Overfitting and Underfitting

Overview

Training Performance: Low (Gorib)
Testing Performance: Low (Gorib)

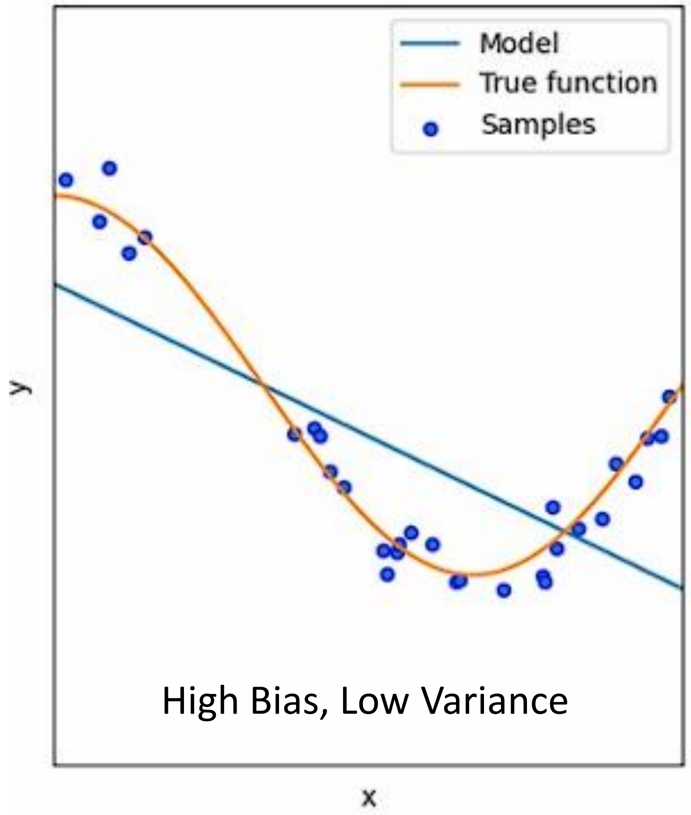


Fig 01: Underfitting

Training Performance: Good
Testing Performance: Good

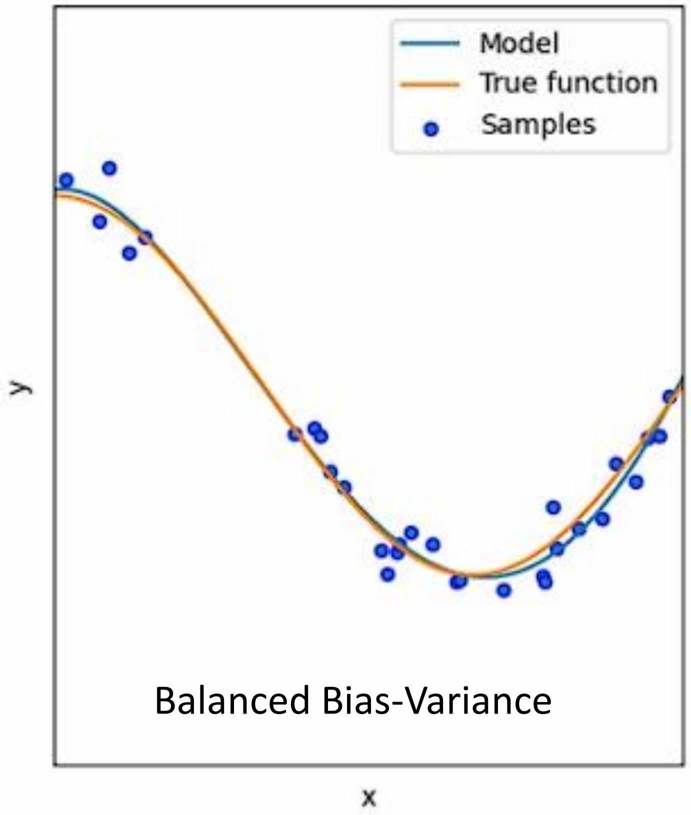


Fig 02: Best fitting

Training Performance: High (Rich)
Testing Performance: Low (Gorib)

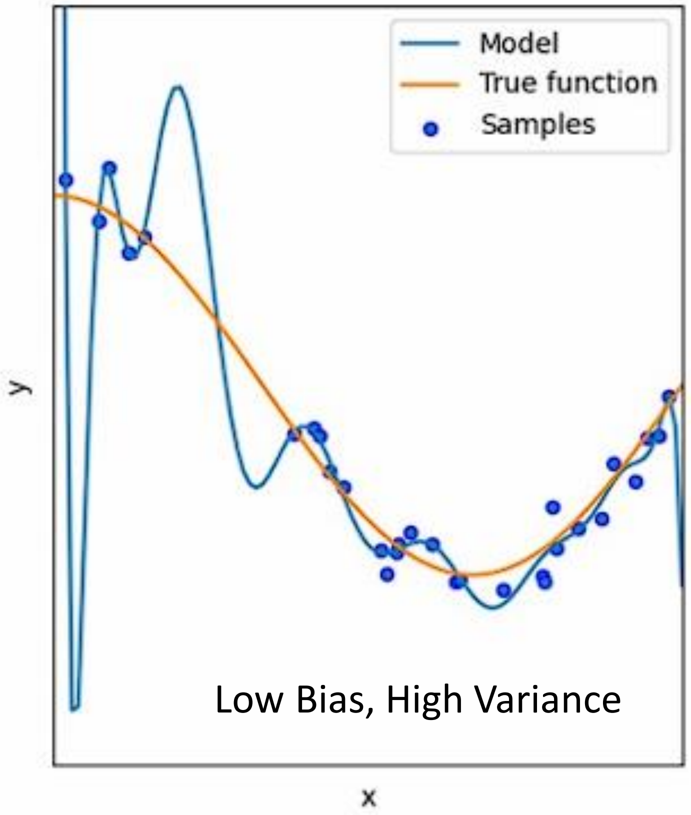


Fig 03: Overfitting

1. **Bias:** The difference between the average predicted value and the true value.
2. **Variance:** The variability of model predictions across different training datasets.

Let's denote:

- **Y**: True value being predicted.
- **f(X)**: The true relationship between features (X) and the target variable (Y).
- **ŷ**: The prediction made by a trained model.
- **E**: Expectation (average) operator.
- **D**: Data.
- **h(D)**: Model trained on dataset D.

1. **Bias**:
   $Bias(\hat{f}(x)) = E[\hat{f}(x)] - f(x)$
   This equation represents the difference between the expected prediction of our model $\hat{f}(x)$ and the true value $f(x)$.
2. **Variance**:
   $Variance(\hat{f}(x)) = E[(\hat{f}(x) - E[\hat{f}(x)])^2]$
   This equation calculates the variability of predictions that our model $\hat{f}(x)$ makes across different training datasets.

Now, let's put it into a combined equation, known as the Bias-Variance Decomposition:

$$Error(\hat{f}(x)) = Bias(\hat{f}(x))^2 + Variance(\hat{f}(x)) + Irreducible\ Error$$

Here, the error of our model ($Error(\hat{f}(x))$) can be decomposed into the sum of squared bias, variance, and an irreducible error term that represents noise in the data that cannot be captured by the model.

In [1]:

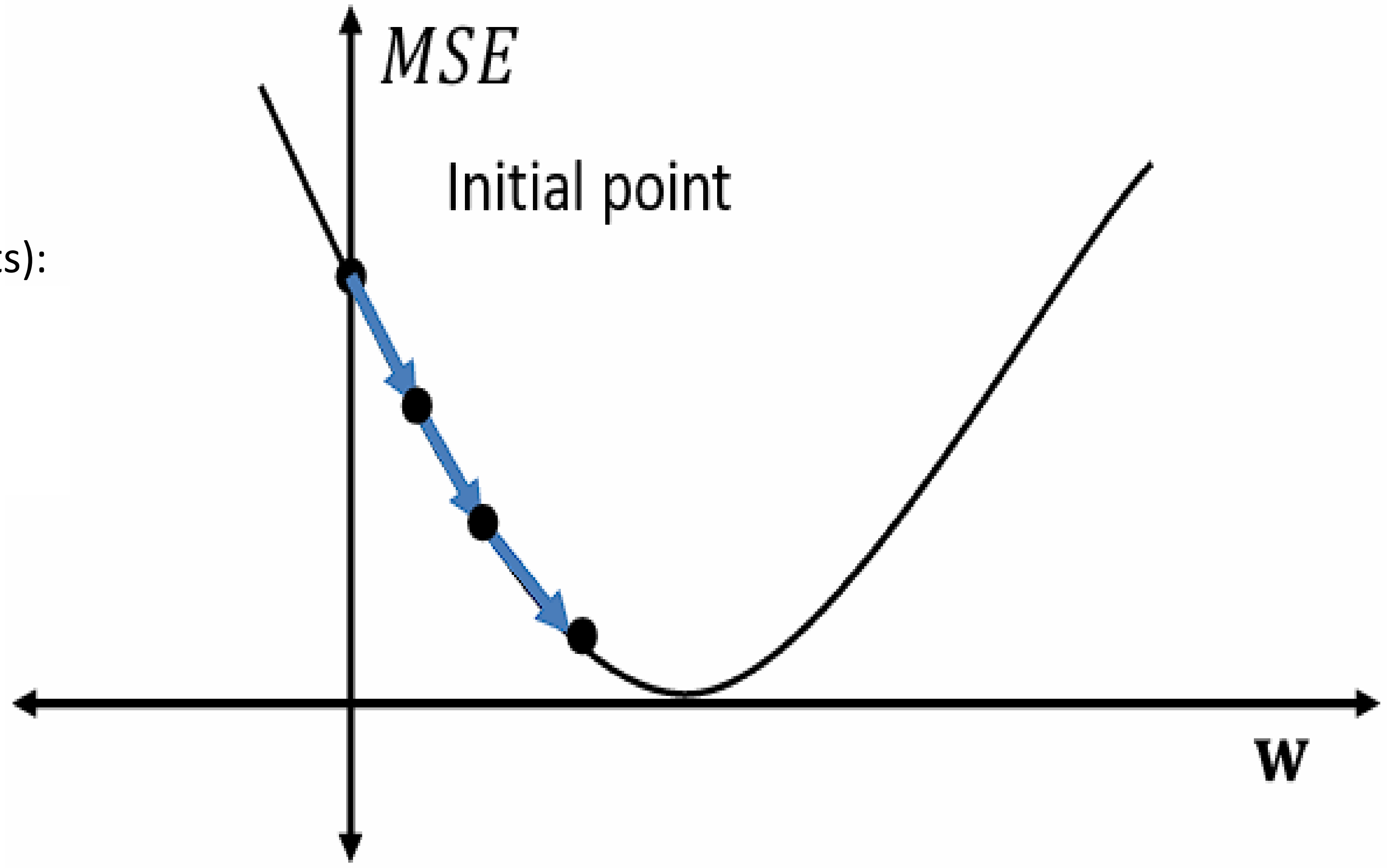
```
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from mlxtend.evaluate import bias_variance_decomp

np.random.seed(0)
X = np.random.rand(100, 1) * 10
y = 2 * X.squeeze() + np.random.randn(100)  # True relationship is y = 2X + noise

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
model = LinearRegression()
model.fit(X_train, y_train)

# Calculate bias and variance using the bias_variance_decomp function
mse, bias, variance = bias_variance_decomp(model, X_train, y_train, X_test, y_test, loss='mse')

print("MSE (Mean Squared Error):", mse)
print("Bias^2:", bias)
print("Variance:", variance)
```

```
MSE (Mean Squared Error): 0.9388721228182039
Bias^2: 0.9178184739745323
Variance: 0.021053648843671263
```

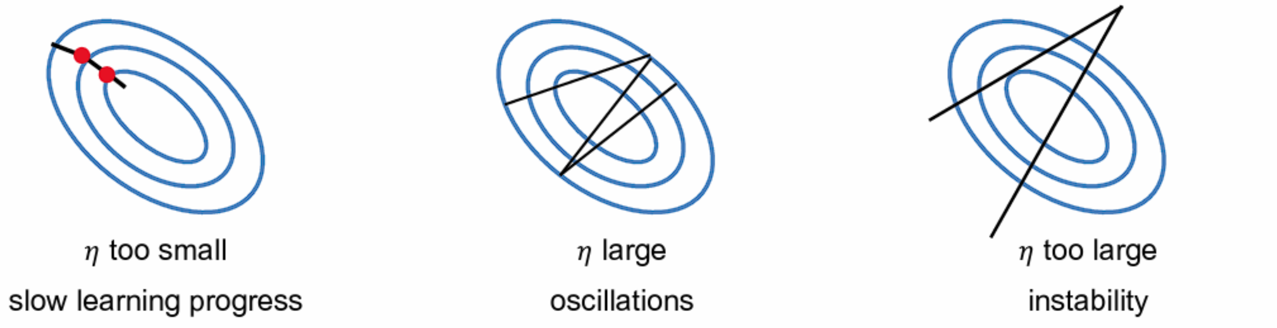
Code Link

Update Parameter (weights):

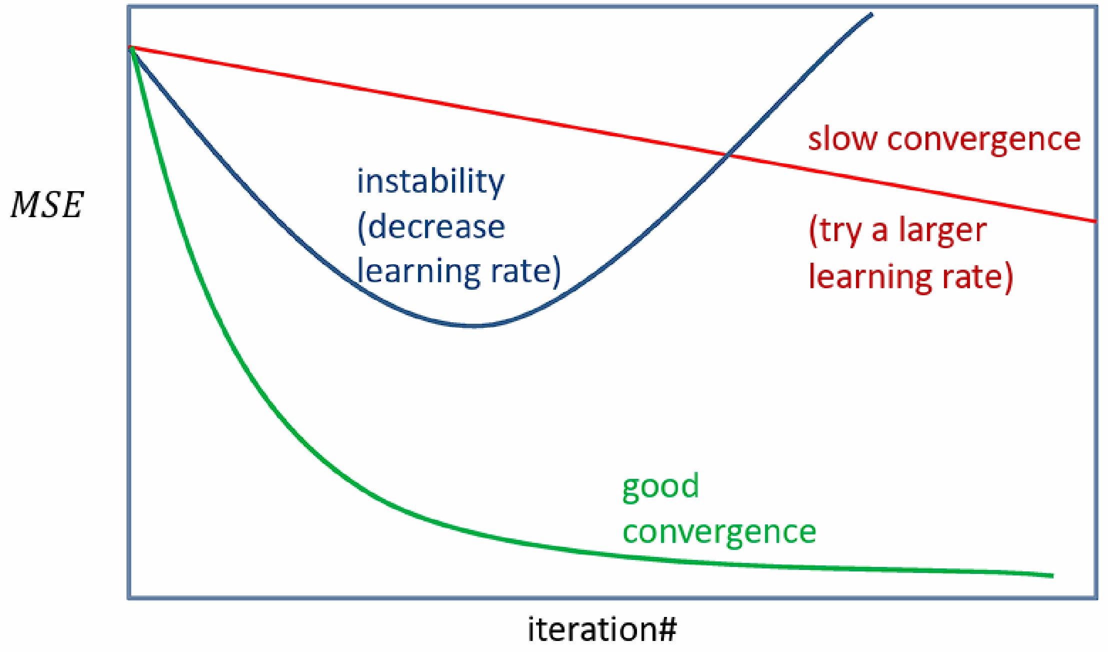
$$\theta_i = \theta_i - \alpha \frac{\partial J(\theta)}{\partial \theta_i}$$



The speed of the local/global minimum is affected from the learning rate.



The training curve could be used to monitor the effect of the learning rate value and observe the convergence. We plot the training loss against the number of training iterations.



The update rule for each parameter θ_i (where i indexes the parameters) in gradient descent can be represented as:

$$\theta_i = \theta_i - \alpha \frac{\partial J(\theta)}{\partial \theta_i}$$

Where:

- α is the learning rate, a hyperparameter that controls the size of the steps taken during optimization.
- $J(\theta)$ is the cost function.
- $\frac{\partial J(\theta)}{\partial \theta_i}$ is the partial derivative of the cost function with respect to θ_i, which gives the gradient of the cost function with respect to that parameter.

Gradient descent continues to update the parameters until convergence, where the algorithm finds parameter values that minimize the cost function.

The Mean Squared Error (MSE) is calculated as the squared difference between the actual values ($y^{(i)}$) and the predicted values ($h_\theta(x^{(i)})$):

$$\text{MSE} = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

1. **Mean Squared Error (MSE)**:
   - MSE quantifies the average of the squared differences between predicted values and actual values across the dataset.
   - The formula is expressed as: $\text{MSE} = \frac{1}{n}\sum_{i=0}^{n}(y_i - \hat{y}_i)^2$, where:
     - y_i represents the actual value from the dataset.
     - $\hat{y}_i$ denotes the predicted value by the model.
     - n signifies the total number of data points.

2. **Substitution of $\hat{y}_i$ with $mx_i + c$**:
    - In linear regression, predictions ($\hat{y}_i$) can be computed using the equation of a straight line, $y = mx + c$.
    - Here, m denotes the slope of the line, x_i is the input feature value, and c represents the y-intercept.
3. **Revised MSE Formula**:
    - After replacing $\hat{y}_i$ with the linear equation $mx_i + c$, the MSE is recalculated as:
        - $\text{MSE} = \frac{1}{n}\sum_{i=0}^{n}(y_i - (mx_i + c))^2$
    - This adjusted formulation is utilized to evaluate the performance of a linear regression model, aiming to minimize the MSE by identifying optimal values for m and c through model training.

Linear Regression using Gradient Descent

Algorithm

Step: 01

Gradient (m) = 0
Intercept (c) = 0
Learning Rate (L) = ~0.0001

Step: 02

Calculate the partial derivative of the Cost function with respect to m. Let the partial derivative of the Cost function with respect to m be Dm.

$$D_m = \frac{\partial(Cost\ Function)}{\partial m} = \frac{\partial}{\partial m}\left(\frac{1}{n}\sum_{i=0}^{n}(y_i - y_{i\,pred})^2\right)$$

$$= \frac{1}{n}\frac{\partial}{\partial m}\left(\sum_{i=0}^{n}(y_i - (mx_i + c))^2\right)$$

$$= \frac{1}{n}\frac{\partial}{\partial m}\left(\sum_{i=0}^{n}(y_i^2 + m^2x_i^2 + c^2 + 2mx_ic - 2y_imx_i - 2y_ic)\right)$$

$$= \frac{-2}{n}\sum_{i=0}^{n}x_i(y_i - (mx_i + c))$$

$$= \frac{-2}{n}\sum_{i=0}^{n}x_i(y_i - y_{i\,pred})$$

Step: 03

Similarly, let's find the partial derivative with respect to c. Let the partial derivative of the Cost function with respect to c be Dc.

$$D_c = \frac{\partial(Cost\ Function)}{\partial c} = \frac{\partial}{\partial c}\left(\frac{1}{n}\sum_{i=0}^{n}(y_i - y_{i\,pred})^2\right)$$

$$= \frac{1}{n}\frac{\partial}{\partial c}\left(\sum_{i=0}^{n}(y_i - (mx_i + c))^2\right)$$

$$= \frac{1}{n}\frac{\partial}{\partial c}\left(\sum_{i=0}^{n}(y_i^2 + m^2x_i^2 + c^2 + 2mx_ic - 2y_imx_i - 2y_ic)\right)$$

$$= \frac{-2}{n}\sum_{i=0}^{n}(y_i - (mx_i + c))$$

$$\frac{-2}{n}\sum_{i=0}^{n}(y_i - y_{i\,pred})$$

Derivative	Integral (Antiderivative)
$\frac{d}{dx}n = 0$	$\int 0\ dx = C$
$\frac{d}{dx}x = 1$	$\int 1\ dx = x + C$
$\frac{d}{dx}x^n = nx^{n-1}$	$\int x^n\ dx = \frac{x^{n+1}}{n+1} + C$
$\frac{d}{dx}e^x = e^x$	$\int e^x\ dx = e^x + C$
$\frac{d}{dx}\ln x = \frac{1}{x}$	$\int \frac{1}{x}\ dx = \ln x + C$
$\frac{d}{dx}n^x = n^x \ln x$	$\int n^x\ dx = \frac{n^x}{\ln n} + C$
$\frac{d}{dx}\sin x = \cos x$	$\int \cos x\ dx = \sin x + C$
$\frac{d}{dx}\cos x = -\sin x$	$\int \sin x\ dx = -\cos x + C$
$\frac{d}{dx}\tan x = \sec^2 x$	$\int \sec^2 x\ dx = \tan x + C$
$\frac{d}{dx}\cot x = -\csc^2 x$	$\int \csc^2 x\ dx = -\cot x + C$
$\frac{d}{dx}\sec x = \sec x \tan x$	$\int \tan x \sec x\ dx = \sec x + C$
$\frac{d}{dx}\csc x = -\csc x \cot x$	$\int \cot x \csc x\ dx = -\csc x + C$
$\frac{d}{dx}\arcsin x = \frac{1}{\sqrt{1-x^2}}$	$\int \frac{1}{\sqrt{1-x^2}}\ dx = \arcsin x + C$
$\frac{d}{dx}\arccos x = -\frac{1}{\sqrt{1-x^2}}$	$\int -\frac{1}{\sqrt{1-x^2}}\ dx = \arccos x + C$
$\frac{d}{dx}\arctan x = \frac{1}{1+x^2}$	$\int \frac{1}{1+x^2}\ dx = \arctan x + C$
$\frac{d}{dx}\operatorname{arc}\cot x = -\frac{1}{1+x^2}$	$\int -\frac{1}{1+x^2}\ dx = \operatorname{arc}\cot x + C$
$\frac{d}{dx}\operatorname{arc}\sec x = \frac{1}{x\sqrt{x^2-1}}$	$\int \frac{1}{x\sqrt{x^2-1}}\ dx = \operatorname{arc}\sec x + C$
$\frac{d}{dx}\operatorname{arc}\csc x = -\frac{1}{x\sqrt{x^2-1}}$	$\int -\frac{1}{x\sqrt{x^2-1}}\ dx = \operatorname{arc}\csc x + C$

Step: 04

Update the value of the gradient and intercept.

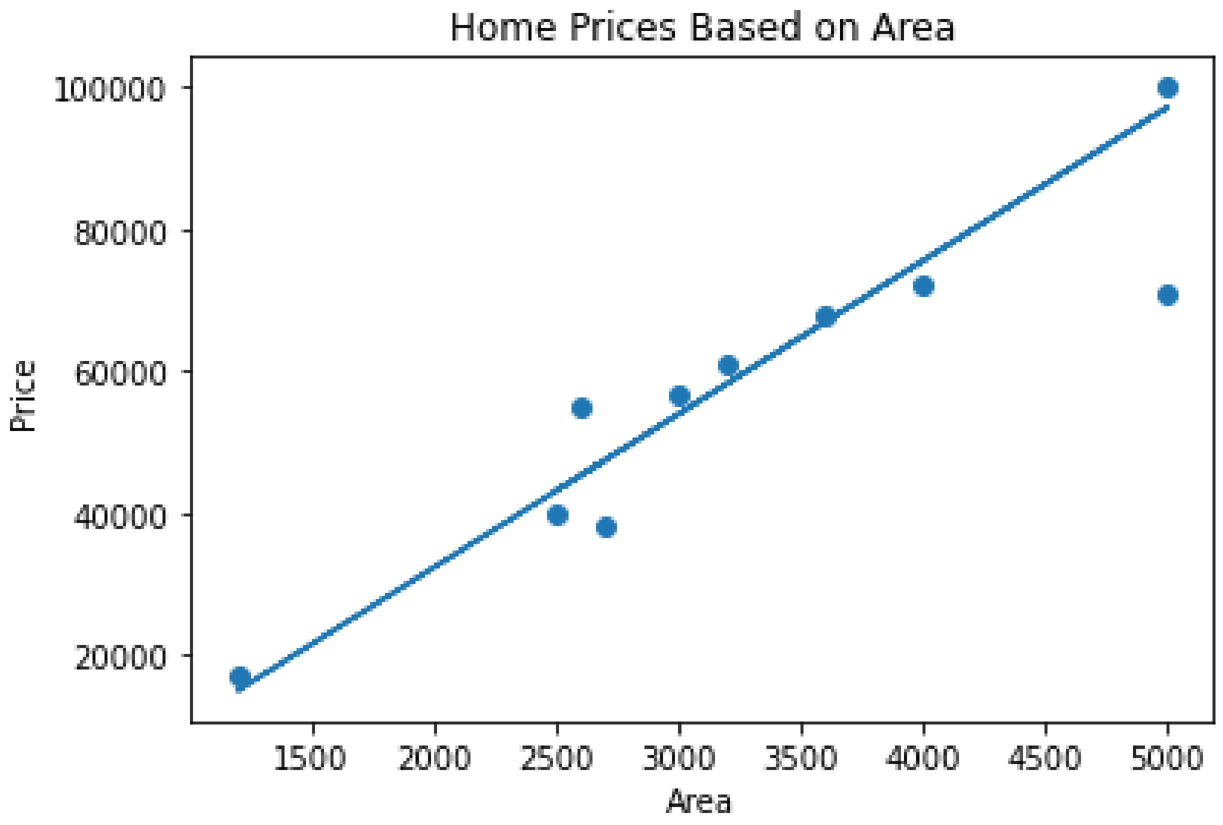
$$m = m - L \times D_m$$

$$c = c - L \times D_c$$

Repeat the steps!
1000 times

Overview:

- Single Variable Linear Regression
- Multiple Variable Linear Regression
- Single vs Multiple
- Cost Function
- Gradient Decent
- Accuracy
  - R2 Value
- Implementing with Python



y = mx + b ; or,
Y = 21.43* X + 4980.13

Coefficient = 21.43
Intercept = 4980.13

Linear Regression with Multiple Variables

Mathematical Representation

predictor, 'x-variable',
independent variable,
explanatory variable

coefficient

$$Y = \underbrace{\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ \dots \ + \beta_p x_p}_{\text{linear predictor}}$$

response, dependent variable,
observation, 'y-variable'

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}$$

where, for $i = n$ observations:

y_i = dependent variable

x_i = expanatory variables

β_0 = y-intercept (constant term)

β_p = slope coefficients for each explanatory variable

Mathematical Representation

Single

$$y = b_0 + b_1 {*} x_1$$

Dependent variable (DV)   Independent variables (IVs)

Multiple

$$y = b_0 + b_1 {*} x_1 + b_2 {*} x_2 + \dots + b_n {*} x_n$$

R Squared Value / Model Accuracy

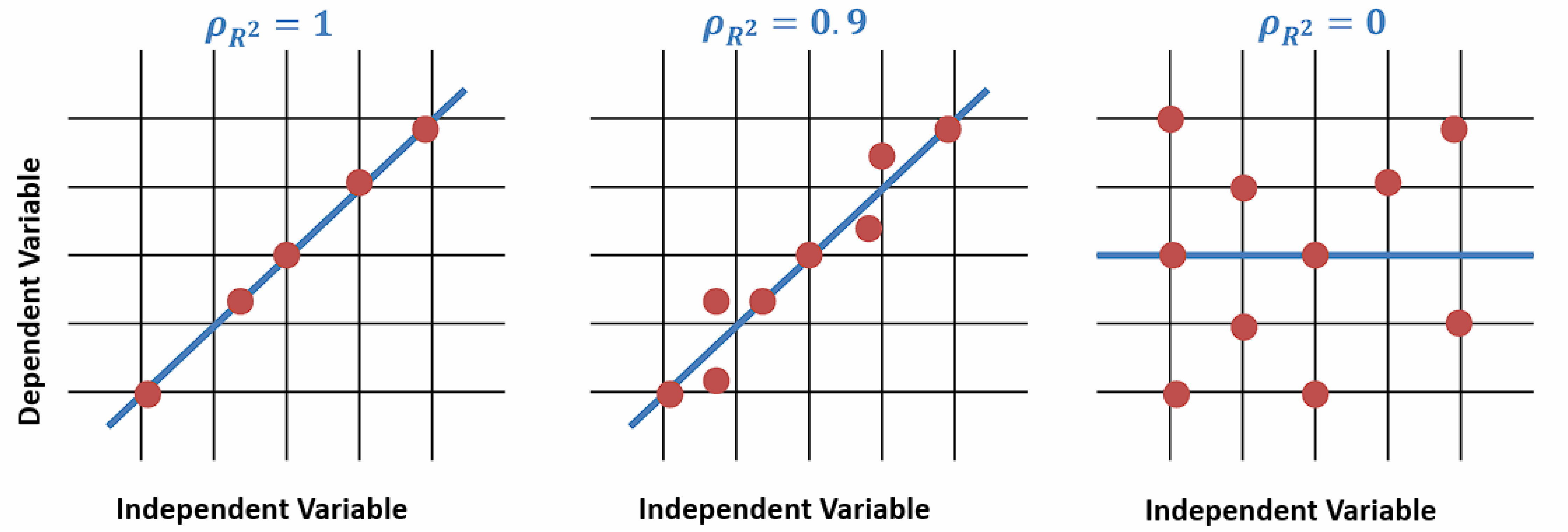
Mathematical Calculation

$$R^2 = 1 - \frac{SS_{RES}}{SS_{TOT}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \overline{y})^2}$$

- Residual sum of squared errors of our regression model (SSres)
- Total sum of squared errors (SStot)

R Squared Value / Model Accuracy

Mathematical Calculation



R Squared Value / Model Accuracy

Python Implementation

Way no: 01

```
reg.score(xtest, ytest)
```

Way no: 02

```
y_pred = reg.predict(xtest) #Predicted y
from sklearn.metrics import r2_score
Score = r2_score(ytest, y_pred)
```

1. **Misclassification Error (MCE)**:
   - Misclassification Error measures the proportion of incorrectly classified instances in a classification problem.
   - It is calculated as the total number of misclassified instances divided by the total number of instances.
   - Mathematically, MCE can be expressed as:

$$MCE = \frac{\text{Number of misclassified instances}}{\text{Total number of instances}}$$

2. **Accuracy (ACC)**:
   - Accuracy measures the proportion of correctly classified instances in a classification problem.
   - It is calculated as the total number of correctly classified instances divided by the total number of instances.
   - Mathematically, Accuracy can be expressed as:

$$ACC = \frac{\text{Number of correctly classified instances}}{\text{Total number of instances}}$$