Day 2: Linear Regression

Summer STEM: Machine Learning

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NYU Tandon School of Engineering
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Outline

Continuing on Vectorize Programming

Demo on vectorize programming.

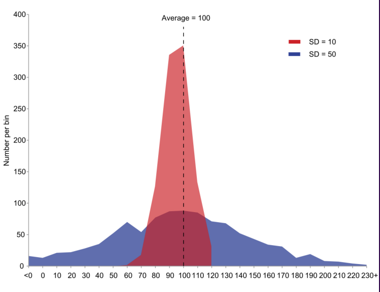
Demo: Plotting Functions

- 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

Basic Concepts

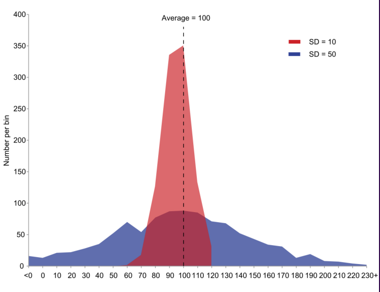
- Let $x = \begin{bmatrix} x_1 & x_2 & \dots & x_N \end{bmatrix}$
- **Mean** (average value): $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$



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

Variance

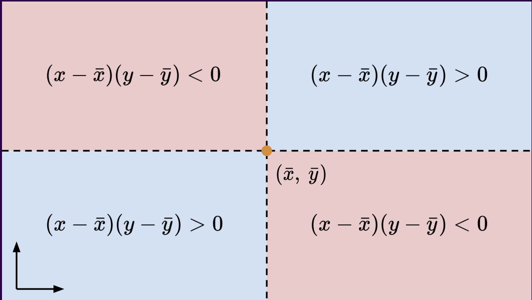
- Variance: $\sigma_x^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2$
- Describes the spread of the data with respect to the mean.



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

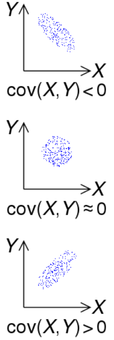
Covariance

- Let $x = \begin{bmatrix} x_1 & x_2 & \dots & x_N \end{bmatrix}$ and $y = \begin{bmatrix} y_1 & y_2 & \dots & y_N \end{bmatrix}$
- Covariance: $\sigma_{xy} = \dfrac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})$
- 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

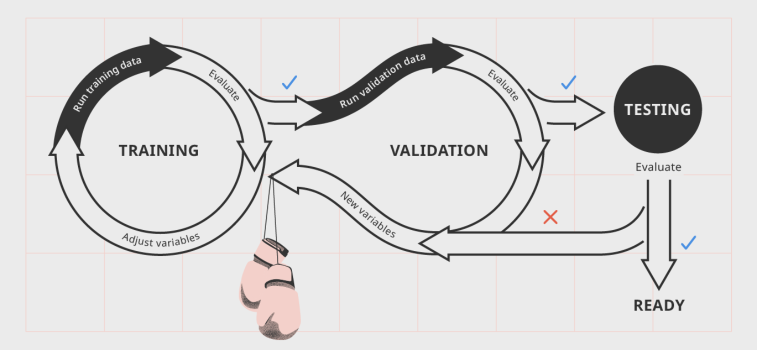
- Columns have labels in the first row
- Collected data (numbers, words) follow below
- Let's export it to a Comma-Separated Values (CSV) file and open it

Outline

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

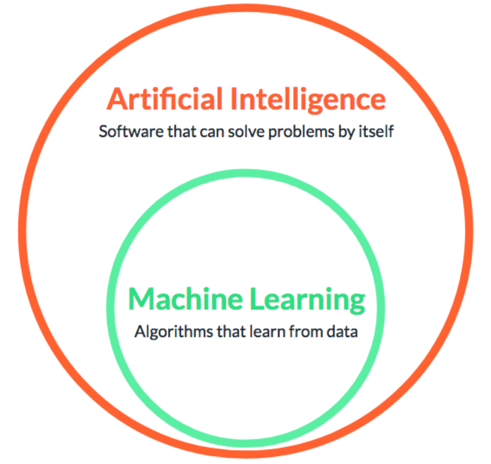


https://lionbridge.ai/articles/how-does-ai-training-work/

Artificial Intelligence

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

Machine Learning



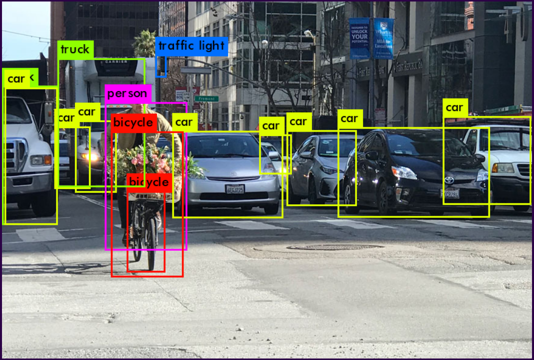
Why is Machine Learning so Prevalent?

- 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

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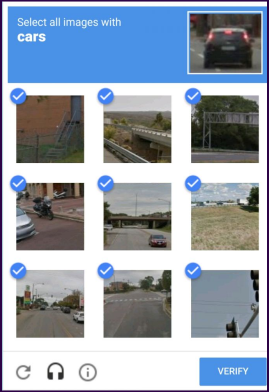
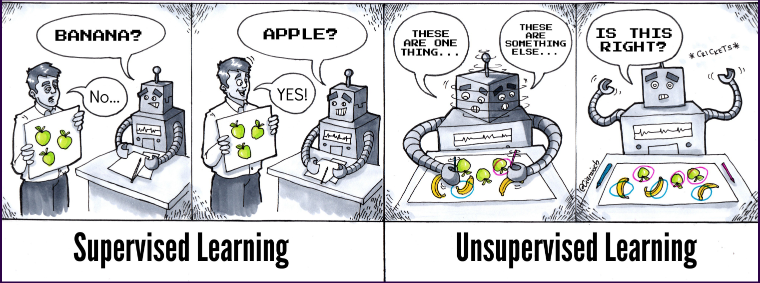
https://towardsdatascience.com/yolo-you-only-look-once-17f9280a4

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

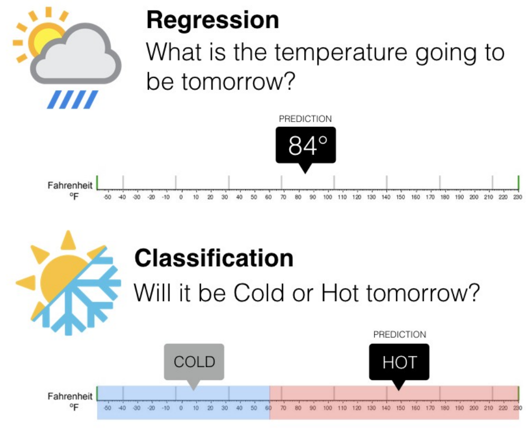


twitter.com/athena_schools/status/1063013435779223553/photo/1

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



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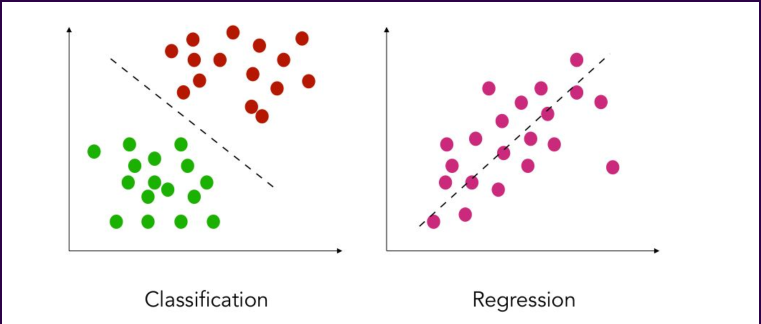
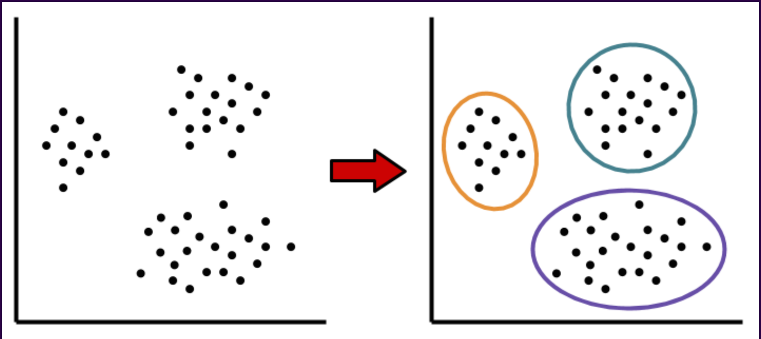
Classification Vs. Regression



https://maelfabien.github.io/machinelearning/ml_base/

Unsupervised Learning



source: the dish on science

Outline

Linear Regression 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 $f(x)$.

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 dataset are representation 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.

Linear Regression 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.

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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.
- $f(x) = w_1 x + w_0$.
- $f(x) = w_2 x^2 + w_1 x + w_0$.
- $f(x) = \dfrac{1}{e^{-(w_1 x + w_0)} + 1}$.
- The numbers w_0, w_1 and w_2 are called model parameters.
- We often write the model as $f(x; \mathbf{w})$, 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), $i = 1, 2, 3, \ldots$
- 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 $f(x_i) = y_i$.
- 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 $f(x) = w_1 x + w_0$.
- 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.

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

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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:

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

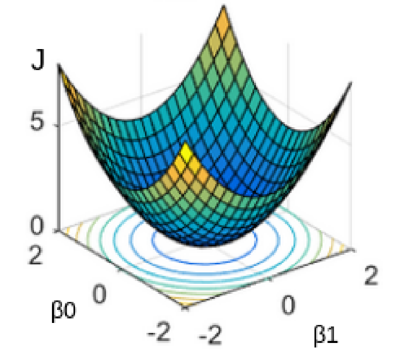
- Loss:

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

- 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 Pseudo-Inverse

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

$$\begin{aligned}\hat{y}_1 &= w_0 + w_1 x_1\\ \hat{y}_2 &= w_0 + w_1 x_2\\ &\vdots\\ \hat{y}_N &= w_0 + w_1 x_N.\end{aligned}$$

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.

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- 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 $\left\| Y - \hat{Y} \right\|^2$
- **Exercise:** Verify

$$\left\| Y - \hat{Y} \right\|^2 = \| Y - X\mathbf{w} \|^2 = \sum_{i=1}^{N} \| y_i - (w_0 + w_1 x_i) \|^2$$

Linear Least Square

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

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

Multilinear 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 $\hat{y}_i = \begin{bmatrix} 1 & x_{i1} & x_{i2} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$

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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`