Supervised Learning - Linear Regression

NYU K12 STEM Education: Machine Learning

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- Course Website
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Outline

1. Review
2. Python
3. Statistics
4. Supervised Learning
5. Linear Regression
6. Multivariable Linear Regression

Day 1 - Review

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  - Unsupervised Learning
- Artificial Intelligence vs. Machine Learning vs. Deep Learning
- Artificial Narrow Intelligence (ANI) vs. Artificial General Intelligence (AGI)

Outline

Why did we use Vectors and Matrices?

- Open Vectorize Programming Demo from Course Website

Plotting Functions

- Open Plotting Functions Demo from Course Website
- Generate and plot the following functions in Python:
  - Scatter plot of points: $(0,1),(2,3),(5,2),(4,1)$
  - Straight Line: $y = mx + b$
  - Sine-wave: $y = sin(x)$
  - Polynomial e.g. $y = x^3 + 2$
  - Exponential e.g. $y = e^{-2x}$
  - Choose a function of your own
- Use Wikipedia and NumPy documentation to search for mathematical formulas and python functions

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Mean

The mean, or average, is the sum of all the values in a dataset divided by the number of values. It provides a measure of the central tendency of the data.

$$\text{Mean}(\mu) = \frac{1}{N}\sum_{i=1}^{N} x_i$$

Example:

For the dataset $X = [2, 4, 6, 8, 10]$,

$$\mu = \frac{2+4+6+8+10}{5} = 6$$

Variance

Variance measures the spread of the data points around the mean. It indicates how much the data varies from the mean.

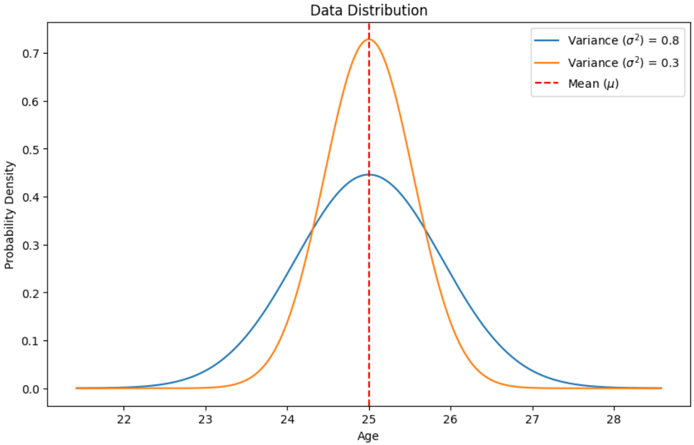
$$\text{Variance}(\sigma^2) = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$$

Example:

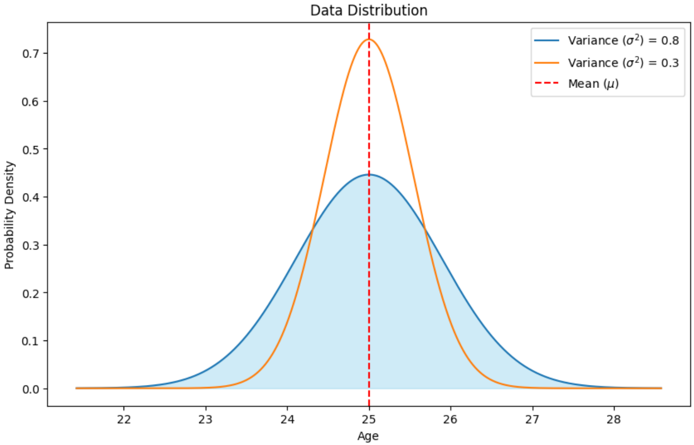
For the dataset $X = [2, 4, 6, 8, 10]$,

$$\sigma^2 = \frac{(2-6)^2 + (4-6)^2 + (6-6)^2 + (8-6)^2 + (10-6)^2}{5} = 8$$

Mean and Variance Visualization



Mean and Variance Visualization



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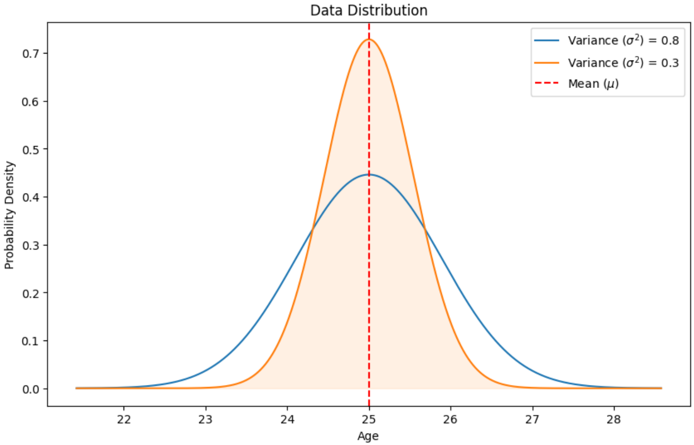


Standard Deviation

Standard deviation is the square root of the variance. It provides a measure of the spread of the data points in the same units as the data itself.

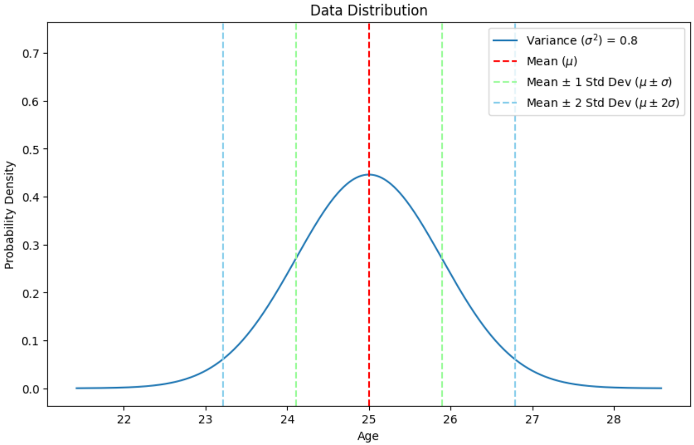
$$\text{Standard Deviation}(\sigma) = \sqrt{\text{Variance}}$$

Example:

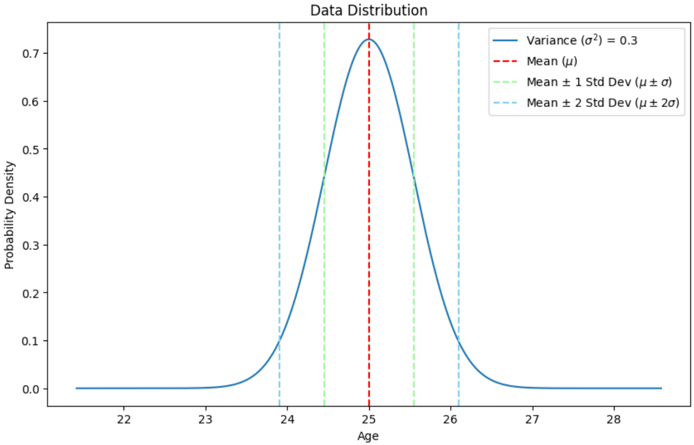
Using the variance calculated previously,

$$\sigma = \sqrt{8} \approx 2.83$$

Standard Deviation Visualization



Standard Deviation Visualization



Covariance

Covariance measures the degree to which two variables change together. If the covariance is positive, the variables tend to increase together; if negative, one variable tends to increase when the other decreases.

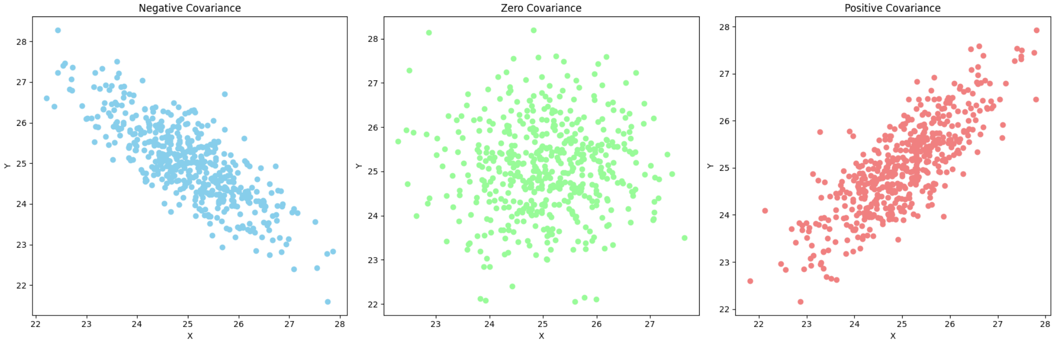
$$\text{Covariance}(\text{Cov}(X, Y)) = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_X)(y_i - \mu_Y)$$

Example:

For the datasets $X = [2, 4, 6]$ and $Y = [3, 6, 9]$,

$$\text{Cov}(X, Y) = \frac{(2-4)(3-6) + (4-4)(6-6) + (6-4)(9-6)}{3} = 6$$

Covariance Visualization



Looking at our ice-breaker data in spreadsheets

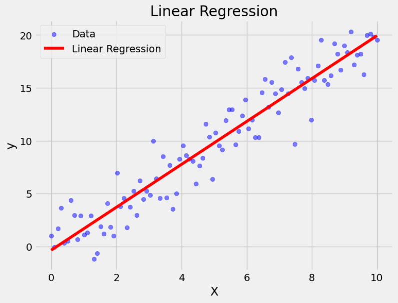
- Open Ice Breaker Dataset Demo from Course Website

Outline

Types of Supervised Learning Problems

Regression

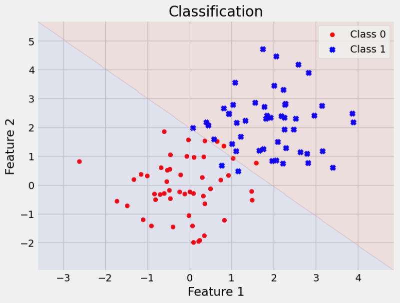
- Used when the output label is a continuous variable
- For example, linear regression, predicts a continuous target variable as a linear combination of input features.



Types of Supervised Learning Problems

Classification

- Used when the output label is categorical.
- For example, linear classification, splits the data into different categories



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Linear Regression in a nutshell

- Consider a function $y = 2x + 1$
- Here we introduce a new notation $y = f(x) = 2x + 1$
- What this means is that we have a function $f(x)$ which has x as its variable.
- If we have different x values we will have different values of $f(x)$

Linear Regression in a nutshell

- For $f(x) = 2x + 1$ and setting $x = 1$ we have $f(x) = 3$
- For $f(x) = 2x + 1$ and setting $x = 0$ we have $f(x) = 1$
- For $f(x) = 2x + 1$ and setting $x = -1.5$ we have $f(x) = -2$

Linear Regression in a nutshell

- We believe that datasets are a representation of underlying models.
- Models which can be represented as functions of features i.e. input to output mappings.
- For example, we can build a model to forecast weather, we can use the features humidity, current temperature and wind speed to estimate what the temperature will be tomorrow.
- Here we have $f(x)$ representing the tomorrow's temperature and x being a vector containing humidity, current temperature and wind speed.

Linear Regression in a nutshell

- Our task here is to figure out what $f(x)$ is, using the data available to us.
- Here $f(x)$ is called a model.
- In other words, we want to find a model that fits the data.

Linear Regression in a nutshell

- It would be easier to have a “framework” of the model ready and find the model parameters using the data.
  - $f(x) = w_1 x + w_0$
  - $f(x) = w_2 x^2 + w_1 x + w_0$
  - $f(x) = \frac{1}{e^{-(w_1 x + w_0)} + 1}$
- The numbers w_0, w_1 and w_2 are called model parameters.
- We often write the model as $f(x; w)$, stacking all parameters to a vector w.

Structure of a dataset

- In a dataset we have many data.
- We can represent each piece of data as (x_i, y_i), $i = 1, 2, 3, \ldots$
- x_i is called the feature and y_i is called the label.
- The relationship between x_i and y_i and the model f is $f(x_i) = y_i$

How would you fit a line?

Can you find a line that passes through $(0, 0)$ and $(1, 1)$?

- The "framework" of the model is $f(x) = w_1 x + w_0$
- The data is ($x = 0$, $f(x) = y = 0$) and ($x = 1$, $f(x) = y = 1$).
- The process of finding a model to fit the data is to find the values of w_1 and w_0.

What model do we use for this dataset?

- Open Linear Regression Demo from Course Website
- Can you find a line that goes through ALL of the data points? Why?

Is Your Model a Good Fit?

- How would you determine if your model is a good fit or not?
  - How will you determine this?
  - Is there a quantitative way?
- We now introduce a new notation $f(x_i) = \hat{y}_i$ here the $\hat{\cdot}$ represents $f(x_i)$ is a prediction of y_i.

Error Functions

- An **error function** quantifies the discrepancy between your model and the data.
  - They are non-negative, and go to zero as the model gets better.
- Common Error Functions:
  - Mean Squared Error:

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N} ||y_i - \hat{y}_i||^2$$

  - Mean Absolute Error:

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N} |y_i - \hat{y}_i|$$

- In later units, we will refer to these as **cost functions** or **loss functions**.

Linear Regression

- Linear models: For scalar-valued feature x, this is $f(x) = w_1 x + w_0$
- One of the simplest machine learning model, yet very powerful.

Least Square Solution

- Model:

$$f(x) = w_1 x + w_0$$

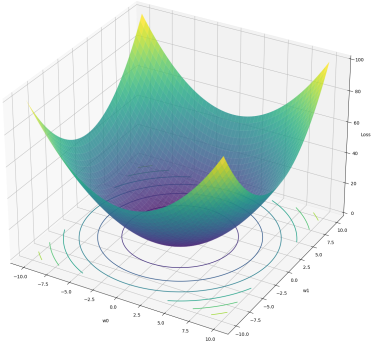
- Loss:

$$J(w_0, w_1) = \frac{1}{N} \sum_{i=1}^{N} ||y_i - f(x_i)||^2$$

- Optimization: Find w_0, w_1 such that $J(w_0, w_1)$ is the least possible value (hence the name “least square”).

Loss Landscape

$$J(w_0, w_1) = \frac{1}{N}\sum_{i=1}^{N} ||y_i - f(x_i)||^2$$



Least Square Solution: Using Pseudo-Inverse

For N data points (x_i, y_i) we have,

$$\hat{y_1} = w_0 + w_1 x_1$$
$$\hat{y_2} = w_0 + w_1 x_2$$
$$\vdots$$
$$\hat{y_N} = w_0 + w_1 x_N$$

Least Square Solution: Using Pseudo-Inverse

In matrix form we have,

$$\begin{bmatrix} \hat{y_1} \\ \hat{y_2} \\ \vdots \\ \hat{y_N} \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

We can write it as $\hat{Y} = X \times W$. We call X the design matrix.

Least Square Solution: Using Pseudo-Inverse

- We can put the desired labels in matrix form as well:

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

- Our goal is to minimize the error between Y and $\hat{Y}$ which can be written as $||Y - \hat{Y}||^2$
- **Exercise:** Verify

$$||Y - \hat{Y}||^2 = ||Y - XW||^2 = \sum_{i=1}^{N} ||y_i - (w_0 + w_1 x_i)||^2$$

Linear Least Square

$$\min_{W} \frac{1}{N} ||Y - XW||^2$$

The solution looks like this,

$$W = (X^T X)^{-1} X^T Y$$

Outline

Multivariable Linear Regression

What if we have multivariable data with x being a vector?

Example:

$$x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \end{bmatrix}$$

$$\begin{aligned} \hat{y_1} &= w_0 + w_1 x_{11} + w_2 x_{12} \\ \hat{y_2} &= w_0 + w_1 x_{21} + w_2 x_{22} \\ &\vdots \\ \hat{y_N} &= w_0 + w_1 x_{N1} + w_2 x_{N2} \end{aligned}$$

Multivariable Linear Regression

The model can be written in matrix-vector form as:

$$\begin{bmatrix} \hat{y_1} \\ \hat{y_2} \\ \vdots \\ \hat{y_N} \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ \vdots & \vdots & \vdots \\ 1 & x_{N1} & x_{N2} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$$

Solution remains the same $W = (X^T X)^{-1} X^T Y$

- **Exercise:** Open Multivariable Linear Regression Demo from Course Website