

$$\hat{y} = \hat{B}_0 + \hat{B}_1 x_1 + \ldots + \hat{B}_p x_p$$

• We can estimate  $B_0, B_1, \ldots, B_p$  as the values that minimize the sum of the squared residuals:

$$RSS = \sum_{i=0}^{n} (y_i - \hat{y}_i)^2$$

• This can be done using standard statistical software.

# Parameter $\beta_0, \beta_1, \dots \beta_p$ estimation

- There is two main ways.
  - Using Linear Algebra and the Normal Equation:
    - <a href="https://towardsdatascience.com/performing-linear-regression-using-the-normal-equation-6372ed3c57">https://towardsdatascience.com/performing-linear-regression-using-the-normal-equation-6372ed3c57</a>
  - Or using some kind of optimization algorithm (e.g. Gradient Descent) to minimize a cost function
    - We will see in a future class



## 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

$$\widehat{sales} = 7.0325 + 0.0475 * TV$$



### Assessing the Overall Accuracy of the Model

• We compute the **Residual Standard Error** 

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

- where the **residual sum-of-squares** is  $RSS = \sum_{i=1}^{n} (y_i \hat{y}_i)^2$ .
- RSE provides an absolute measure of lack of the fit of the model to the data. Since, it is measured in the units of Y, it is not always clear what constitutes a good RSE.

### Assessing the Overall Accuracy of the Model

• **R-squared** or fraction of variance explained is

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

where  $TSS = \sum_{i=1}^{n} (y_i - \bar{y})^2$  is the **total sum of squares** and <u>measures</u> the total variance in the response.

- $\mathbb{R}^2$  measures the proportion of variability in Y that can be explained using X.
- 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:

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

## Advertising data results

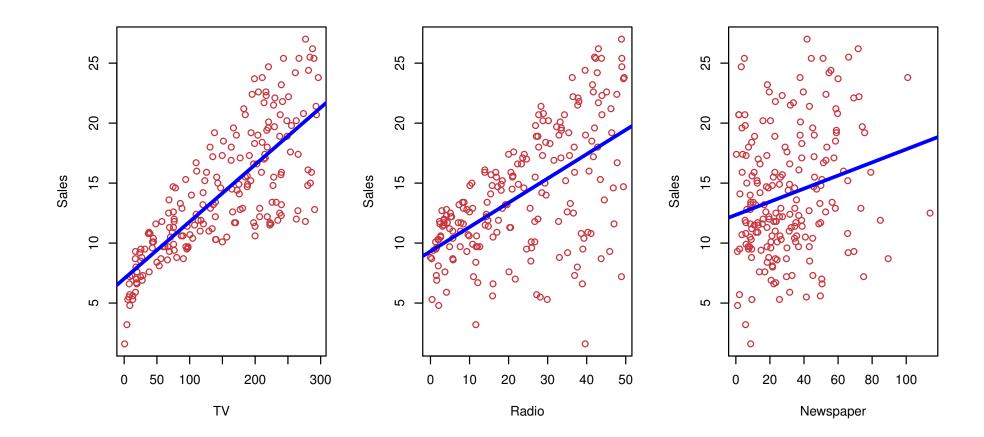
Quantity	Value
Residual Standard Error	3.26
$R^2$	0.612
F-statistic	312.1



# Multiple Linear Regression

The model:

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p + \epsilon$$



• We interpret  $\beta_j$  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:

sales = 
$$\beta_0 + \beta_1 x TV + \beta_2 x radio + \beta_3 x newspaper + \epsilon$$

### Interpreting regression coefficients

- The ideal scenario is when the predictors are uncorrelated
  - Each coefficient can be estimated and tested separately.
  - Interpretations such as "a unit change in  $X_j$  is associated with a  $\beta_j$  change in Y, while all the other variables stay fixed", are possible.
- Correlations amongst predictors cause problems:
  - The variance of all coefficients tends to increase, sometimes dramatically
  - ullet Interpretations become hazardous when  $X_i$  changes, everything else changes.

Claims of causality should be avoided for observational data.



#### Estimation and Prediction for Multiple Regression

ullet Given <u>estimates</u>  $\hat{eta}_0,\hat{eta}_1,\ldots,\hat{eta}_p$  , we can make predictions using the formula

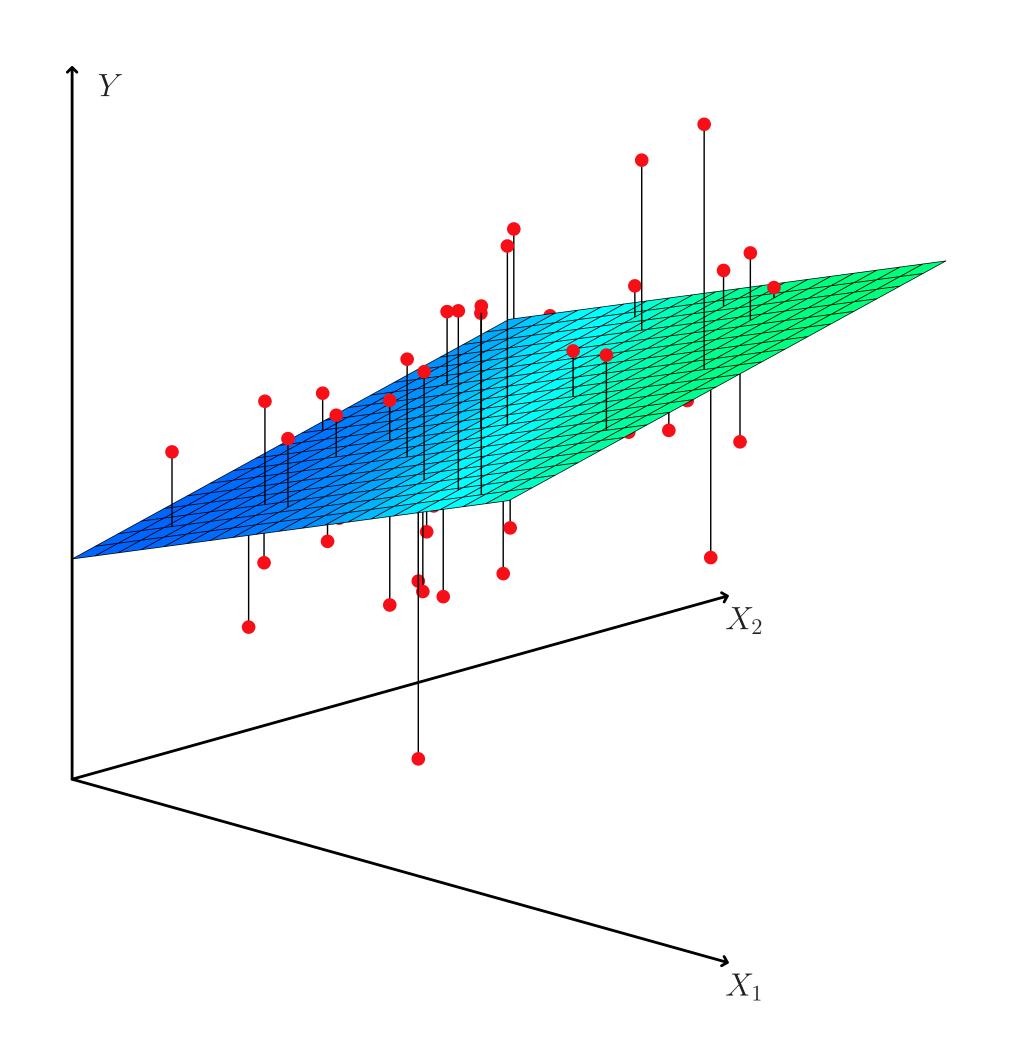
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p$$

ullet We estimate  $eta_0,eta_1,\ldots,eta_p$  as the values that minimize the sum of the squared residuals

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} + \dots + \hat{\beta}_p x_{ip})^2$$

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



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

	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 interesting questions

**Q1:** Is at least one of the predictors  $X_1, X_2, \ldots, X_p$  useful in predicting the response?

**Q2:** Do all the predictors help to explain Y, or is only a subset of the predictors useful?

Q3: How well does the model fit the data?

**Q4:** Given a set of predictor values, what response value should we predict, and how accurate is our prediction?



### Q1: Is at least one predictor useful?

• In the multiple regression setting with p predictors, we need to ask whether all of the regression coefficients are zero. We test the null hypothesis:

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

versus the alternative:

- $H_a$ : at least one of  $\beta_i$  is non-zero
- This hypothesis test is performed by computing the F-statistic

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

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



### Q2: 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.
- 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 billion models! Instead we need an automated approach that searches through a subset of them. We discuss two commonly use approaches next.



### Q2: Forward selection

- Use 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.
- Add to that model the variable that results in the lowest <u>RSS</u> 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.



### Q2: 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.
- 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.
- Intead of using p-value, other measures or methodologies can be used



#### Q3: How well the model fits the 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
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newspaper	-0.001	0.0059	-0.18	0.8599

Quantity	Value
Residual Standard Error	1.69
$R^2$	0.8972
F-statistic	570



#### Q3: How well the model fits the data

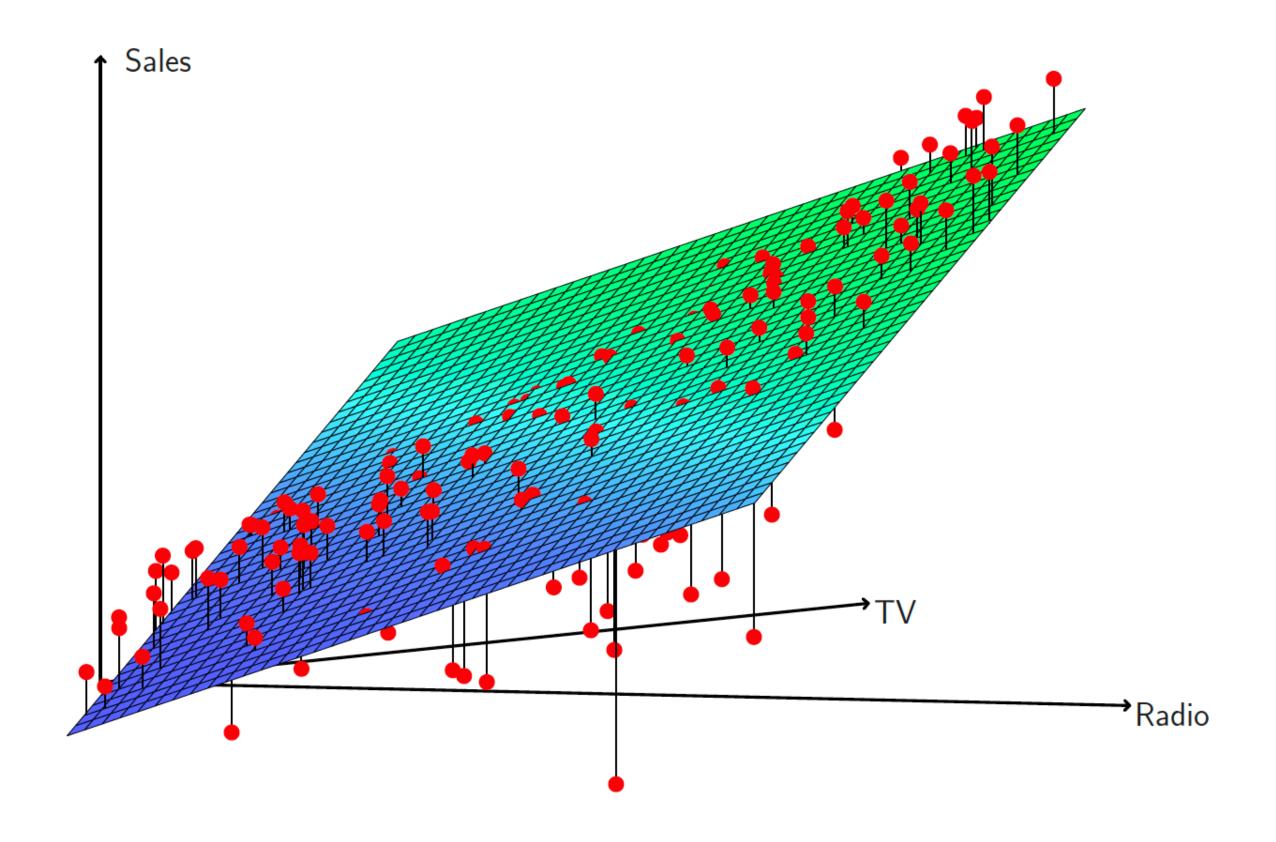
#### with newspaper:

Quantity	Value
Residual Standard Error	1.686
$R^2$	0.8972

#### without newspaper:

Quantity	Value
Residual Standard Error	1.681
$R^2$	0.89719





The model seems to overestimate estimate sales for instances in which most of the advertising money was spend exclusively on either TV OR radio.

It underestimates sales for instances where the budget was split between to medias





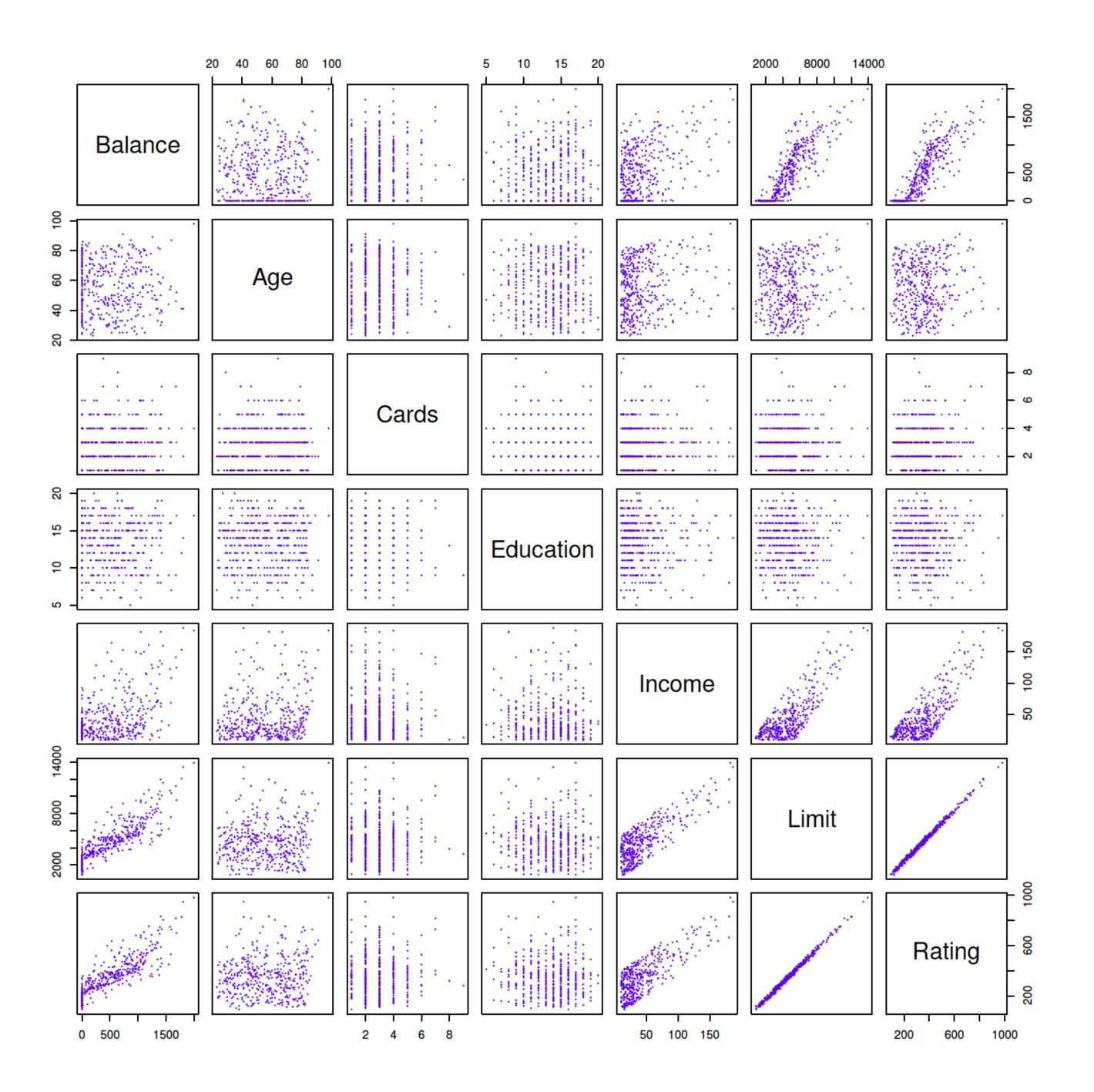
Categorical data?



## Categorical data

- Some times our data is not quantitative but qualitative. For example: gender, ethnicity, city,...
- 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: (student status), status (marital status), and ethnicity (Caucasian, African American (AA) or Asian).







### Qualitative Predictors

• 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:

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

### Credit card data

#### Results for gender model:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	509.80	33.13	15.389	< 0.0001
gender[Female]	19.73	46.08	0.429	0.6690



#### Qualitative predictors with more than two levels

- What happens if there is more than two levels?
- For example, for the **ethnicity**?



#### 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 levers

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

$$yi = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + e_i \begin{cases} \beta_0 + \beta_1 + e_i & \text{if $i$th person is Asia} \\ \beta_0 + \beta_2 + e_i & \text{if $i$th person is Caucasian} \\ \beta_0 + e_i & \text{if $i$th person is AA} \end{cases}$$

• 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 the previous analysis on the Advertising data, it is assumed that the effect on sales of increasing one advertising medium is independent of the amount spent on the other media
  - For example, the linear model

$$\widehat{sales} = \beta_0 + \beta_1 x TV + \beta_2 x radio + \beta_3 x newspapers$$

states that the average effect on sales of a one-unit increase in TV is always  $eta_1$ , regardless of the amount spent on radio

### Interactions

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



### Modeling interactions - Adverstising data

Model takes the form:

$$sales = \beta_0 + \beta_1 x TV + \beta_2 x radio + \beta_3 x (radio x TV) + e$$

	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	0.0000	20.73	< 0.0001

# Interpretation

- The results in this table suggests that interactions are important.
- The p-value for the interaction term  $TV \ x \ radio$  is extremely low, indicating that there is strong evidence for  $H_A: \beta_3 = 0$ .
- The  $\mathbb{R}^2$  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.

#### Interactions

- 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 hierarchy 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.



#### Interactions between qualitative and quantitative 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:

$$balance_{i} \approx \beta_{0} + \beta_{1} x income_{i} + \begin{cases} \beta_{2} & \text{if } student \\ 0 & \text{if } not student \end{cases}$$

$$= \beta_{1} x income_{i} + \begin{cases} \beta_{0} + \beta_{2} & \text{if } student \\ \beta_{0} & \text{if } not student \end{cases}$$

#### Interactions between qualitative and quantitative 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:

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$$= \beta_{1} x income_{i} + \begin{cases} \beta_{0} + \beta_{2} & \text{if } student \\ \beta_{0} & \text{if } not student \end{cases}$$

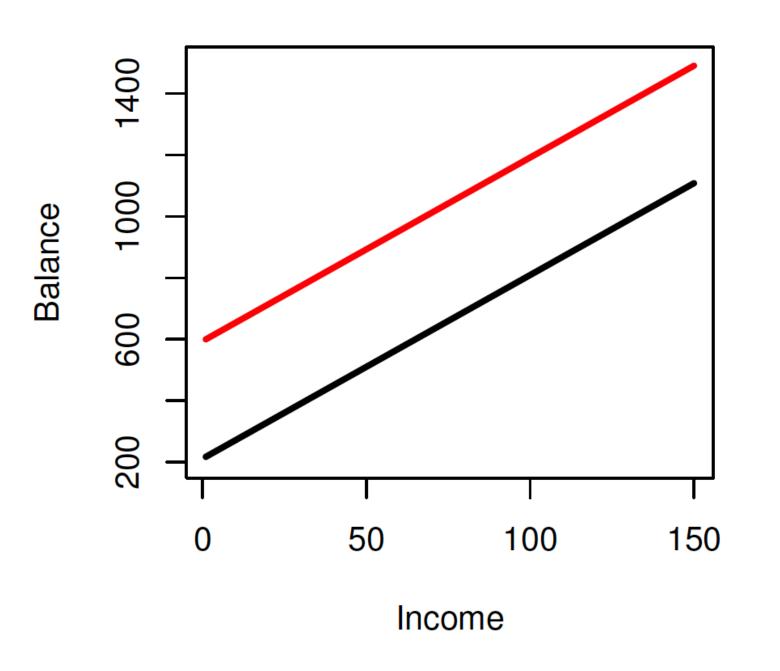
• With interactions, it takes the form:

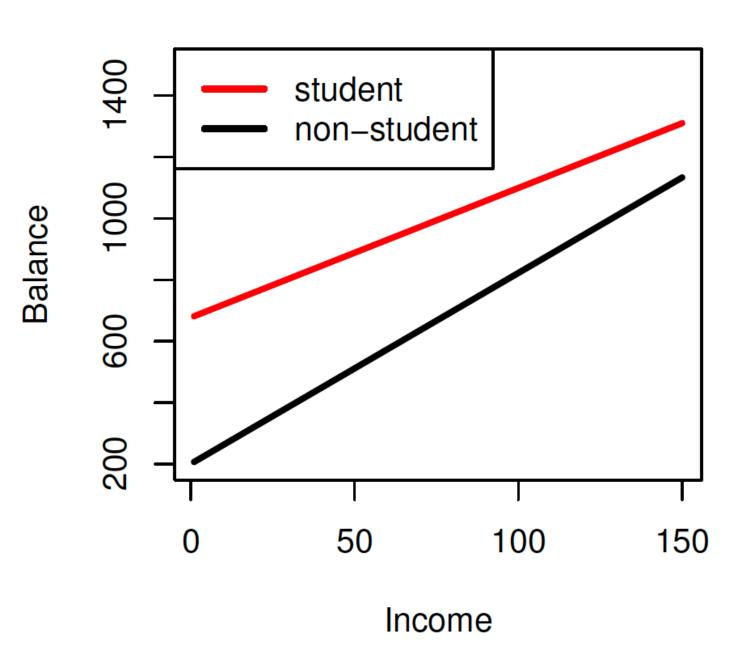
$$balance_{i} \approx \beta_{0} + \beta_{1} x income_{i} + \begin{cases} \beta_{2} + \beta_{3} x income_{i} & \text{if } student \\ 0 & \text{if } notstudent \end{cases}$$

$$= \begin{cases} (\beta_{0} + \beta_{2}) + (\beta_{1} + \beta_{3}) x income_{i} & \text{if } student \\ \beta_{0} + \beta_{1} x income_{i} & \text{if } notstudent \end{cases}$$

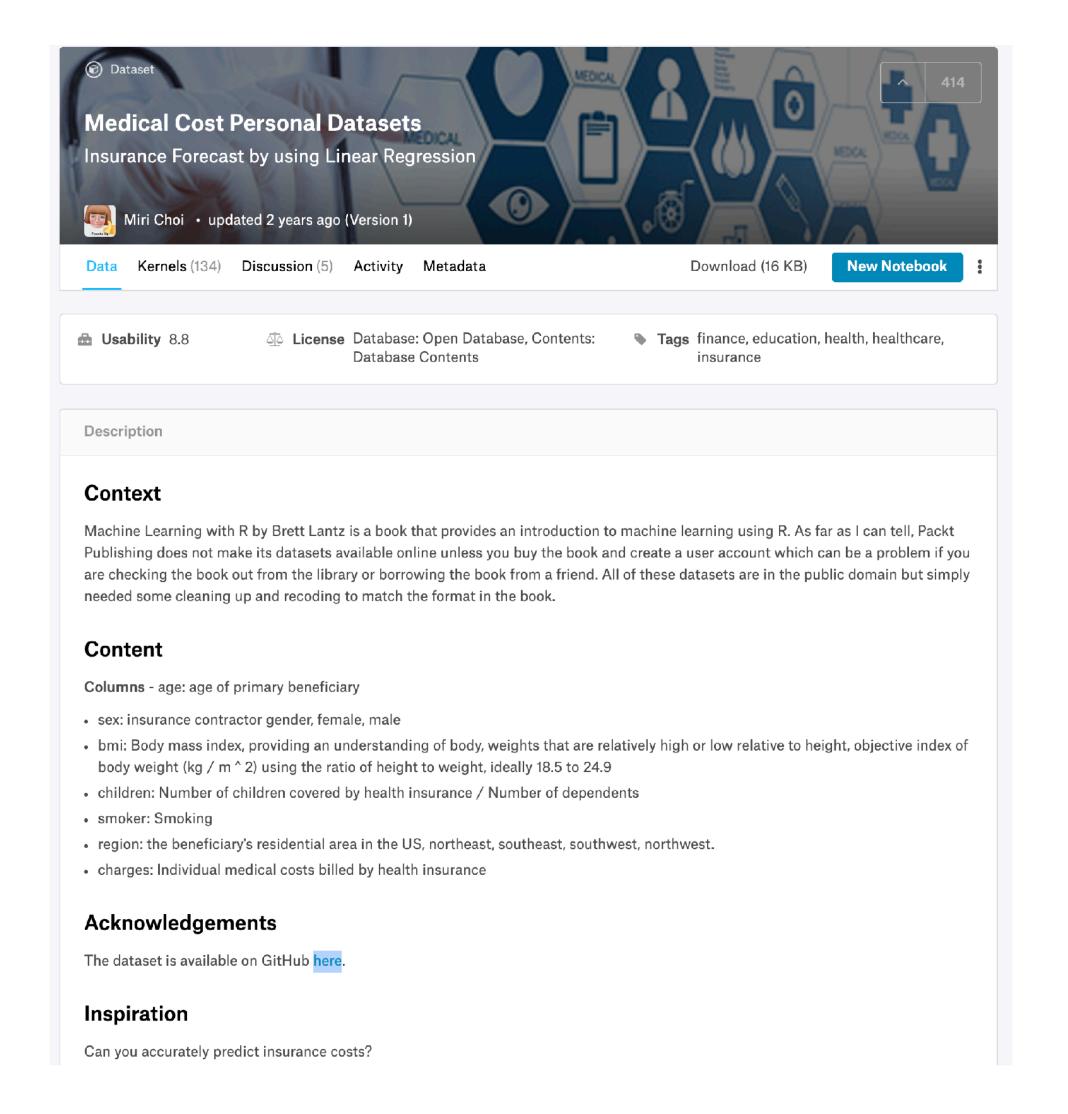
#### **Without interactions**

#### With interactions











#### Task: Can you accurately predict insurance costs?

#### **Experience:**

1338 examples with the following features:

sex: insurance contractor gender, female, male

**bmi**: Body mass index, providing an understanding of body, weights that are relatively high or low relative to height, objective index of body weight (kg / m ^ 2) using the ratio of height to weight, ideally 18.5 to 24.9

children: Number of children covered by health insurance / Number of dependents

smoker: Smoking

region: the beneficiary's residential area in the US, northeast, southeast, southwest, northwest.

charges: Individual medical costs billed by health insurance



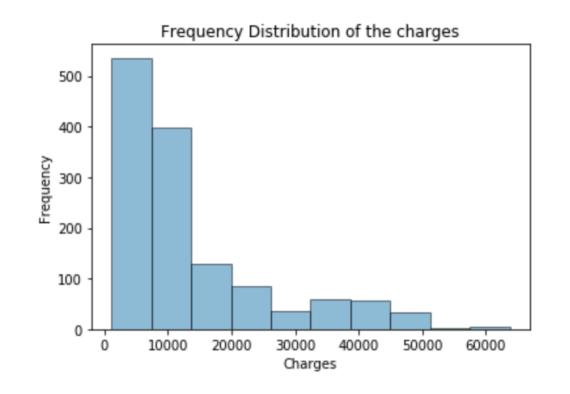
Is data preparation needed here? What should we consider?

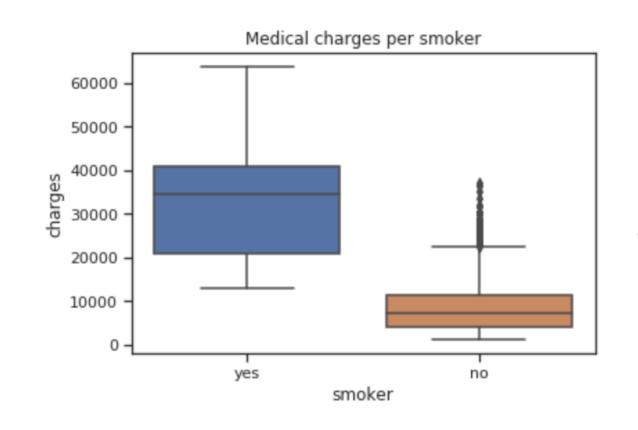
We have 3 categorical features: "sex", "smoker", "region"

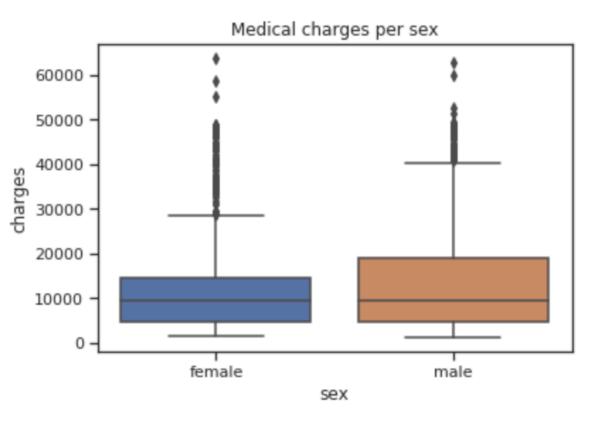
Is there any missing value?

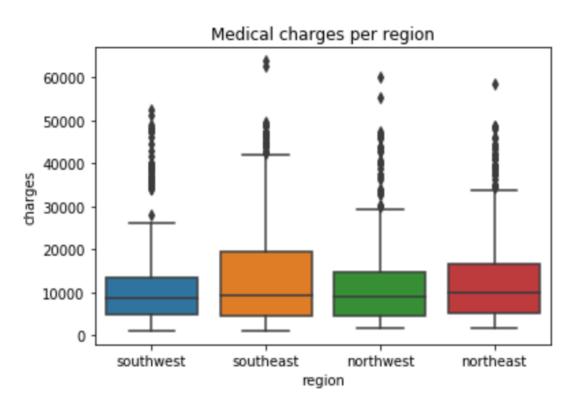
Which is the feature distribution?



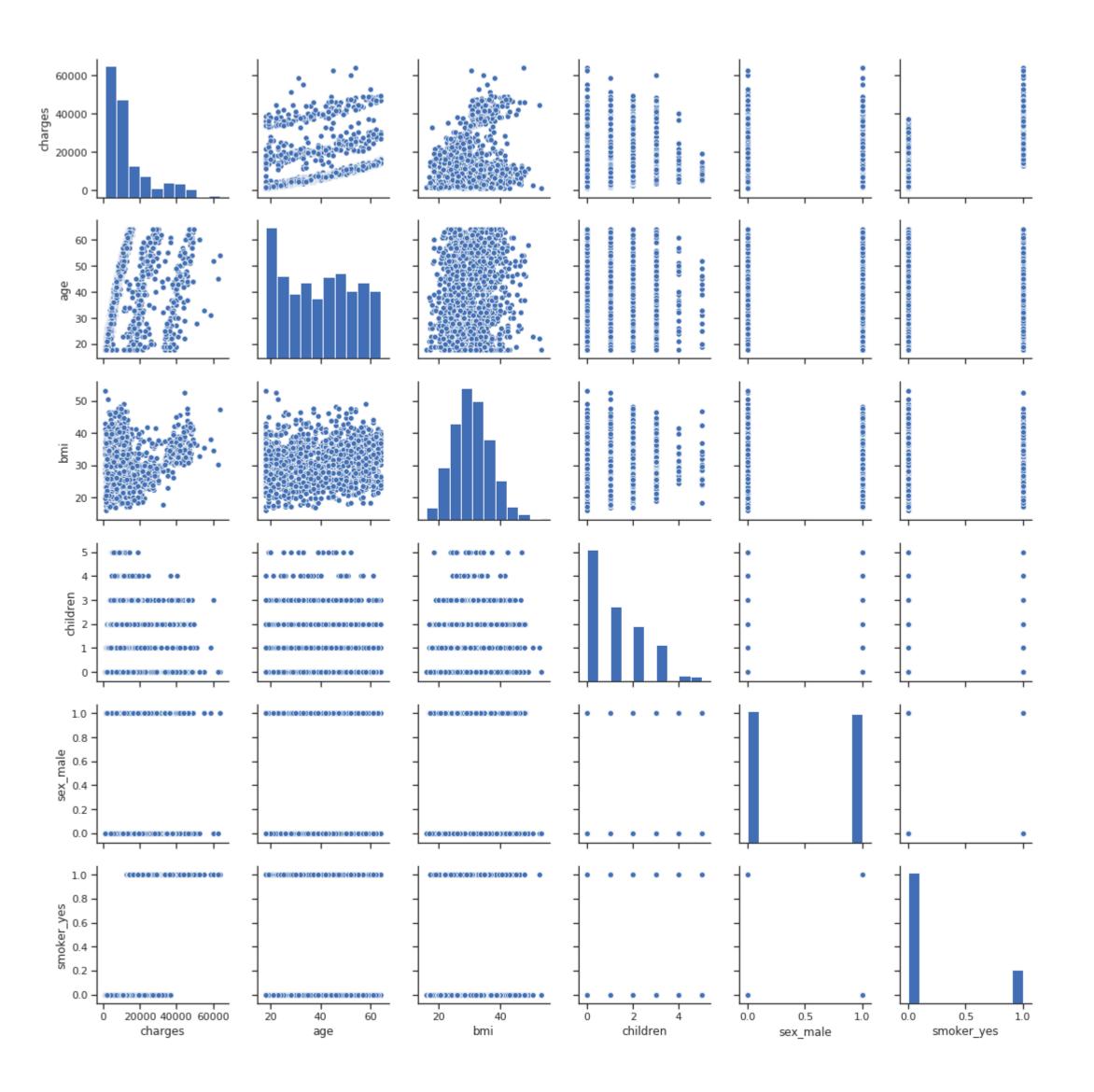












	charges	age	bmi	children	sex_0	smoker_0
count	1338.000000	1338.000000	1338.000000	1338.000000	1338.000000	1338.000000
mean	13270.422265	39.207025	30.663397	1.094918	0.494768	0.795217
std	12110.011237	14.049960	6.098187	1.205493	0.500160	0.403694
min	1121.873900	18.000000	15.960000	0.000000	0.000000	0.000000
25%	4740.287150	27.000000	26.296250	0.000000	0.000000	1.000000
50%	9382.033000	39.000000	30.400000	1.000000	0.000000	1.000000
75%	16639.912515	51.000000	34.693750	2.000000	1.000000	1.000000
max	63770.428010	64.000000	53.130000	5.000000	1.000000	1.000000

There is no missing values!:)





	age	bmi	children	sex_male	smoker_yes
charges	0.299008	0.198341	0.067998	-0.057292	0.787251
age		0.109272	0.042469	0.020856	-0.025019
bmi			0.012759	-0.046371	0.003750
children				-0.017163	0.007673
sex_0					-0.076185

	Coefficient
age	255.765700
bmi	325.533716
children	586.352547
sex_male	392.430723
smoker_yes	23770.069109

^--#:-:--t

**Feature Correlations** 

**Linear Regression Features** 





We are ready to learn a regression MODEL.

Let's divide the data into two sets: training(75%) and test (25%)

#### **Linear regression MODEL**

$$\hat{y} = B_0 + B_1 x_1 + \ldots + B_p x_p$$

	Coefficient
age	252.277070
bmi	308.930902
children	359.000639
sex_male	257.252678
smoker_yes	24069.017691

 $R^2 = 0.7314$ RMSE = 6009.79

**Linear Regression Features** 

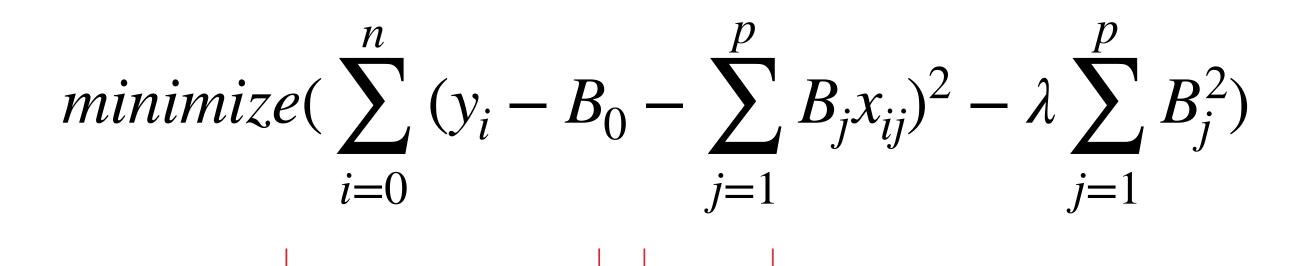
Regularization means making the model less complex which can allow it to generalize better (i.e. avoid overfitting) and perform better on a new data.

• Linear Regression:

minimize 
$$(\sum_{i=0}^{n} (y_i - B_0 - \sum_{j=1}^{p} B_j x_{ij})^2)$$

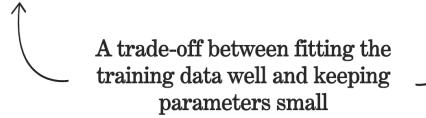
• Ridge Regression:

L2 penalty / Penalty Term / Regularisation Term



Fit training data well (OLS)

Keep parameters small





• Linear Regression:

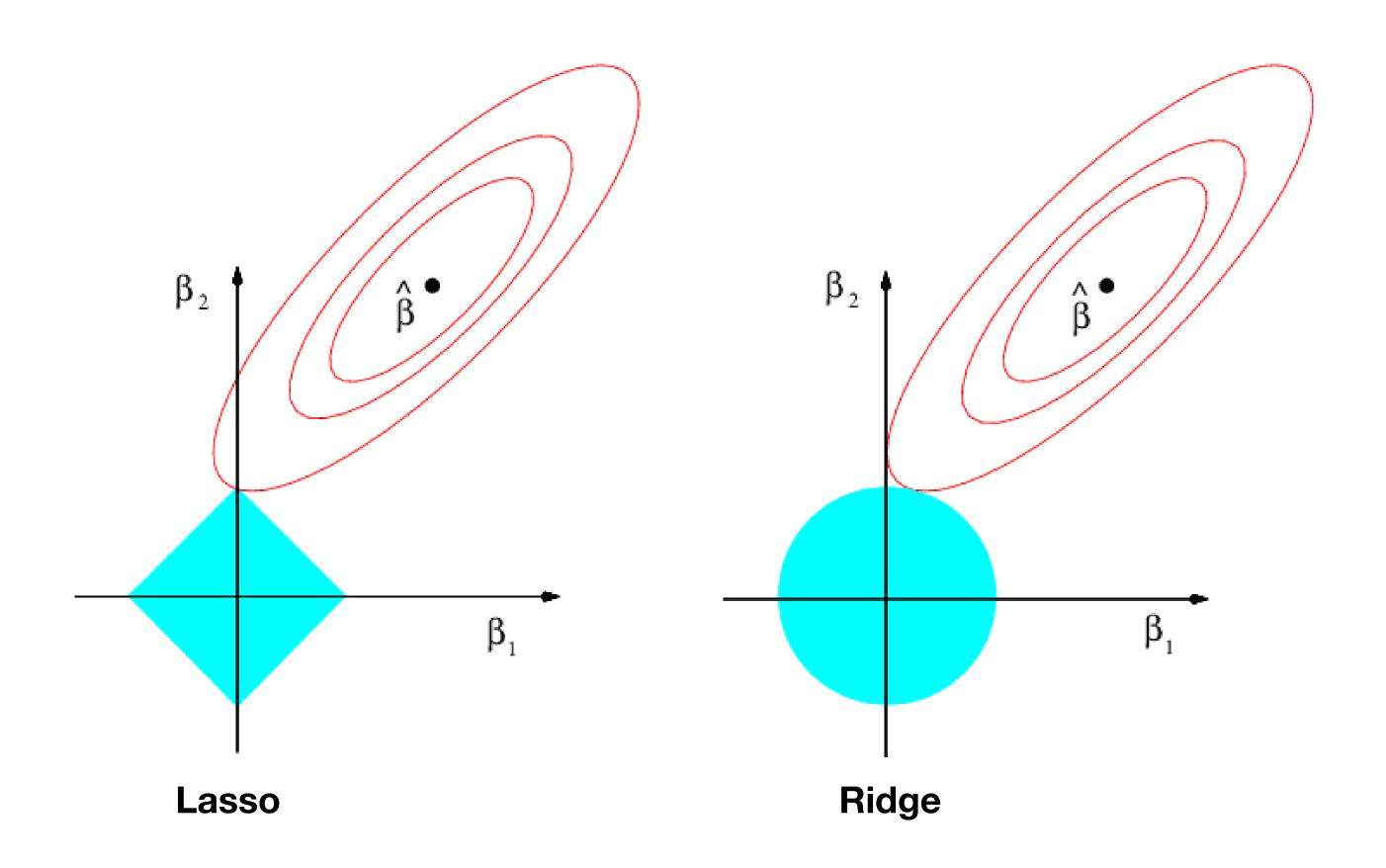
minimize 
$$(\sum_{i=0}^{n} (y_i - B_0 - \sum_{j=1}^{p} B_j x_{ij})^2)$$

• Ridge Regression:

minimize 
$$(\sum_{i=0}^{n} (y_i - B_0 - \sum_{j=1}^{p} B_j x_{ij})^2 - \lambda \sum_{j=1}^{p} B_j^2)$$

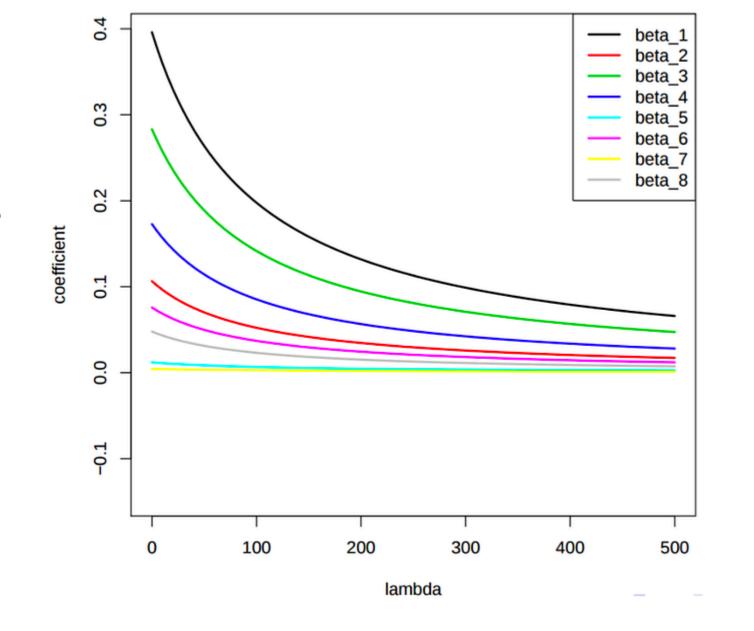
Lasso

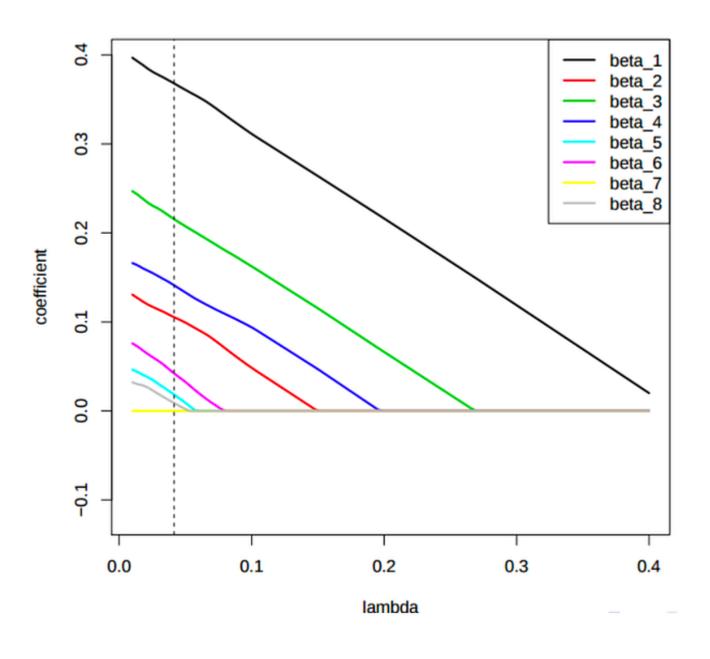
minimize 
$$(\sum_{i=0}^{n} (y_i - B_0 - \sum_{j=1}^{p} B_j x_{ij})^2 - \lambda \sum_{j=1}^{p} |B_j|)$$





An example







### Elastic Net

- The LASSO method has some limitations:
  - In small-n-large-p dataset (high-dimensional data with few examples), the LASSO selects at most n variables before it saturates.

- If there is a group of highly correlated variables, LASSO tends to select one variable from a group and ignore the others.
- To overcome these limitations, the elastic net adds a quadratic part to the L1 penalty, which when used alone is a ridge regression



# Any Idea of non Linear Methods?