



University of Pittsburgh

ECE 2195: Special Topics – Computers Machine Learning

Linear Regression

Mai Abdelhakim, PhD

ECE Department

Swanson School of Engineering

University of Pittsburgh

maia@pitt.edu



This unit

- Linear regression model
- Coefficient estimation
- Inference: Measure association between target and features
 - T-statistics
 - P-value
- Linear regression with multiple features
- Feature selection
- Performance metrics

Linear Regression

- Regression: **Quantitative response prediction, supervised** learning
- Linear regression: assumes linear relation between predictors/features (X_1, X_2, \dots, X_p) and the response Y

- **Parametric Model**

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

β_i : Coefficients or parameters

- Easy to **interpret** the parameters
 - β_1 is the **average increase in Y when there is one unit increase in X_1 and all other features are constant**
- Linear regression is extremely useful both conceptually and practically.

Linear Regression

- **Population line/Actual functions:** $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$
- **Estimated line:** $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \dots + \hat{\beta}_p X_p$
- Given training data, what are the **coefficients** that fit the available training data well
 - Get n training observations: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
 - How to estimate β'_i s?
- One method to estimate coefficients is the **least square method**

Simple Linear Regression – Single Feature

Linear Regression with one feature

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

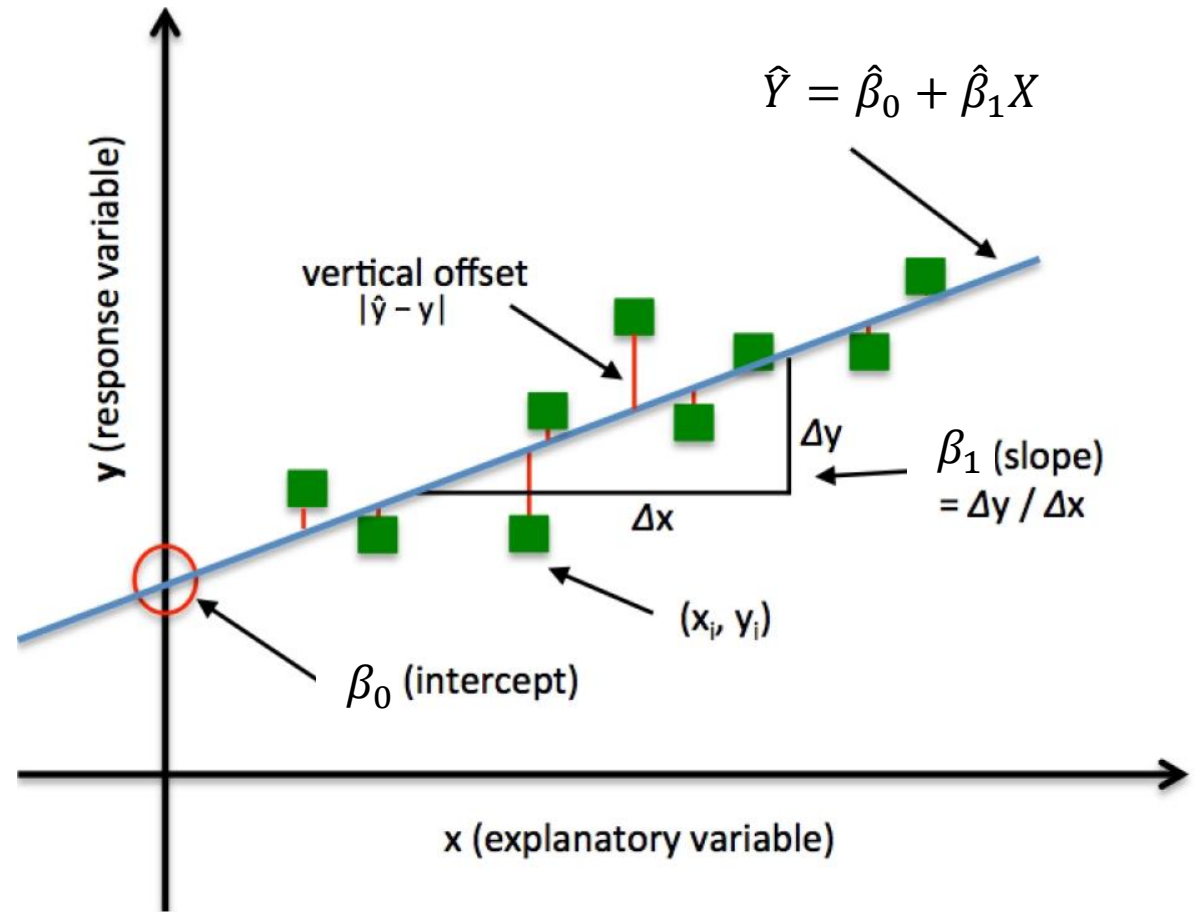
- β_0 is called the **intercept** or **bias term**
- β_1 is the **slope**
- The **coefficients (parameters)** β_0 and β_1 are unknown
- Before we make predictions, coefficients must be estimated

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

How would the fit look like if

$$\beta_1 = 0?$$

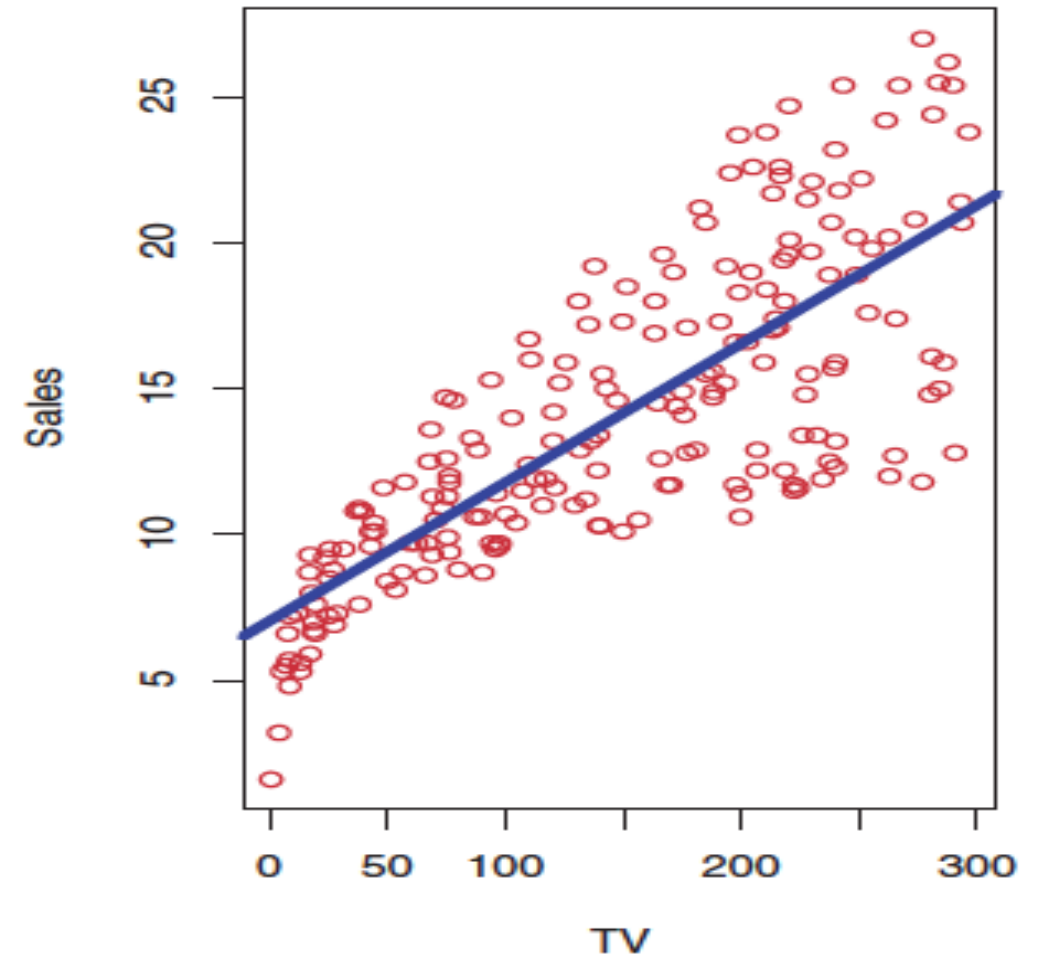
$$\beta_0 = 0?$$



Ref: Raschka, Python Machine Learning

Example

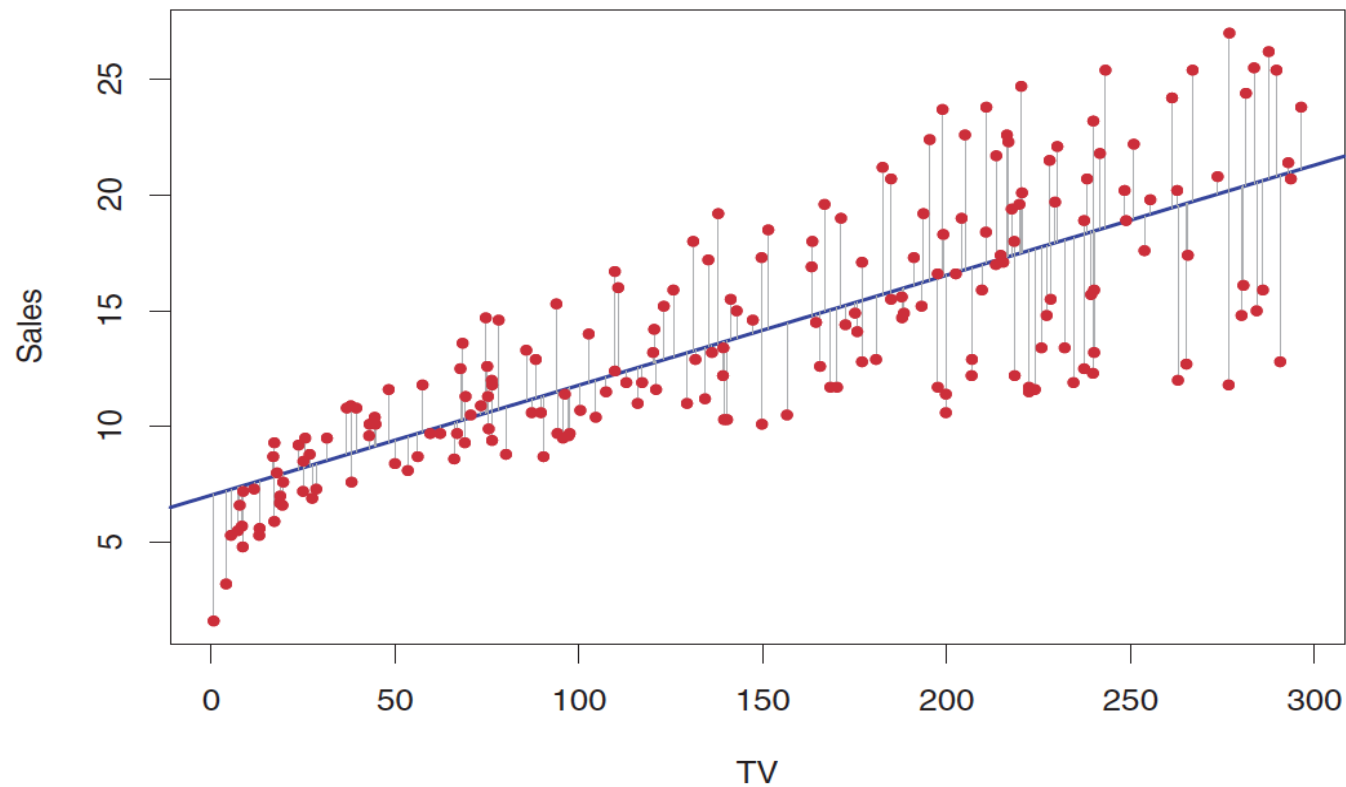
- In the Advertising example, this data set consists of the TV advertising budget and product sales in $n = 200$ different markets
- Linear regression model:
$$\text{sales} \approx \beta_0 + \beta_1 \times \text{TV}$$
- How to get β_0 and β_1 ?



Least Square Method

- Error term of each sample in the training data is:

$$e_i = \hat{y}_i - y_i$$



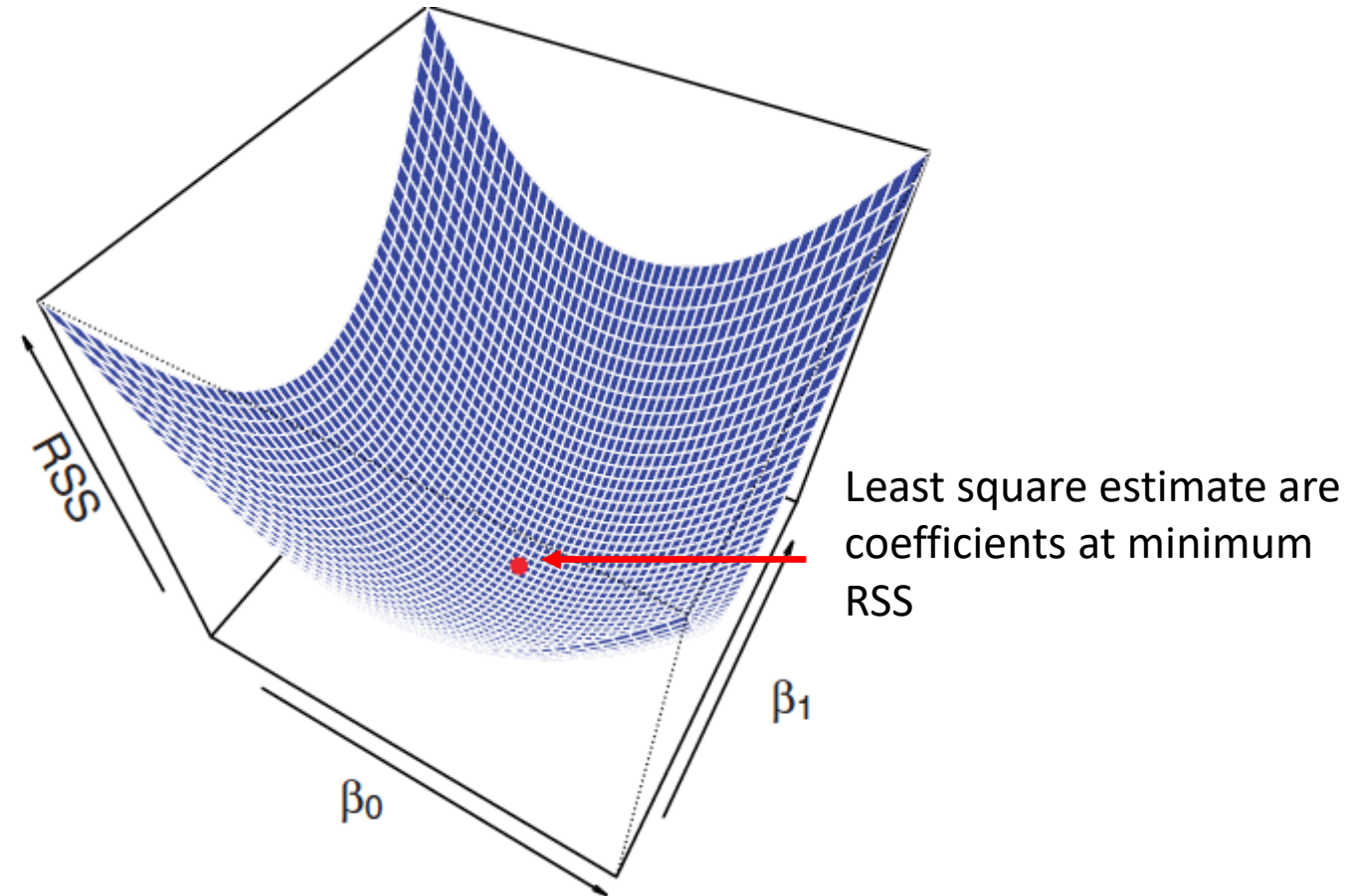
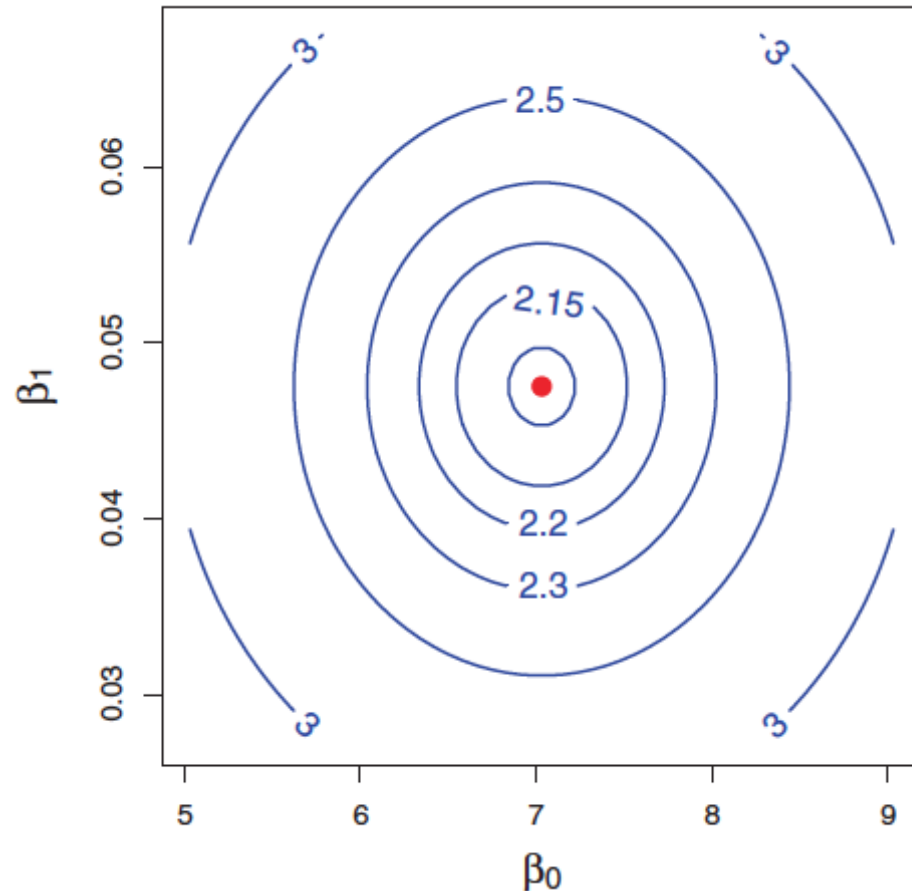
Training Set

TV budget	Sales
x_1	y_1
x_2	y_2
x_n	y_n

Least Square Method

- RSS: residual sum of squares:

$$\text{RSS} = e_1^2 + \dots + e_n^2 = \sum_{i=1}^n [\hat{y}_i - y_i]^2 = \sum_{i=1}^n [\hat{\beta}_0 + \hat{\beta}_1 x_i - y_i]^2$$



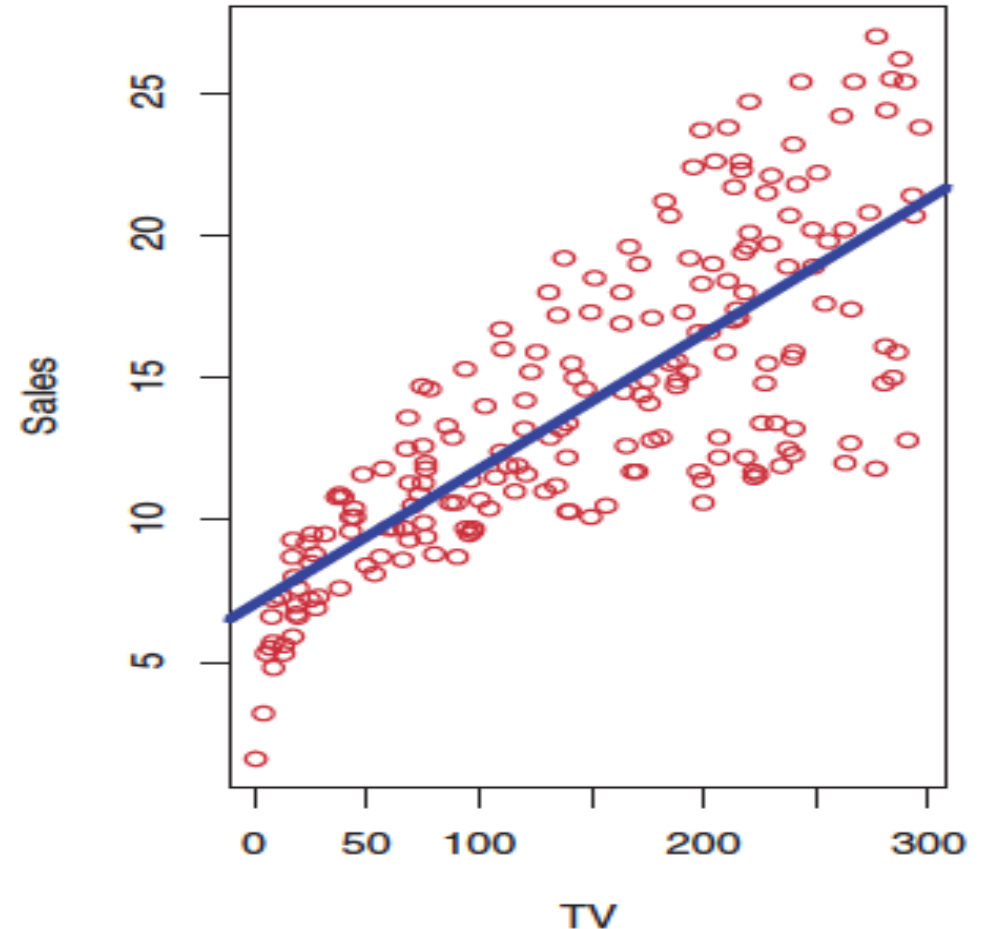
Least Square Method

- Define cost function as mean square error (MSE):

$$J(\hat{\beta}_0, \hat{\beta}_1) = \frac{1}{n} \sum_{i=1}^n [\hat{y}_i - y_i]^2 = \frac{1}{n} \sum_{i=1}^n [\hat{\beta}_0 + \hat{\beta}_1 x_i - y_i]^2 = \frac{1}{n} RSS$$

- **Least square method finds the coefficients that minimizes $J(\beta_0, \beta_1)$**
 - This also **minimizes RSS**

$$\text{minimize}_{\beta_0, \beta_1} J(\beta_0, \beta_1)$$



Approach: Least Square Method

- **Model:** $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$
- **Parameters:** estimate β_0 and β_1
- **Optimization/cost function:** $J(\beta_0, \beta_1)$
 - $J(\hat{\beta}_0, \hat{\beta}_1) = \frac{1}{n} \sum_{i=1}^n [\hat{\beta}_0 + \hat{\beta}_1 x_i - y_i]^2 = \frac{1}{n} RSS$
 - *Sometimes defined as* $J(\hat{\beta}_0, \hat{\beta}_1) = \frac{1}{2n} \sum_{i=1}^n [\hat{\beta}_0 + \hat{\beta}_1 x_i - y_i]^2 = \frac{1}{2n} RSS$
 - The cost function can also be defined to be just equal *RSS*: $J(\hat{\beta}_0, \hat{\beta}_1) = RSS$
- **Goal:** find coefficients that minimize the cost functions
$$\underset{\beta_0, \beta_1}{\text{minimize}} J(\beta_0, \beta_1)$$

Methods for Finding the Optimal Coefficients

- Get derivative of the cost function then set to zero → closed form method
- Gradient descent

Ordinary Least Square (OLS) – Closed Form Solution

- We get the partial derivative of cost function (or RSS) with respect to β_i , then equate to zero to get the coefficients

$$\frac{\partial RSS}{\partial \beta_0} = 0, \frac{\partial RSS}{\partial \beta_1} = 0$$

- Using some calculus, show that β_0 and β_1 that minimize the RSS are

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

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

where $\bar{y} = \frac{\sum_{i=1}^n y_i}{n}$ $\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$

Least Square Method Optimization – Gradient Descent

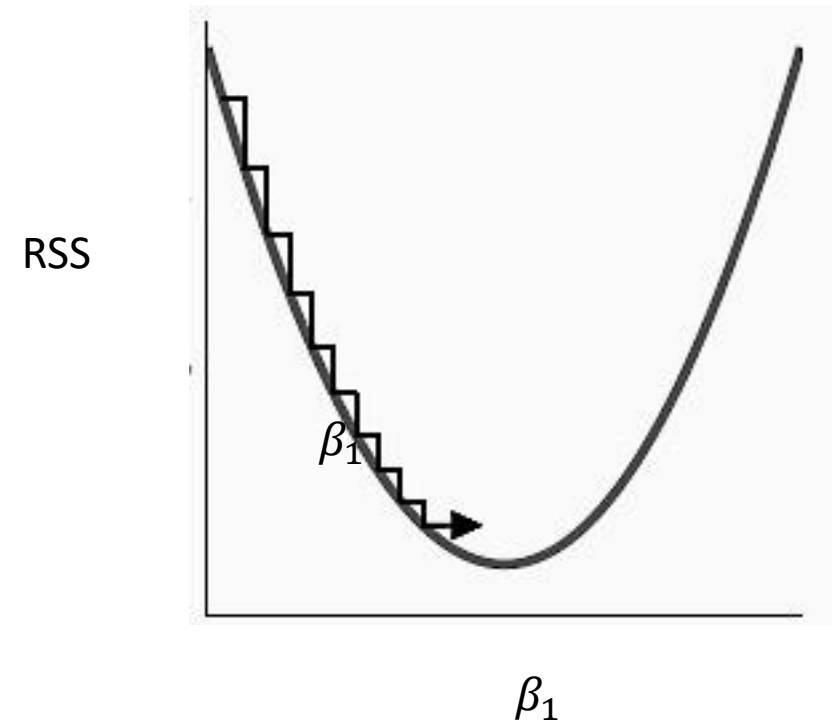
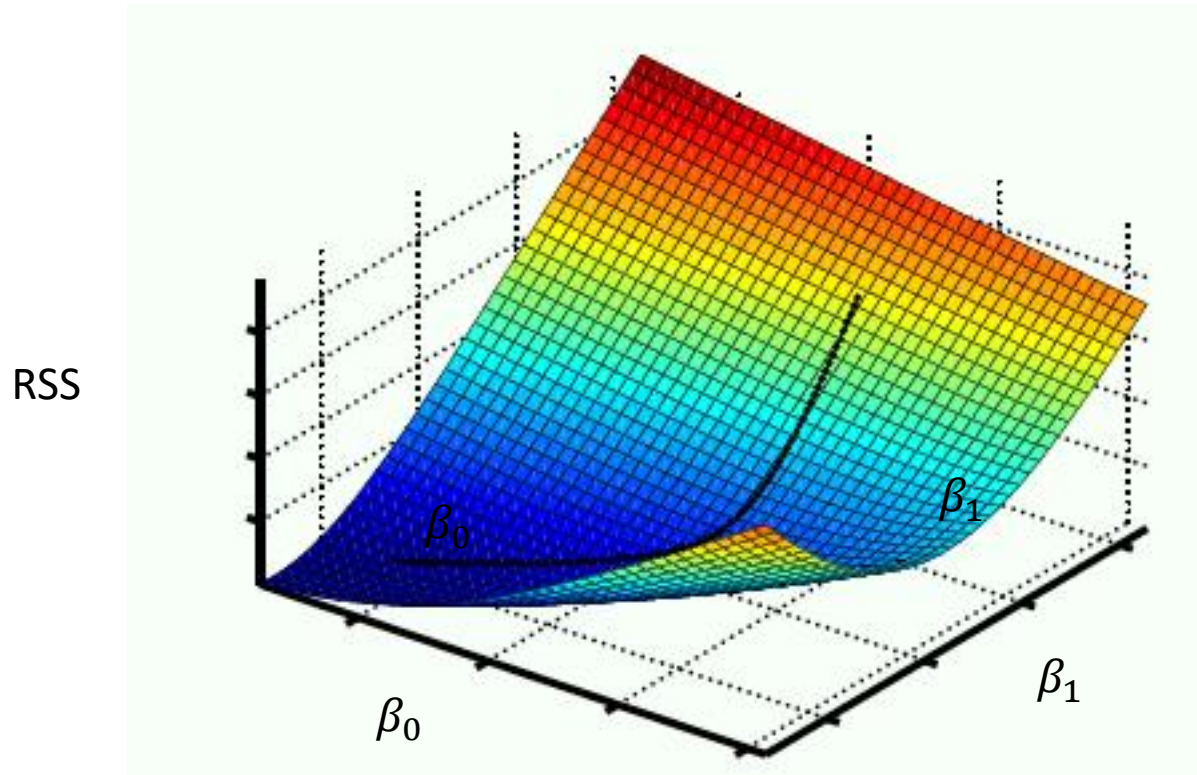
- Another method to find optimal parameters
- Used when finding closed form solution is difficult or computationally expensive
- Iterative method to find the optimal values of coefficients
 - Start with some values for the parameters (β_0 and β_1)
 - Calculate the gradient and then update all parameters simultaneously

$$\beta_i := \beta_i - \alpha \frac{\partial}{\partial \beta_i} J(\beta), \quad \alpha \text{ is the learning rate}$$

- Keep changing the parameters to reduce the objective function $J(\hat{\beta}_0, \hat{\beta}_1)$ until the **minimum value of the objective function** is obtained or a **predefined stopping condition** is met.

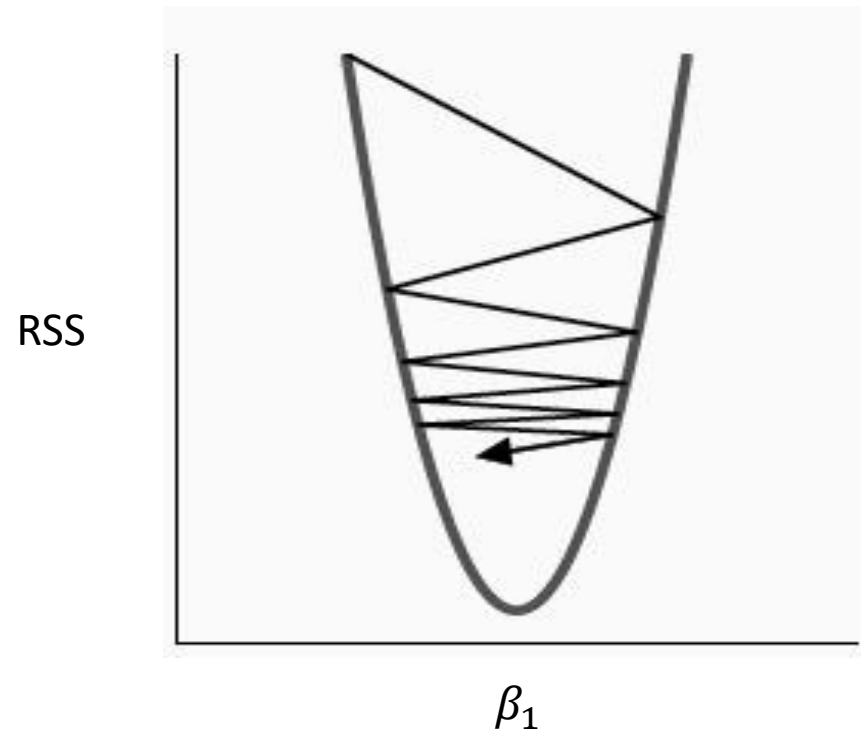
Impact of Learning Rate

- With a small learning rate, e.g. $\alpha=0.1$, convergence is slow

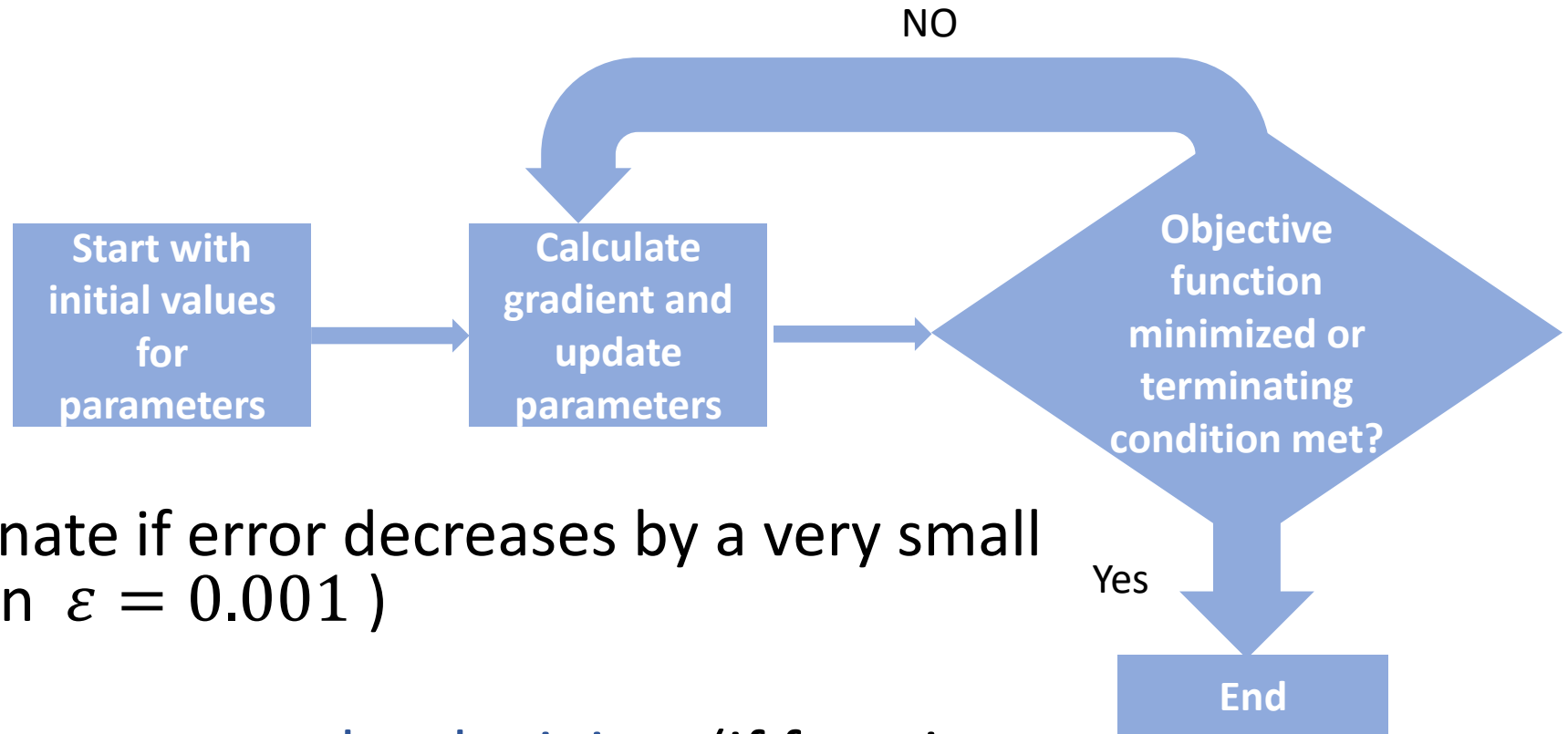


Impact of Learning Rate

- Large learning rate, e.g. $\alpha=2$, the algorithm may not converge



Optimization – Gradient Descent



- **Converge**: e.g., terminate if error decreases by a very small amount (e.g. less than $\varepsilon = 0.001$)
- **Disadvantage**: may **converge at a local minima** (if function not convex, e.g. in neural networks)
- **Variants** – e.g. stochastic gradient descent (update weight using one training example at a time)

Linear Regression in Python – Model

- Let's generate a synthetic data
- Assume the actual line is: $y=2+3X+\epsilon$, with ϵ be normal error with zero mean and unit variance

$$y = \text{beta0} + \text{beta1} * x + \text{error}$$

Linear Regression in Python

```
from sklearn.model_selection import train_test_split
```

```
from sklearn.linear_model import LinearRegression
```

```
X_train, X_test, Y_train, Y_test= train_test_split(x, y, random_state= 0)
```

```
linreg= LinearRegression().fit(X_train, Y_train)
```

```
print("The intercept is: ", linreg.intercept_)
```

```
print("The coefficient of TV feature is:",linreg.coef_)
```

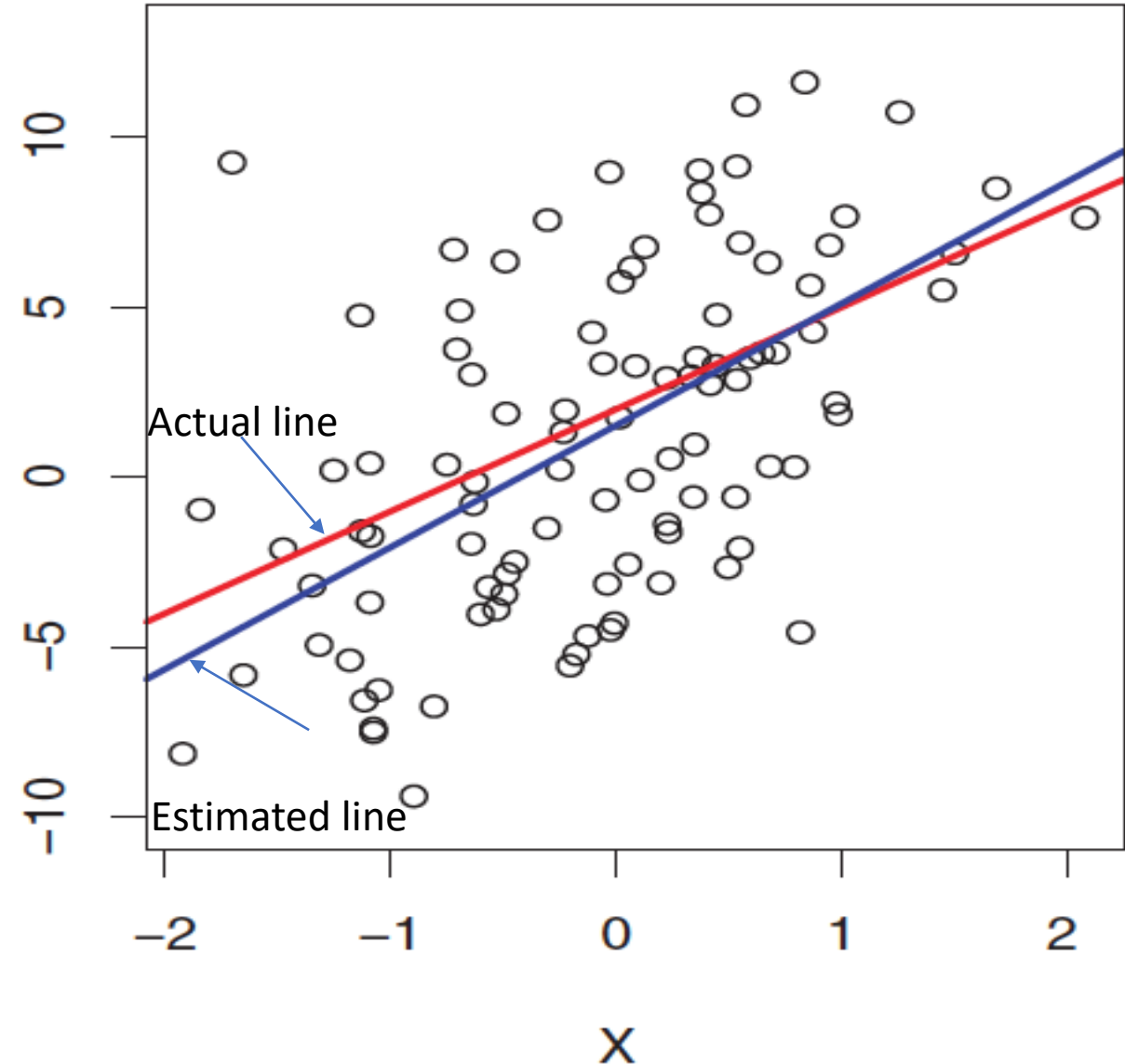
Plot the Data and the Fitted Model

```
estimated_linearmodel= linreg.intercept_ + linreg.coef_ * x
```

```
plt.plot(x, estimated_linearmodel, 'b-')
```

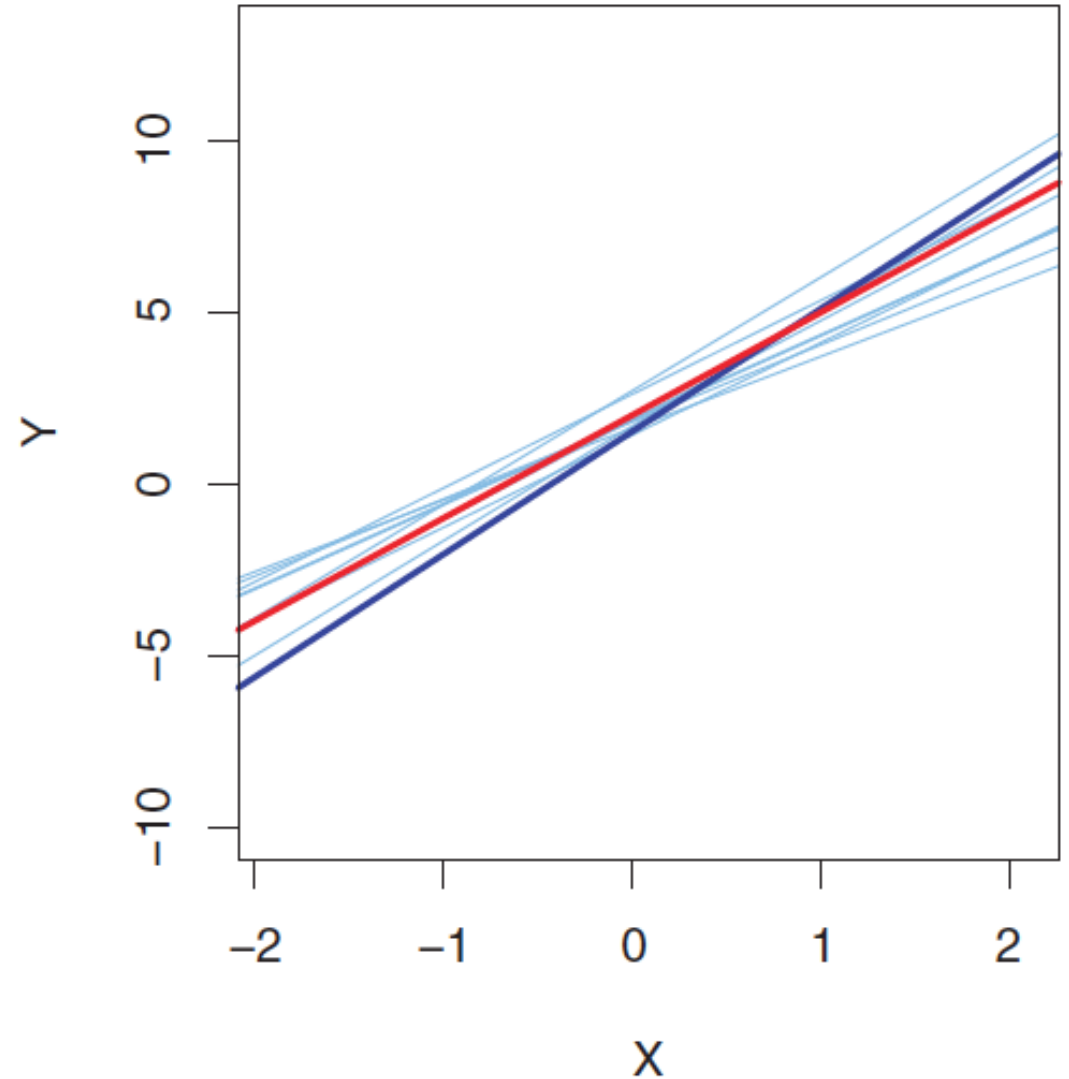
Accuracy of Coefficient Estimates

- Red line: actual $f(x) = \beta_0 + \beta_1 X$
Population regression, $y = \beta_0 + \beta_1 X + \epsilon$
- Black circles are data points
- Blue line: least square line estimated from 100 training points



Accuracy of Coefficient Estimates

- Fig. shows 10 least square lines (light blue lines), each computed based on 10 random set of training observations
- The fitted model depends on the data
- How accurate is the estimated coefficients?



Accuracy of Coefficient Estimates - Variance

- We can measure the standard error of each coefficient
- $(SE)^2$ is the variance
 - Reflects how the coefficient varies under repeated sampling
 - Let $\sigma^2 = Var(\epsilon)$, variance of error, and \bar{x} be the average of feature x , n is the number of observations

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

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

Accuracy of Coefficient Estimates - Confidence Interval

- **Confidence interval:** 95% confidence interval is the range of values that with 95% probability the range will contain the **true unknown value** of the coefficient.
- For β_1 , 95% confidence interval is approximately equal to:

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

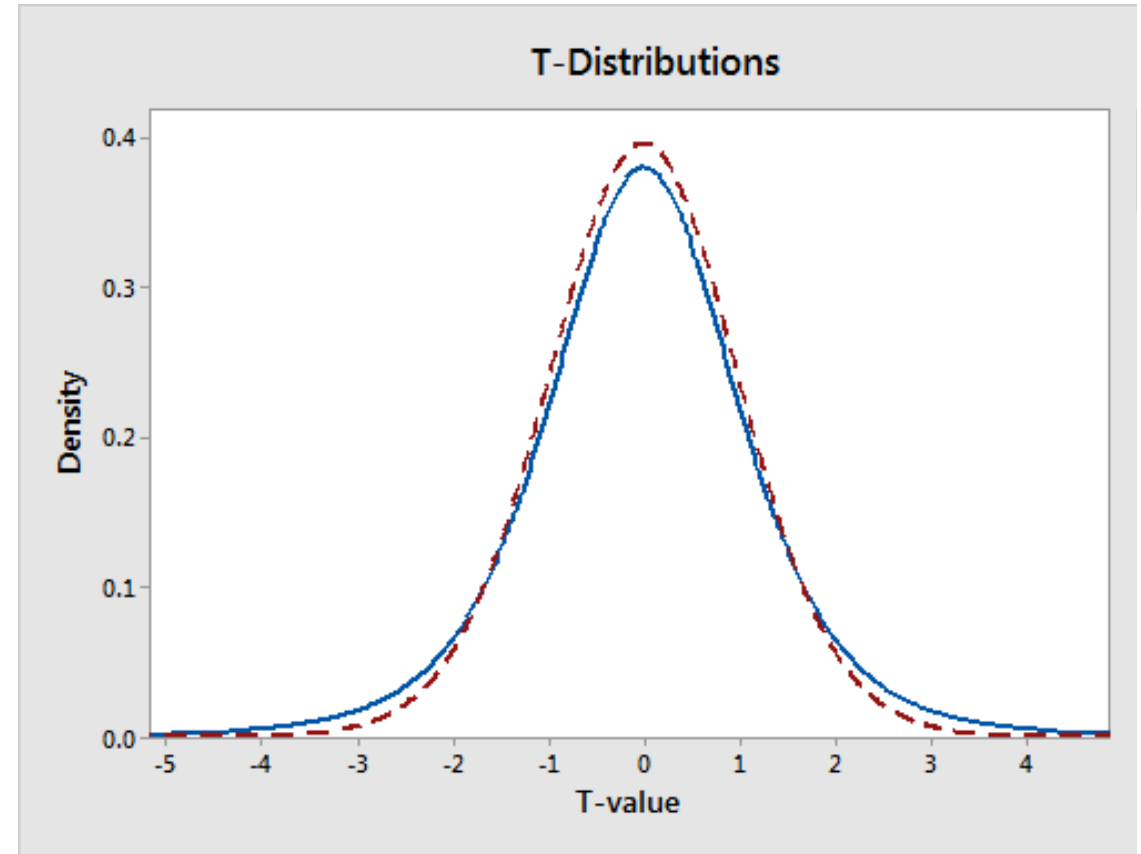
- Question: is there actual association between the feature and the target? Is the feature important in prediction?

Association Between Feature and Response Modeled as Hypothesis test

- **Hypothesis test:** procedure for deciding whether to accept or reject the assertion based on the observed data
 - A hypothesis is an assertion about a random thing
- Hypothesis test:
 - **Null hypothesis H_0 :** No association between feature and response, i.e.
$$\beta_1 = 0$$
 - **Alternative hypothesis H_1 :** There is an association between feature and response, i.e.
$$\beta_1 \neq 0$$

Test the Null Hypothesis – T-statistics and P-value

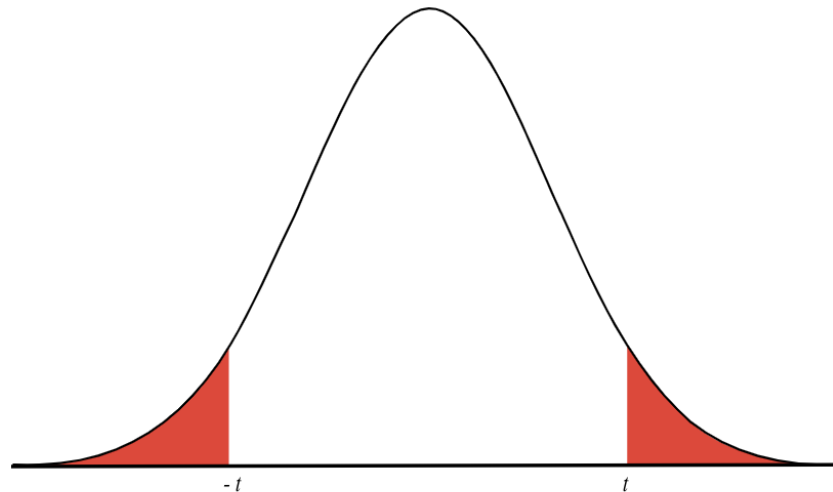
- **t-statistics:** $t = \frac{\hat{\beta}_1 - 0}{SE(\hat{\beta}_1)}$
 - Measures how far $\hat{\beta}_1$ is away from 0 (Null hypothesis).
 - If t-statistics is large, this reflects association between feature and response



Under Null hypothesis

Test the Null Hypothesis – T-statistics and P-value

- **P-value:** is the probability of observing a statistical value (here we use t-statistics) equal to the **observed ($|t|$) or larger if there is no association between response and the feature** (i.e when Null hypothesis is true)
 - Small value reflects that there is an association between features and output
 - Large value reflects low association between features and output



Association Between Feature and Response

- We care about the terms corresponding to the features (not the intercept)

	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

Calculate Statistical Summary in Python

- Get advertising dataset from courseweb or from this link: <http://www-bcf.usc.edu/~gareth/ISL/data.html>

```
from pandas import read_csv  
AdvertisingData=read_csv('Advertising.csv')
```

- Use statsmodels python module, to get **statistical summary** for ordinary least square: <http://www.statsmodels.org/stable/index.html>

```
import statsmodels.formula.api as smf
```

- The statistical summary you will get includes:

Coefficients, standard error or variance (`std_err`), t statistics, P-value ($P > |t|$), confidence interval (`[0.025, 0.975]`)

- **Q:** what is the confidence interval of TV coefficient generated by the code?
 - Does the confidence interval include 'zero'? What does that imply?

Linear Regression – Multiple Features

Linear Regression with Multiple Features

- $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$

β_j is the average effect on Y of one unit increase in X_j holding other features fixed

- *Challenge: In practice, features can be correlated and may change with each other (will be discussed)*

- Make predictions using

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

- **Estimate coefficients** $(\beta_0, \beta_1, \beta_2 \dots \beta_p)$ that minimizes the MSE or RSS

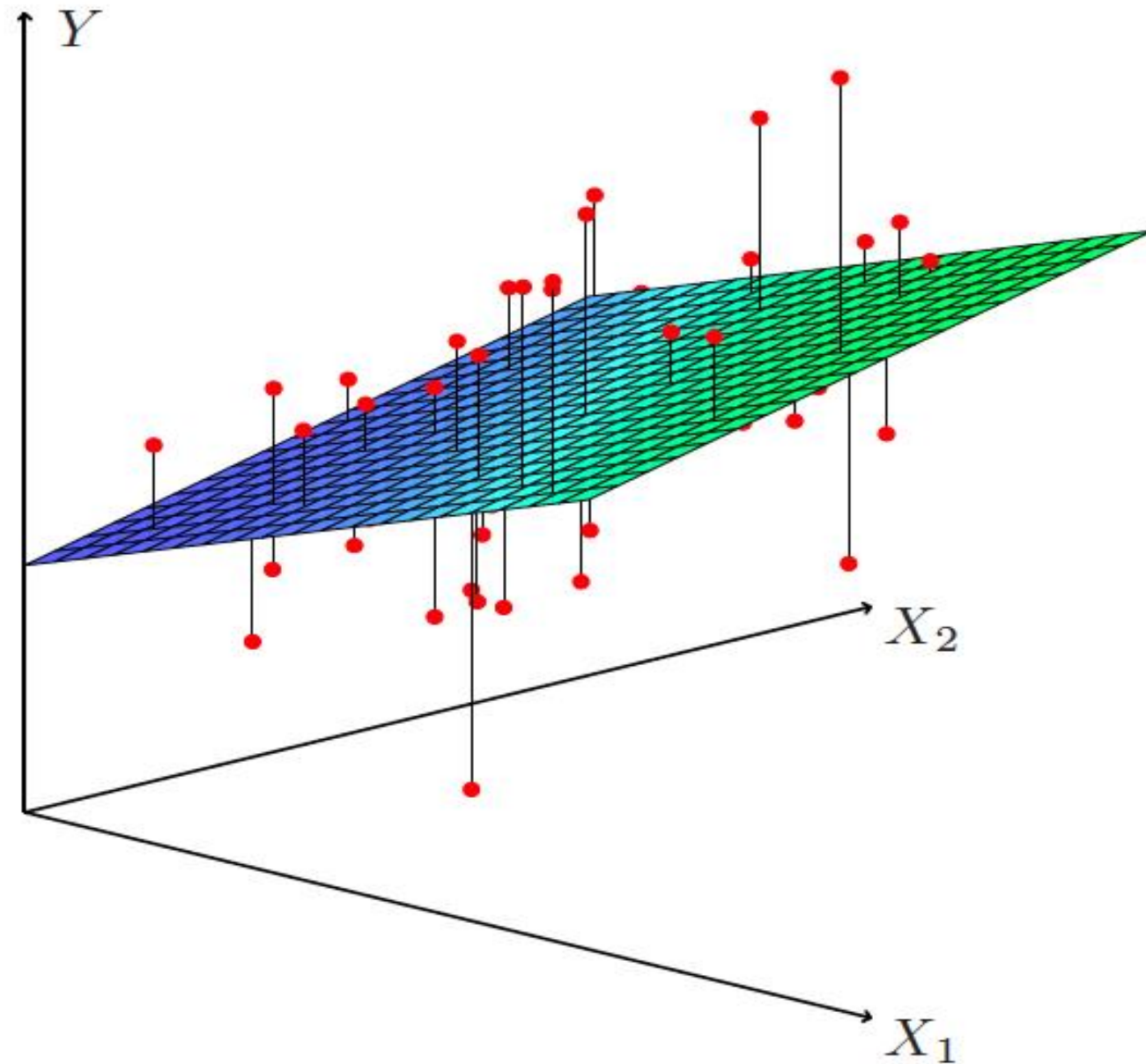
$$\text{RSS} = \sum_{i=1}^n (\hat{y}_i - y_i)^2$$

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

x_{ij} : j th feature
of i th training
point

Multiple least squares regression estimate

**Rule: number of observation
points/training must be larger than
number of features, i.e., $P < n$**



Least Square Method: Matrix Form Closed-Form Solution

- Matrix form:

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} \dots & x_{1p} \\ 1 & x_{21} \dots & x_{2p} \\ \vdots & \vdots & \vdots \\ 1 & x_{n1} \dots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

x_{ij} : j th feature of i th training point

- That is: $y = X \beta + \epsilon$
 - y is target of training data ($n \times 1$) vector
 - X is $n \times (p+1)$ matrix, first column is all constant (1's)
 - $\hat{\beta}$ is $(p+1) \times 1$ vector of $[\beta_0 \dots \beta_p]^T$

Closed-form Solution

- $RSS(\hat{\beta}) = (y - X\hat{\beta})^t (y - X\hat{\beta})$
- If we differentiate with respect to β , then equate to zero, we get:

$$\frac{\partial RSS}{\partial \hat{\beta}} = \frac{\partial}{\partial \hat{\beta}} ((y - X\hat{\beta})^t (y - X\hat{\beta})) = 0$$

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

Optimization – Gradient Descent For Multiple Variables

- Same as before
- Objective is $J(\beta) = J(\beta_1 \dots \beta_p) = RSS = \sum_{i=1}^n [\hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \dots + \hat{\beta}_p x_{ip} - y_i]^2$
- Iterative method to find the optimal values of coefficients
 - Start with some values for the parameters $(\beta_0 \dots \beta_p)$
 - Calculate the gradient and then simultaneously update the parameters
$$\beta_i := \beta_i - \alpha \frac{\partial}{\partial \beta_i} J(\beta), \alpha \text{ is the learning rate}$$
- Keep changing the parameters to reduce the objective function until the minimum value of the objective function is obtained.

Features Association: Fitting the Sales with TV and Newspaper Budget

- Find P-value corresponding to Newspaper budget when using **both *TV and Newspaper*** as features.
 - Do both features impact the sales?

	coef	std err	t	P> t	[0.025	0.975]
Intercept	5.7749	0.525	10.993	0.000	4.739	6.811
TV	0.0469	0.003	18.173	0.000	0.042	0.052
Newspaper	0.0442	0.010	4.346	0.000	0.024	0.064

Features Association: Sales Example with Budget Spent on 3 Media

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

- Features with low p-values have association with output

```
import statsmodels.formula.api as smf
```

```
model=smf.ols('Sales ~ TV+Radio+Newspaper', AdvertisingData)
Fitting_results=model.fit()
print(Fitting_results.summary().tables[1])
print('p-values are: \n', Fitting_results.pvalues)
```

	coef	std err	t	P> t	[0.025	0.975]
Intercept	2.9389	0.312	9.422	0.000	2.324	3.554
TV	0.0458	0.001	32.809	0.000	0.043	0.049
Radio	0.1885	0.009	21.893	0.000	0.172	0.206
Newspaper	-0.0010	0.006	-0.177	0.860	-0.013	0.011

High p-value, low association with Sales

- Find P-value corresponding to Newspaper budget when using **both *TV and Newspaper*** as features.
 - Do both features impact the sales?
- Find P-value of Newspaper when using **TV, Radio and Newspaper** as features
 - Which is of least importance?
 - *Here, it is clear that **Newspaper has no impact on Sales!***
 - *Does the confidence interval of Newspaper include zero?*

Recall Correlation

- Finding the correlation between features and target helps in inference
- Covariance between two variables X, Y : $COV(X,Y) = E[(X-\text{mean}(X))(Y-\text{mean}(Y))]$
- If covariance is zero, then X and Y are not correlated
- Correlation coefficient between X, Y ($\rho_{x,y}$) Is a value in the range of $[-1,1]$

$$\rho_{x,y} = \frac{COV(X,Y)}{\sqrt{VAR(X)} \sqrt{VAR(Y)}}$$

- If $\rho_{x,y}=0$, then there is no correlation
- If $\rho_{x,y}=1$, then there is a positive correlation
- If $\rho_{x,y}=-1$, then there is a negative correlation

- Correlation matrix contains correlation coefficient of different variables
- Can be obtained with numpy in python

Import numpy as np

correlation_coef2=np.corrcoef([AdvertisingData.TV, AdvertisingData.Radio, AdvertisingData.Newspaper, AdvertisingData.Sales])

	TV	Radio	Newspaper	Sales
TV	1.000000	0.054809	0.056648	0.782224
Radio	0.054809	1.000000	0.354104	0.576223
Newspaper	0.056648	0.354104	1.000000	0.228299
Sales	0.782224	0.576223	0.228299	1.000000

Each number presents correlation between the corresponding variables (indicated in row and column labels)

Calculate the MSE with and without Newspaper advertisement, you should find the difference is very low!

Features Association: Decide on Important Features

- How to find subset of the most important features
- Find least square fit for all possible subsets of the features, then find best one
- What if the training observations are not sufficient, e.g. $n < p$?
- What if we have large number of features?
 - Very complex to check all subset of important features
 - 40 features, we have over a billion models to fit
- Need more efficient approach to find the best subset of features

Features Association: Decide on Important Features

- Forward selection:
 - Start with null hypothesis
 - Fit p simple linear regression models, then add to the null model the feature that results in lowest RSS
 - Fit $p-1$ models, then add to that model the feature that results in lowest RSS among all two-feature models
 - And so on until stopping criteria is met

When a feature is added it is will not be removed in subsequent iterations

- Backward selection:
 - Start with all variables/features in the model
 - Remove variable with largest p-value
 - The new ($p-1$ features) model is fitted, and feature with largest p-value is removed
 - Repeat until stopping criteria is met: all variables have p-value below some threshold
 - Selection can be based on the accuracy of the model instead of the p-value
 - Backward selection cannot be used if $p > n$

- **Mixed selection:** combination of forward and backward selection
 - Starts with null hypothesis, add one feature at a time (like forward selection)
 - If a feature has its p-value higher than a certain threshold when new features are added to the model, then this feature is removed
 - Unlike forward and backward selection, here it is possible to remove feature after adding it
- **Feature transformation:** discussed later

Scaling and Normalization

- **Feature scaling** and normalization may improve the performance of a learning algorithm
 - House price prediction: area (2000 feet²), number of bedrooms [1-5]
- **Essential when using gradient descent**
 - The derivative will lead to multiplying by a feature value. This will make the rate of parameter update depend on the value of the feature
- Python functions: MinMaxScaler or StandardScaler

Assessing Model Accuracy

- How well the model fits the data?

- Metrics:

- Mean squared error : $MSE = \frac{1}{n} \sum_{i=1}^n [\hat{y}_i - y_i]^2 = \frac{1}{n} RSS$

- Root mean squared error: $RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n [\hat{y}_i - y_i]^2} = \sqrt{\frac{1}{n} RSS}$

- R^2 metric

- Others

Assessing Model Accuracy

- R^2 metric is a number between [0,1]

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

- TSS is the total sum of squares $TSS = \sum (y_i - \bar{y})^2$
 - Measures total variance in the response Y (variability in Y) before the regression is performed
- R^2 measures the proportion of variability in Y that can be explained using feature (X) .

Assessing Model Accuracy

- R^2 metric is a number between [0,1]

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

- TSS is the total sum of squares $\text{TSS} = \sum (y_i - \bar{y})^2$
- Higher R^2 metric is desired

R² metric Calculations

Calculate the R² metric of OLS using the training in the table

Training Index (<i>i</i>)	Target (<i>y_i</i>)	Feature (<i>x_i</i>)
1	5	6
2	7	9
3	8	10
4	10	12
5	11	13
6	13	16

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

$$\text{RSS} = e_1^2 + \dots + e_n^2 = \sum_{i=1}^n [\hat{y}_i - y_i]^2 = \sum_{i=1}^n [\hat{\beta}_0 + \hat{\beta}_1 x_i - y_i]^2$$

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

R² metric Calculations

Calculate the R² metric using the training in the table

Training index	Target (y _i)	Feature (x _i)	y _i x _i	x _i ²
1	5	6	30	36
2	7	9	63	81
3	8	10	80	100
4	10	12	120	144
5	11	13	143	169
6	13	16	208	256
sum	54	66	644	786

$$n=6 \quad \bar{y} = \frac{\sum_{i=1}^n y_i}{n} = 9 \quad \bar{x} = \frac{\sum_{i=1}^n x_i}{n} = 11$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n y_i x_i - \bar{y} \sum_{i=1}^n x_i}{\sum_{i=1}^n x_i^2 - \bar{x} \sum_{i=1}^n x_i} \Rightarrow \hat{\beta}_1 = \frac{644 - 9 \times 66}{786 - 11 \times 66} = 0.83$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \Rightarrow \hat{\beta}_0 = 9 - 0.83 \times 11 = -0.13$$

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i = -0.13 + 0.83 x_i$$

R² metric Calculations

Calculate the R² metric using the training in the table

Training index	Target (y _i)	Feature (x _i)	
1	5	6	4.85
2	7	9	7.34
3	8	10	8.17
4	10	12	9.83
5	11	13	10.66
6	13	16	13.15
sum	54	66	

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \\ = -0.13 + 0.83 x_i$$

$$n=6 \quad \bar{y} = \frac{\sum_{i=1}^n y_i}{n} = 9 \quad \bar{x} = \frac{\sum_{i=1}^n x_i}{n} = 11$$

$$\text{RSS (on training data)} = \sum_{i=1}^n [\hat{y}_i - y_i]^2 = 0.334$$

$$\text{TSS} = \sum_{i=1}^n [\bar{y} - y_i]^2 = 42$$

$$\text{Training R}^2 \text{ metric in this example} = (\text{TSS} - \text{RSS}) / \text{TSS} = 0.99$$

Note that we access the model using test data, which can be evaluated in a similar manner but using a test dataset

R² in python

- Using the score method:
Fitted_model.score(X_test,Y_test)
- Or use metric module in sklearn
from **sklearn.metrics** import **r2_score**
predicted_target= fitted_model.**predict**(X_test)
r2score=**r2_score**(Y_test, predicted_target)