

Day 2: Linear Regression

Summer STEM: Machine Learning

Department of Electrical and Computer Engineering
NYU Tandon School of Engineering
Brooklyn, New York

Outline

- 1** Python libraries
- 2** Statistics Basics
- 3** Introduction to Machine Learning
- 4** Linear Regression

Continuing on Vectorize Programming

Demo on vectorize programming.

Demo: Plotting Functions

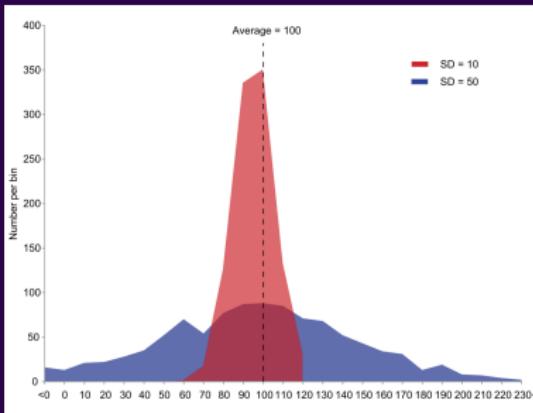
- Generate and plot the following functions in Python:
 - Scatter plot of points: (0,1), (2,3), (5,2), (4,1)
 - Straight Line: $y = mx + b$
 - Sine-wave $y = \sin(x)$
 - Polynomial e.g. $y = x^3 + 2$
 - Exponential e.g. $y = e^{-2x}$
 - Choose a function of your own
- Use Wikipedia and Numpy Documentation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

Outline

- 1** Python libraries
- 2** Statistics Basics
- 3** Introduction to Machine Learning
- 4** Linear Regression

Basic Concepts

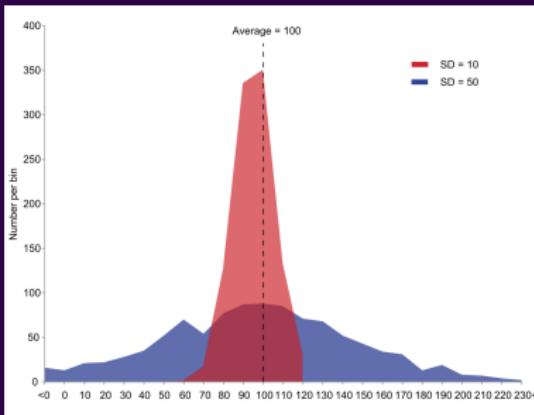
- Let $x = [x_1 \quad x_2 \quad \dots \quad x_N]$
- **Mean** (average value): $\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$



<https://en.wikipedia.org/wiki/Variance>

Variance

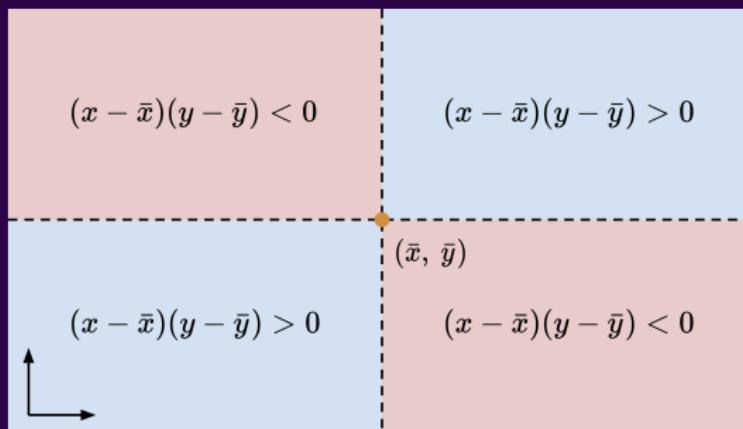
- Variance: $\sigma_x^2 = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2$
- Describes the spread of the data with respect to the mean.



<https://en.wikipedia.org/wiki/Variance>

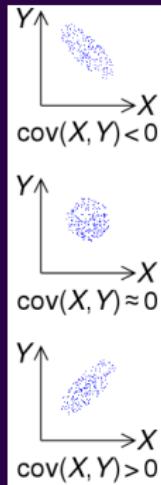
Covariance

- Let $x = [x_1 \ x_2 \ \dots \ x_N]$ and $y = [y_1 \ y_2 \ \dots \ y_N]$
- Covariance: $\sigma_{xy} = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})$
- Describes the relationship between two variables.



Covariance

■ Covariance: $\sigma_{xy} = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})$



<https://en.wikipedia.org/wiki/Covariance>

Looking at our ice-breaker data in spreadsheets

- Columns have labels in the first row
- Collected data (numbers, words) follow below
- Let's export it to a Comma-Separated Values (CSV) file and open it

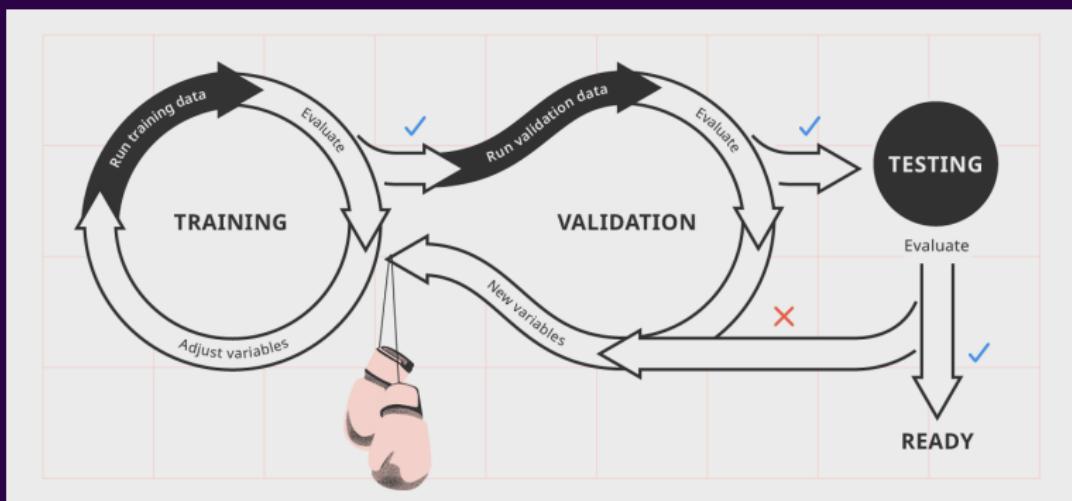
Outline

- 1** Python libraries
- 2** Statistics Basics
- 3** Introduction to Machine Learning
- 4** Linear Regression

What is Machine Learning

- Recognize patterns from data
- Make predictions based on the learnt patterns
- A very effective tool where human expertise is not available

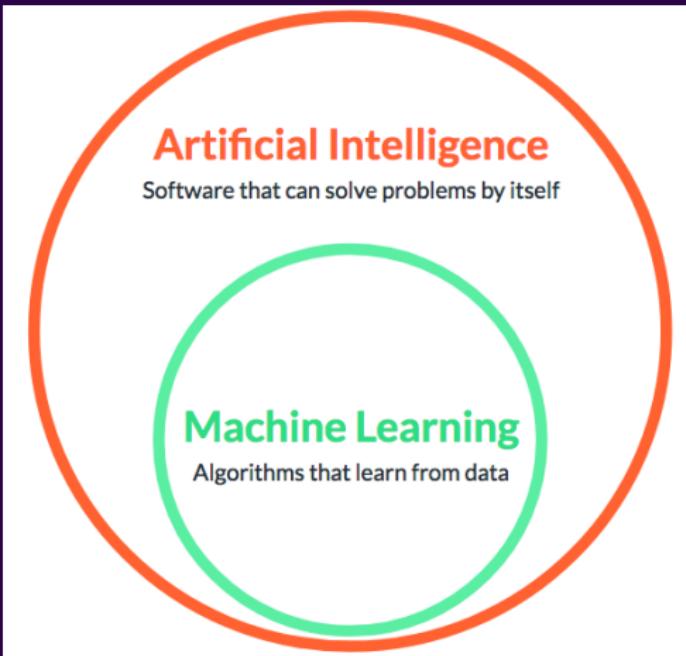
Machine Learning Pipeline



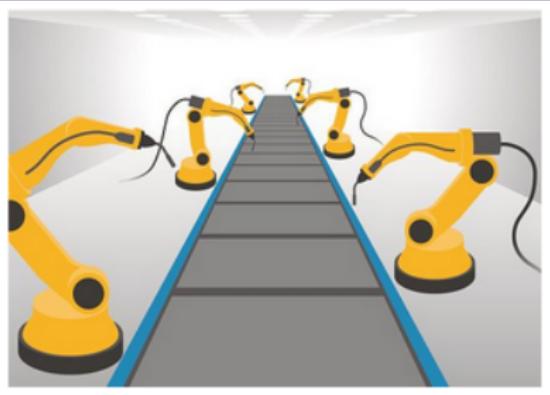
Artificial Intelligence

- Search
- Reasoning and Problem Solving
- Knowledge Representation
- Planning
- Learning
- Perception
- Natural Language Processing
- Motion and Manipulation
- Social and General Intelligence

Machine Learning



Autonomous vs. Automated



Autonomous Example: Self-driving car



■ Waymo Video

<https://www.tesmanian.com/blogs/tesmanian-blog/tesla-autopilot-full-self-driving-fsd-improvements-video>

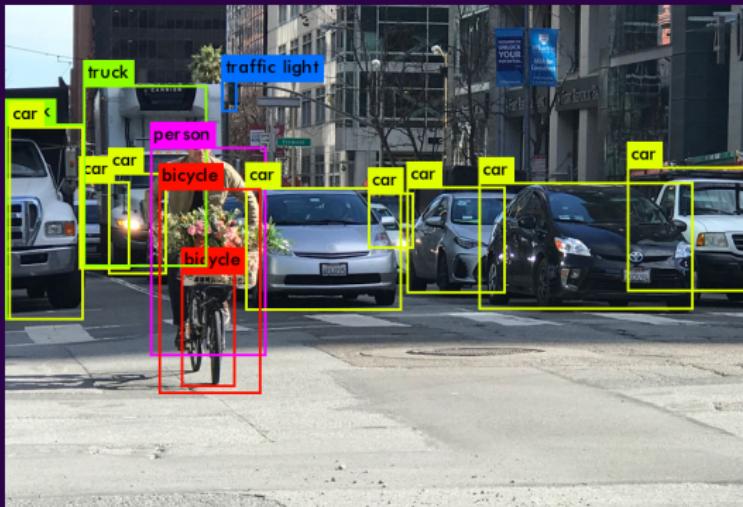
Why is Machine Learning so Prevalent?

- Database mining
- Medical records
- Computational biology
- Engineering
- Recommendation systems
- Understanding the human brain

Why Now?

- Big Data
 - Massive storage. Large data centers
 - Massive connectivity
 - Sources of data from internet and elsewhere
- Computational advances
 - Distributed machines, clusters
 - GPUs and hardware

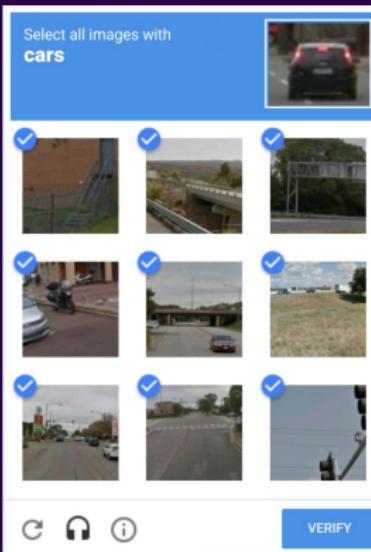
Labelled Data



■ YOLO v2

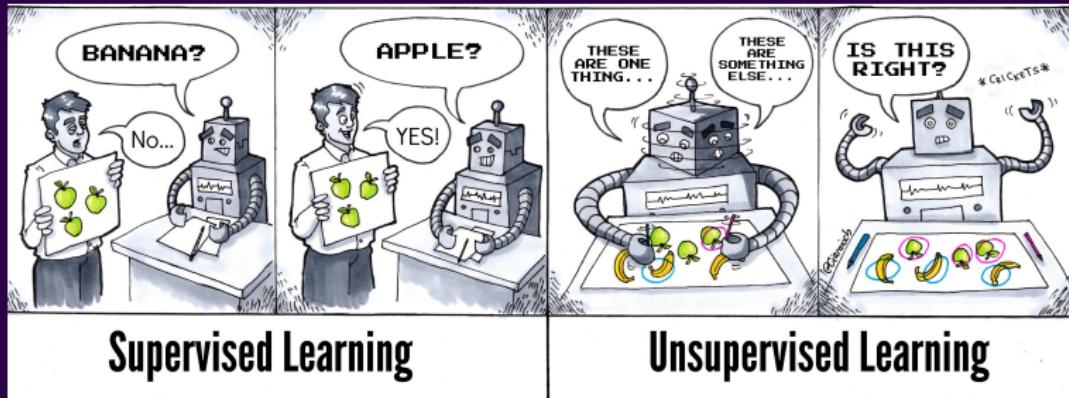
<https://towardsdatascience.com/yolo-you-only-look-once-17f9280a41b0> | NYU TANDON SCHOOL OF ENGINEERING

How labels are generated



<https://devrant.com/rants/1758134/select-all-images-with-cars-i-did-and-its-not-correct-why-not>

Supervised Vs. Unsupervised Learning

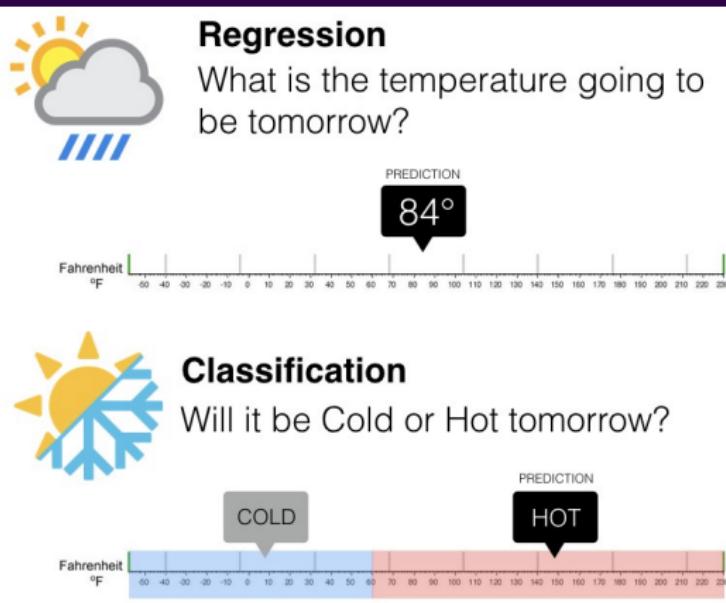


twitter.com/athena_schools/status/1063013435779223553/photo/1 NYU TANDON SCHOOL OF ENGINEERING

Supervised Vs. Unsupervised Learning

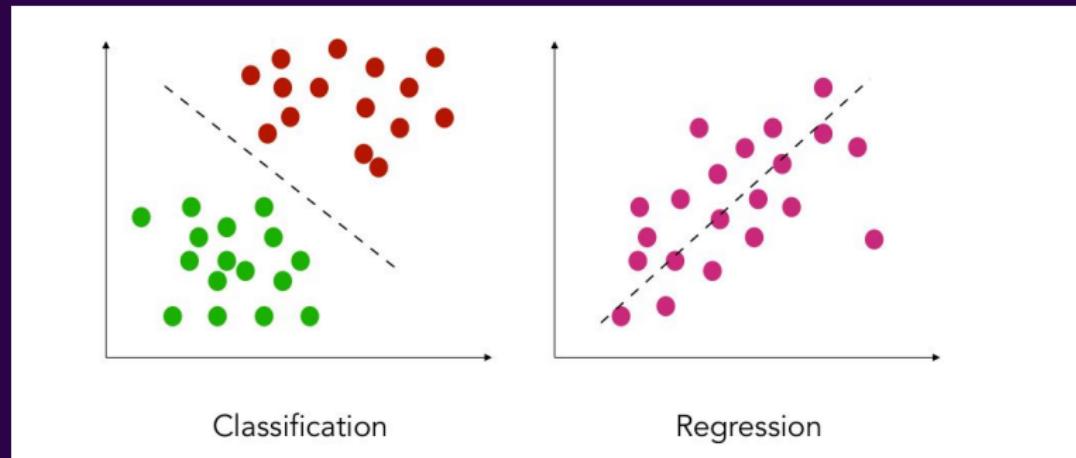
- The main difference between supervised and unsupervised learning is the existence of a supervisor, which in many cases is in the form of a data label.
- The label of the data is what we want the machine learning algorithm to predict.

Classification Vs. Regression

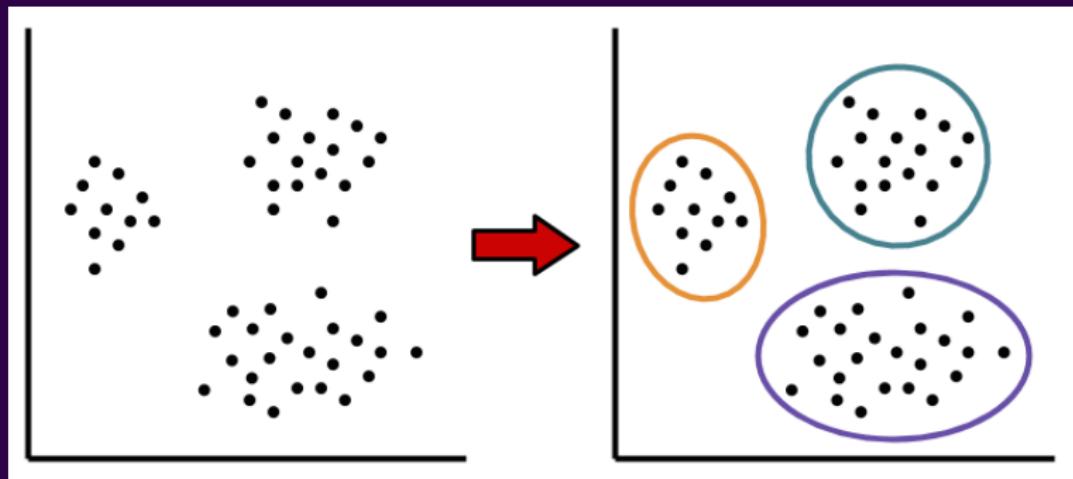


<https://www.pinterest.com/pin/672232681855858622/?lp=true>

Classification Vs. Regression



Unsupervised Learning



source: the dish on science

Outline

- 1** Python libraries
- 2** Statistics Basics
- 3** Introduction to Machine Learning
- 4** Linear Regression

Supervised learning in a nutshell

- Consider a function $y = 2x + 1$.
- Here we introduce a new notation $f(x) = 2x + 1$.
- 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 $f(x)$.

Supervised learning 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 $f(x) = -2$

Supervised learning in a nutshell

- We believe that datasets are representations of underlying models which can be represented as functions of features.
- 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.

Supervised learning in a nutshell

- But many times we do have $f(x)$ available, 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.

Supervised learning in a nutshell

- It would be easier to have a "framework" of the model ready and find the model parameters using the data.
- $f(x) = w_1x + w_0$.
- $f(x) = w_2x^2 + w_1x + w_0$.
- $f(x) = \frac{1}{e^{-(w_1x+w_0)} + 1}$.
- The numbers w_0 , w_1 and w_2 are called model parameters.
- We often write the model as $f(x; \mathbf{w})$, stacking all parameters to a vector \mathbf{w} .

Structure of a dataset

- In a dataset we have many data.
- We can represent each piece of data as (x_i, y_i) , $i = 1, 2, 3, \dots$
- 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 $f(x_i) = y_i$.
- For example, if the weather forecast says it will be $21^\circ C(69.8^\circ F)$ if it turns out to be $22^\circ C(71.6^\circ F)$ you won't be yelling at the TV.

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 $f(x) = w_1x + w_0$.
- 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 .

How would you fit a quadratic curve?

Can you find a quadratic curve that passes through $(0, 0)$, $(1, 1)$ and $(-1, 1)$?

- The "framework" of the model is $f(x) = w_2x^2 + w_1x + w_0$.
- The data is $(x = 0, f(x) = y = 0)$, $(x = 1, f(x) = y = 1)$ and $(x = -1, f(x) = y = 1)$.
- The process of finding a model to fit the data is to find the values of w_2 , w_1 and w_0 .

What model do we use for this dataset?

- Open `demo_boston_housing_one_variable.ipynb`
- Can you find a line that go 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: $MSE = \frac{1}{N} \sum_{i=1}^N \|y_i - \hat{y}_i\|^2$
 - Mean Absolute Error: $MAE = \frac{1}{N} \sum_{i=1}^N |y_i - \hat{y}_i|$
- In later units, we will refer to these as **cost functions** or **loss functions**.
- **Exercise :** Compute the MSE and the MAE on your model

Linear Regression

- Linear models: For scalar-valued feature x , this is
$$f(x) = w_1x + w_0$$
- One of the simplest machine learning model, yet very powerful.

Least Square Solution

- Model:

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

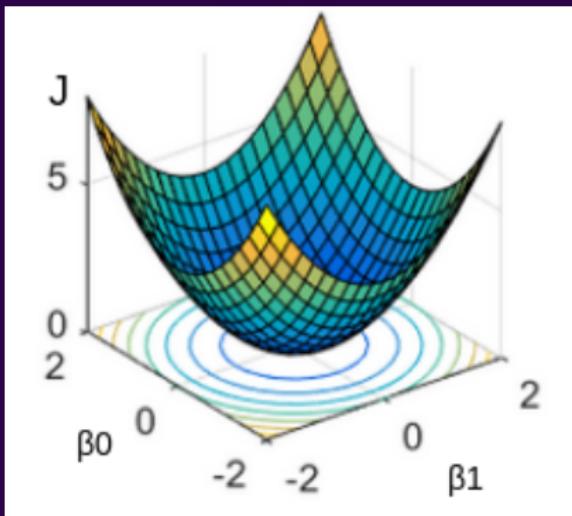
- Loss:

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

- 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 Statistics

■ Solution:

$$f(x) = \bar{y} + \frac{\sigma_{xy}}{\sigma_x^2}(x - \bar{x})$$

$$w_1 = \frac{\sigma_{xy}}{\sigma_x^2}, \quad w_0 = \bar{y} - w_1 \bar{x}$$

■ Prediction:

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

Least Square Solution: Using Pseudo-Inverse

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

$$\hat{y}_1 = w_0 + w_1 x_1$$

$$\hat{y}_2 = w_0 + w_1 x_2$$

$$\vdots$$

$$\hat{y}_N = w_0 + w_1 x_N.$$

Linear Regression

- 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 $\hat{Y} = X\mathbf{w}$. We call X the design matrix.

- 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

$$\|Y - \hat{Y}\|^2 = \|Y - Xw\|^2 = \sum_{i=1}^N \|y_i - (w_0 + w_1x_i)\|^2$$

Linear Least Square

- $\min_{\mathbf{w}} \frac{1}{N} \|Y - X\mathbf{w}\|^2$
- The solution looks like this,

$$\mathbf{w} = (X^T X)^{-1} X^T Y.$$

Linear Regression

- What if we have multivariate data with \mathbf{x} being a vector?
- Ex: $\mathbf{x}_i = [x_{i1}, x_{i2}]^T$

$$\hat{y}_1 = w_0 + w_1 x_{11} + w_2 x_{12}$$

$$\hat{y}_2 = w_0 + w_1 x_{21} + w_2 x_{22}$$

$$\vdots$$

$$\hat{y}_N = w_0 + w_1 x_{N1} + w_2 x_{N2}$$

- The model can be written as $\hat{y}_i = [1 \quad x_{i1} \quad x_{i2}] \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$

Multilinear Regression

- In matrix-vector form

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_{n2} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$$

- Solution remains the same $\mathbf{w} = (X^T X)^{-1} X^T Y$
- Exercise: open `demo_multilinear.ipynb`