Introduction to MACHINE LEARNING

BY DATAROCKIE

- What is Data Science? -
- What is Machine Learning?

15 mins

- 4 Steps in Machine Learning 30 mins
- Algorithms You Need to Know 60 mins

What is DATA SCIENCE?

Data + Science

What is Data?

Data is new electricity.

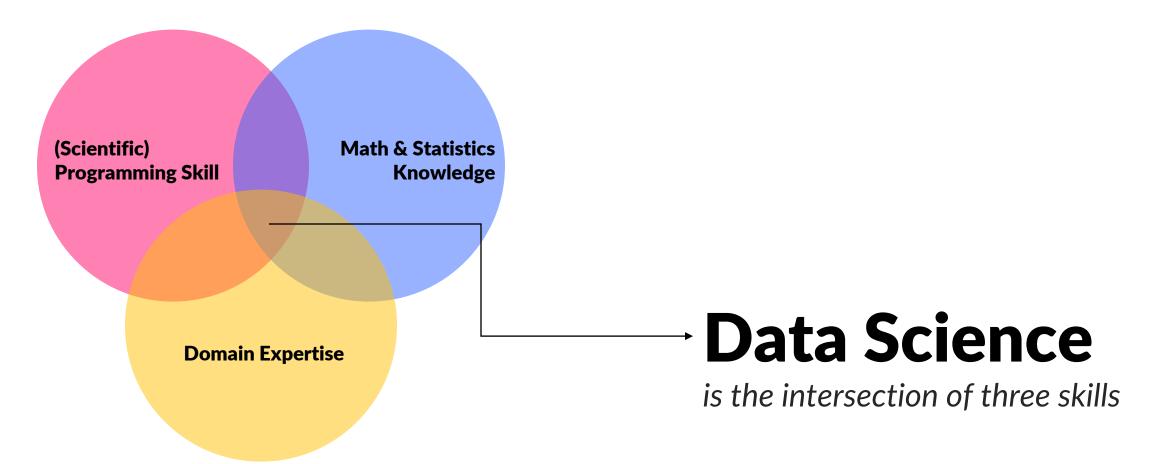
Science as we know it.

Andrew Ng

Scientists use data to test hypothesis, theory formation.



DS Venn Diagram



http://drewconway.com/zia/2013/3/26/the-data-science-venn-diagram

Essential Knowledge

Programming skill

- R
- Python
- SQL
- Spark
- Hadoop

(Scientific) **Math & Statistics Programming Skill** Knowledge **Domain Expertise**

Math & Statistics

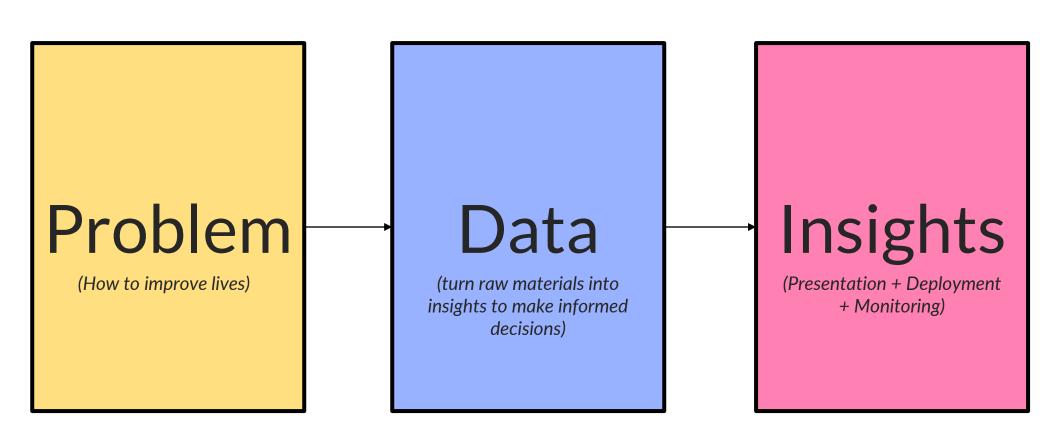
- Linear algebra
- Calculus
- Descriptive statistics
- Inferential statistics
- Bayesian statistics
- Probability

Domain Expertise

- Marketing | Business
- Medical | Health
- Politic
- Engineer
- Could be anything

Always

Good data science starts with good question



What is MACHINE LEARNING?

Can you guess?

x (input)	1	2	3	4	5	6	7	8	9	10
y (output)	1	4	9	16	25	36	49	64	81	

You guess the function is x^2



Right! Can you guess this one?

	X1	X2	Х3	X4	Υ
Occasion 1	Restaurant	Many	Friday	Good	Yes
Occasion 2	Pub Bar	Many	Saturday	OK	Yes
Occasion 3	Pub Bar	Few	Monday	ОК	No
Occasion 4	Restaurant	Few	Friday	Bad	Yes
Occasion 5	Restaurant	Many	Friday	Good	No
Occasion 6	Pub Bar	Few	Saturday	OK	Yes
Occasion 7	Pub Bar	Many	Monday	Good	No
Occasion 8	Restaurant	Few	Saturday	OK	No
Occasion 9	Pub Bar	Many	Friday	Bad	No
Occasion 10	Restaurant	Few	Friday	Good	

Yes or No?

Machine Learning is function approximation

Machine Learning is inductive reasoning

Learning from experience

ML algorithms trying to MAP inputs (x's) to output (y)

	X1	X2	Х3	X4	Y
Occasion 1	Restaurant	Many	Friday	Good	Yes
Occasion 2	Pub Bar	Many	Saturday	OK	Yes
Occasion 3	Pub Bar	Few	Monday	ОК	
Occasion 4	Restaurant	Few	Friday	Bad	
Occasion 5	Restaurant	Many	Friday	Good	1 Par
Occasion 6	Pub Bar	Few	Saturday	OK	
Occasion 7	Pub Bar	Many	Monday	Good	
Occasion 8	Restaurant	Few	Saturday	OK	
Occasion 9	Pub Bar	Many	Friday	Bad	300
Occasion 10 Restaurant		Few	Friday	Good	

It's good to have lots data but ...

REPRESENTATION

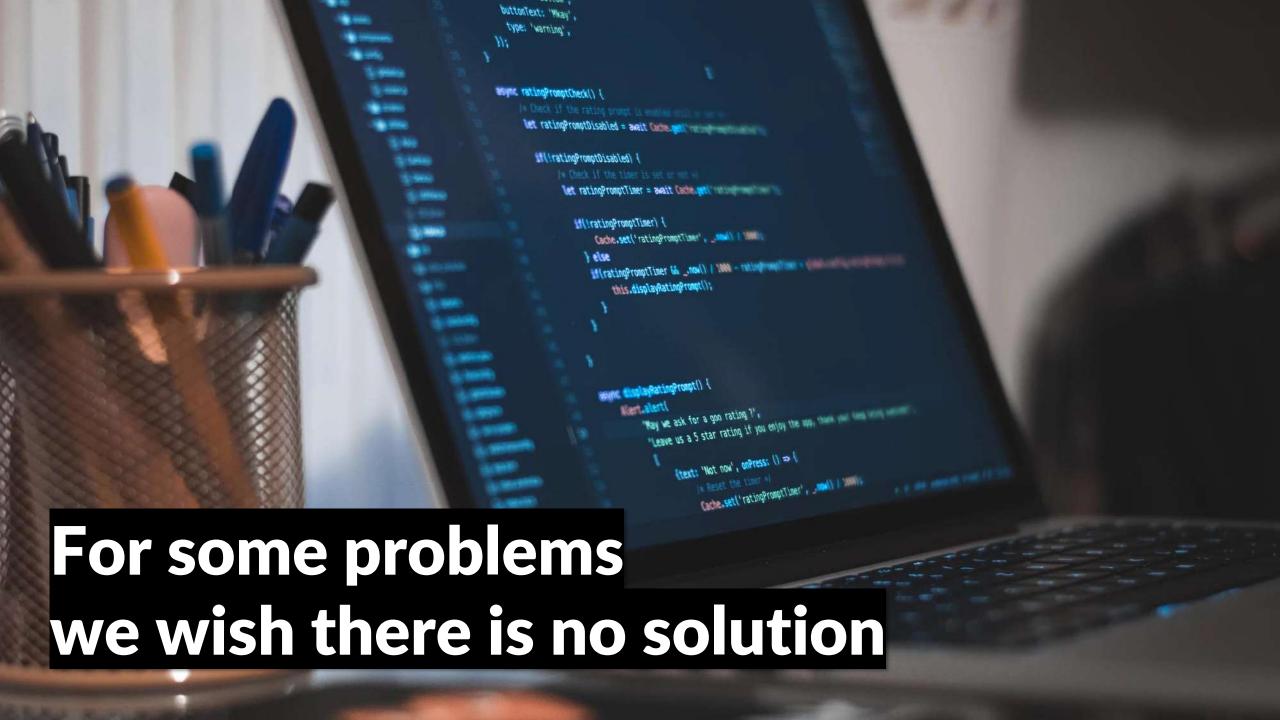
is the quality we desire

ML Example

- Predict breast cancer
- Weather forecast
- Watson analytics
- Google flu trend
- Obama winning the US election







A proper definition of ML

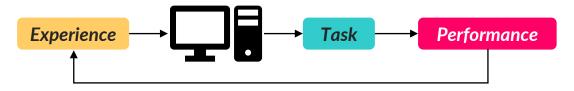
Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.

A more modern def in 1998

Well posed Learning Problem: A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.



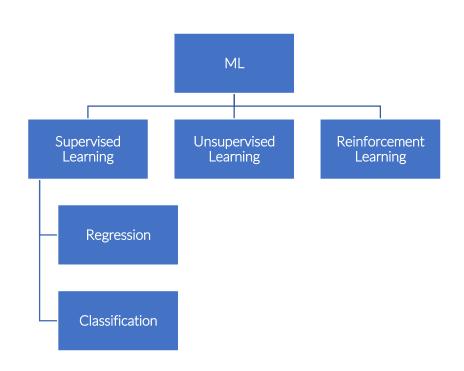
Tom Mitchell (1998)



Can we improve computer's ability to perform task T over time (without being explicitly programmed)?

Types of ML algorithms

- 1. Supervised Learning
 - i. Regression
 - ii. Classification
- 2. Unsupervised Learning
- 3. Reinforcement Learning



What's Artificial Intelligence



Function approximation Y = f(X) Model = Algorithm (Data)Predicting new unseen data

We build models to represent the world (problem we're trying to solve)



And the goal of Machine Learning is

GENERALIZATION

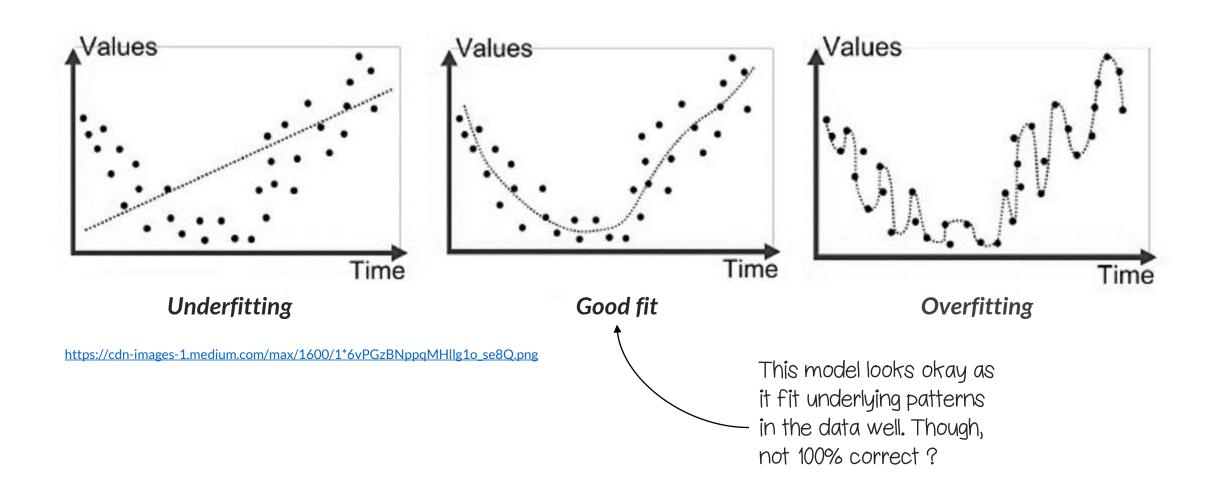
Beyond (past) data you used to build the model

Generalization means we make sure our models don't overfit the data

Also don't underfit

We mean data in the past

If your model can't generalize to new unseen data, then you're in trouble.

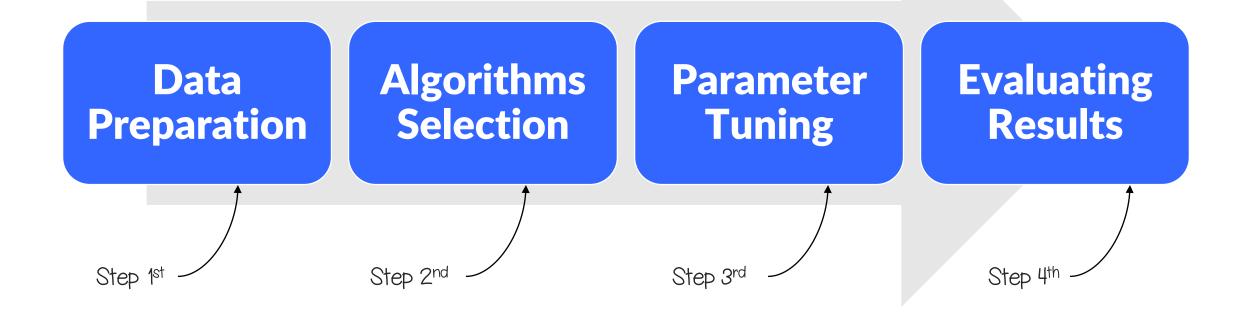


SUMMARY

- Data Science in Thailand is still very young
- ML is data scientist's arsenal tool
- ML is **Function Approximation**, learning from experience
- Representation & Generalization (avoid overfitting | underfitting)
- 3 types of ML algorithms including supervised, unsupervised and reinforcement learning
- Regression predicts numbers | Classification predicts categories



Four key steps in ML



DATA PREPARATION

Data Format

			Target Variable		
	X1	X2	Х3	X4	Υ
Occasion 1	Restaurant	Many	Friday	Good	Yes
Occasion 2	Pub Bar	Many	Saturday	ОК	Yes
Occasion 3	Pub Bar	Few	Monday	ОК	No
Occasion 4	Restaurant	Few	Friday	Bad	Yes
Occasion 5	Restaurant	Many	Friday	Good	No
Occasion 6	Pub Bar	Few	Saturday	OK	Yes
Occasion 7	Pub Bar	Many	Monday	Good	No
Occasion 8	Restaurant	Few	Saturday	ОК	No
Occasion 9	Pub Bar	Many	Friday	Bad	No
Occasion 10	Restaurant	Few	Friday	Good	No

Data Points | **Observations**

Variable Types

- 1. Binary (1/0)
- 2. Categorical
- 3. Integer
- 4. Continuous

Feature Selection

- Choose relevant set of features that represent the problem
- Curse of dimensionality: 2^n

Feature Engineering

- Recode
- Combine multiple variables (PCA)
- Extract new information from existing feature

Gentle intro to Feature Engineering

ID	Name	DOB	Math	Stats	Art	Music	Design
1	Mr. David Beckham	13/05/1975	85	90	50	42	49
2	Ms. Angelina Jolie	20/09/1988	50	60	90	95	88
3	Mr. Khalid Khan	05/01/1950	32	65	70	72	65
4	Mr. Hibino Takamoto	31/12/1995	75	76	80	50	30

Question:

What new variable can we create from this dataset? Think at least 5 new variables

We can use dplyr::mutate() to create new variables

Missing Data

- 1. Approximated
- 2. Predicted (Supervised Learning)
- 3. Removed

If we have large data points and NA is not much, we may consider removing them

Mean | Median

imputation

Approximated or Removed?

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R functions:

complete.cases(df) สำหรับตรวจสอบว่าข้อมูลมี NA หรือเปล่า? tidyr::drop_na(df) สำหรับ drop case ที่มีข้อมูลไม่ครบทิ้ง

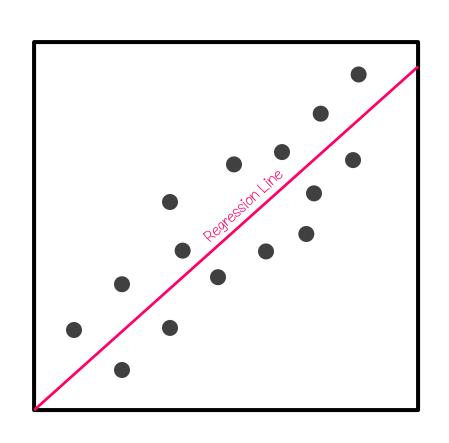
ALGORITHM SELECTION

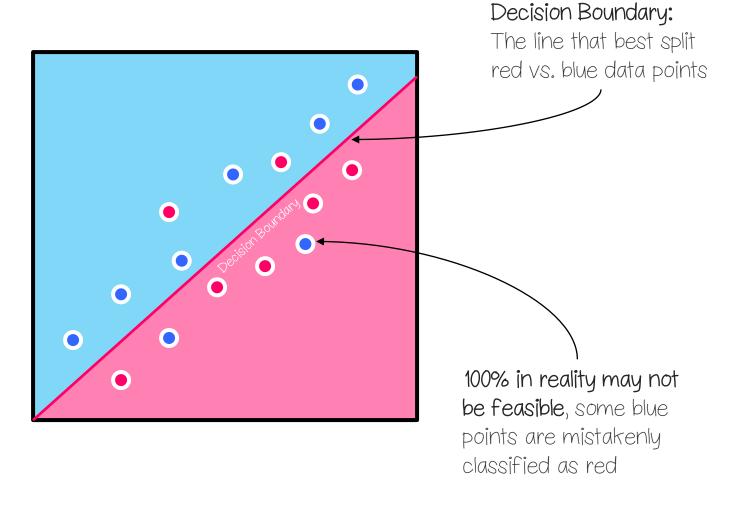
There are 3 types of algorithms

	Algorithms	Main Tasks
Unsupervised learning	K-Means Principal Component Analysis (PCA) Association Rules Social Network Analysis (SNA)	Tell me what patterns exist in my data - descriptive
Supervised learning	Linear Regression Logistic Regression Decision Tree Random Forests KNN Support Vector Machine Neural Networks	Use the pattern in my data to make predictions - predictive
Reinforcement learning	Multi-Armed Bandits (UBC, Thompson Sampling)	Use the pattern in my data to make predictions and – improve – these predictions as more results come in

Source: Data Science For The Layman (2017)

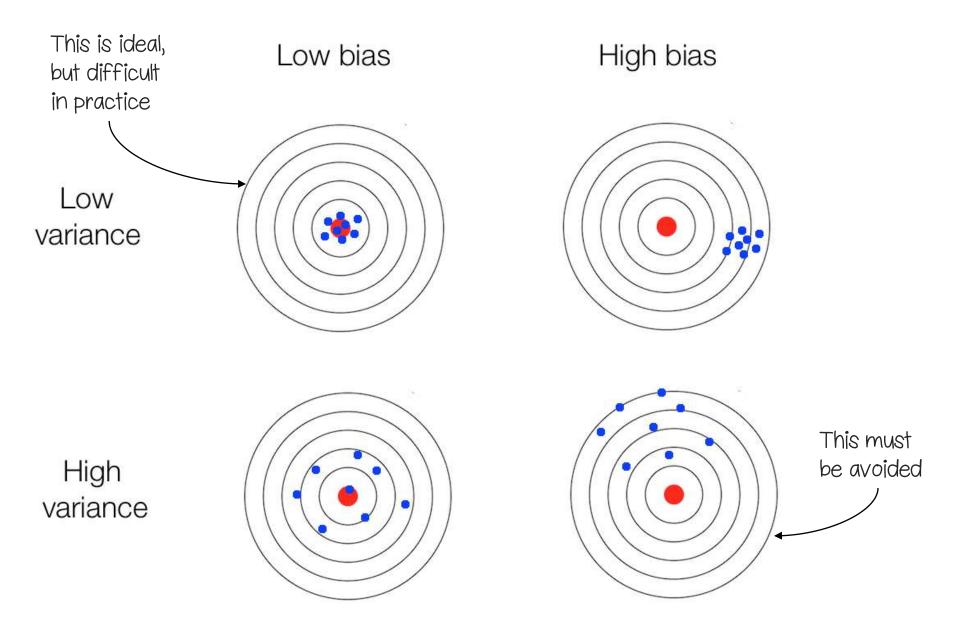
Regression vs. Classification







Our model consists of 3 types of error



Example Models

High Bias

Having lots of assumptions to do function approximation

Linear Regression Logistic Regression Linear Discriminant Analysis

Low Bias

Having little or few assumptions about the function approximation

Decision Tree KNN SVM

Low Variance

New data does not cause model to change much

High Variance

New data causes model to change much i.e. prediction results vary significantly compared to low variance algorithms

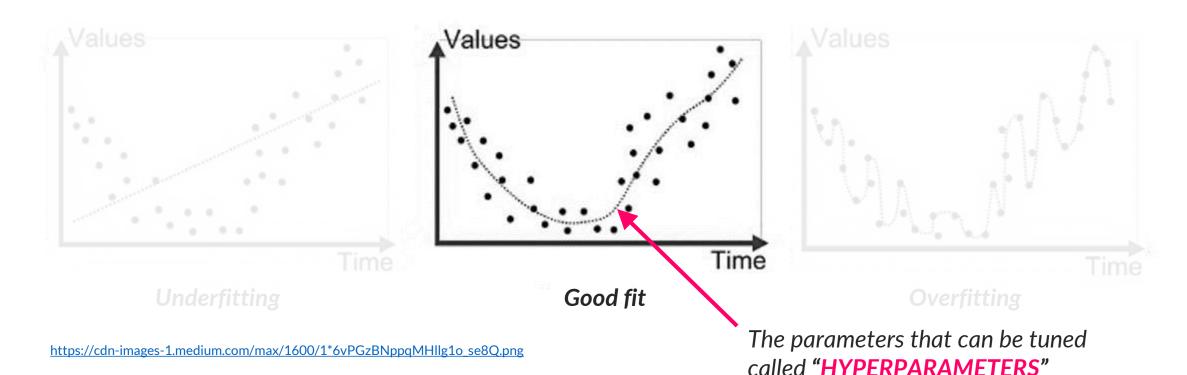
PARAMETER TUNING



There are so many learners.

Even the <u>same</u> learner can have different performances.

We tune parameter to get the best results (GOOD FIT) from our learner.



Some models have hyperparameters, some don't.

Stochastic Gradient Boosting

```
method = 'gbm'
```

Type: Regression, Classification

Tuning parameters:

- n.trees (# Boosting Iterations)
- interaction.depth (Max Tree Depth)
- shrinkage (Shrinkage)
- n.minobsinnode (Min. Terminal Node Size)

Hyperparameters of GBM algorithms

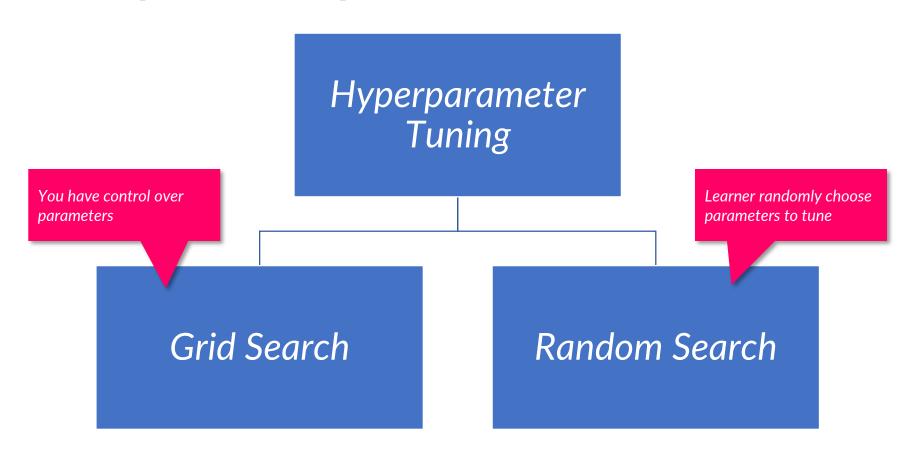
Required packages: gbm , plyr

A model-specific variable importance metric is available.

http://topepo.github.io/caret/train-models-by-tag.html

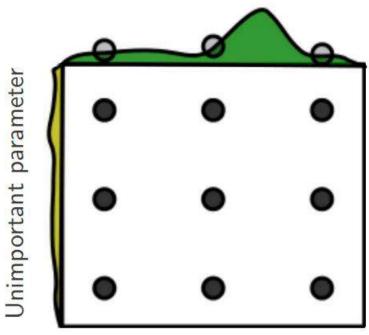
SEARCH for the best tune

ML is optimization problem



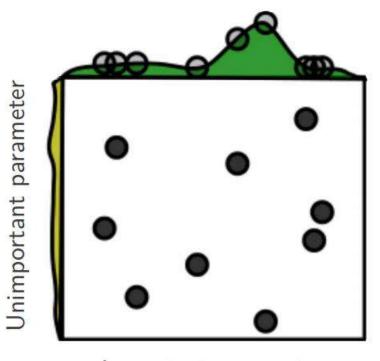
It really depends on the learners. Sometimes it's more efficient to use random search, sometimes it's not.

Grid Layout



Important parameter

Random Layout



Important parameter

http://www.jmlr.org/papers/volume13/bergstra12a/bergstra12a.pdf

EVALUATING RESULTS

Performance Metrics

Classification problems

- Confusion Matrix
- % Accuracy
- Area Under Curve (AUC)
- Logarithmic Loss (Log Loss)
- Cohen's KAPPA #for imbalanced problems

Regression problems

- Mean Absolute Error (MAE)
- Root Mean Squared Error (RMSE)



Confusion Matrix

Total n = 100	Reference		
Predicted	Cancer	No Cancer	
Cancer	60	3	
No Cancer	2	35	

Accuracy is the sum of diagonal divided by total sample size

Confusion Matrix

Total n = 100	Reference		
Predicted	Cancer	No Cancer	
Cancer	60 (A)	3 (B)	
No Cancer	2 (C)	35 (D)	

```
ถ้าผู้ป่วยเป็นมะเร็ง เราทายถูกเท่าไร? (%)

Sensitivity = A / A+C
```

ถ้าผู้ป่วยไม่ได้เป็นมะเร็ง เราทายถูกเท่าไร? (%)

Specificity =
$$D / B + D$$

ผล prediction "cancer" ของเราถูกกี่ %

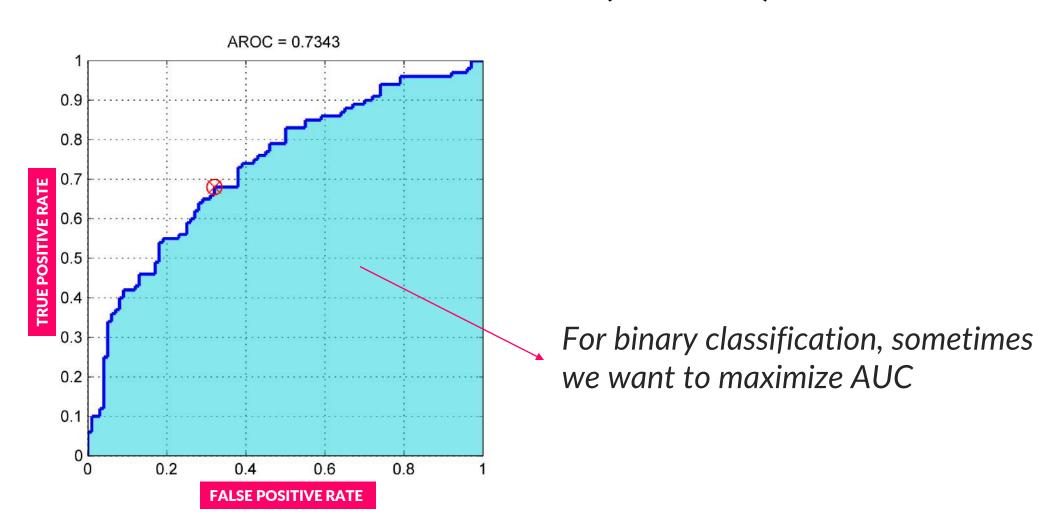
Precision =
$$A / A + B$$

ในผู้ป่วยโรคมะเร็งทั้งหมด เราทำนายถูกเท่าไร? (%)

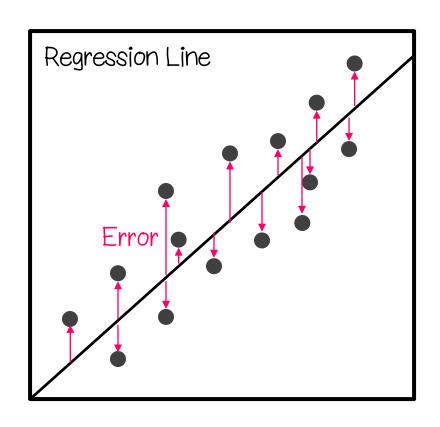
Recall =
$$A / A + C$$

Measure of overall test's accuracy

Area Under Curve (AUC)



Root Mean Squared Error (RMSE)



Mathematical Expression always look scary

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (Actual - Predicted \ y_i)^2}{N}}$$

$$RMSE = \sqrt{\frac{sum(error^2)}{N}}$$

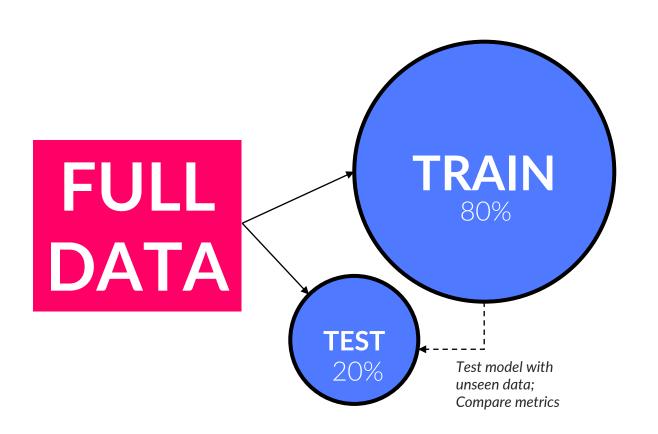
Remember this one

$$RMSE = \sqrt{mean (error^2)}$$

Recall the goal of ML is "GENERALIZATION"

We must test our model on new unseen dataset

Is our model good to go?



Training set (build model)

Testing set (evaluate model)

Decision Criterion:

The model passes the test if tested performance is similar trained performance [metric]

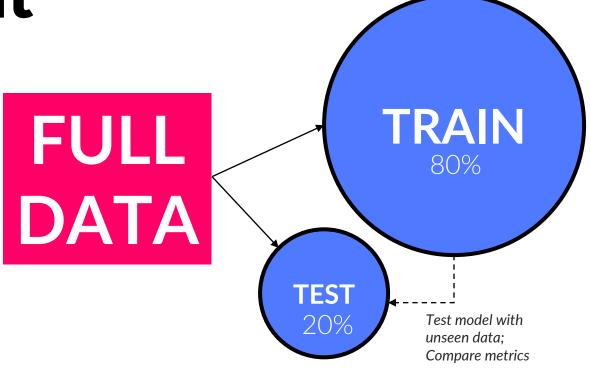
Resampling techniques

- 1. Train-test split
- 2. k-Fold Cross-Validation

This method is preferred but it's very expensive for large dataset

- Repeated k-Fold Cross-Validation
- 4. Bootstrap
- 5. Leave One Out Cross-Validation

The most efficient method is train-test split



K-Fold Cross Validation

FULL DATASET

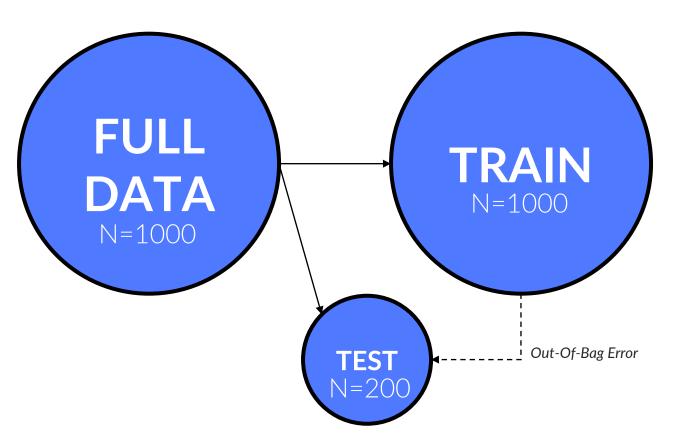


[1]	Train	Train	Train	Train	Test
[2]	Train	Train	Train	Test	Train
[3]	Train	Train	Test	Train	Train
[4]	Train	Test	Train	Train	Train
[5]	Test	Train	Train	Train	Train

People normally do 5, 10 K-Fold

Bootstrap Sampling

(aka. Random sampling with replacement)

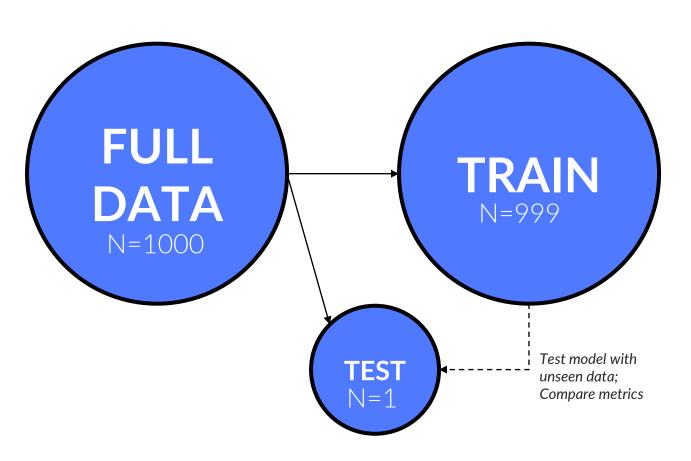


Explanation:

1000 may come from 800 unique data points + 200 repeated data points

Leave One Out CV

This is the most expensive method – time consuming



Explanation:

Leave 1 data point to test the model. For n=1000, this means we need to run model 1000 times

#SIMPLE:)

Data Preparation

Algorithms Selection

Parameter Tuning

Evaluating Results

Clean data
Missing Values
Feature selection
Feature engineering

No Free Lunch

- Bias Variance
- Time Money Accuracy

Hyperparameter Tuning For The Best Results

AvoidingOverfitting

Resampling Methods Performance Metrics

- Accuracy
- AUC
- RMSE

SUMMARY

- Data preparation takes 70-80% of our time.
 - "Garbage in, Garbage out"
 - Feature selection | Feature engineering | Missing Value
- No free lunch theorem
 - Bias vs. Variance Tradeoff
 - Speed vs. Accuracy Tradeoff
- [Hyper]Parameter tuning to get the best out of our learning algorithms
- Resampling techniques used in ML research incl. train-test, k-fold CV, repeated k-fold CV, bootstrap, and LOOCV

OKAY!! Let's recap a bit

- ML is function approximation
- Learn from past data to predict future (unseen) data point
- The goal is representation & generalization (avoid overfitting)
- Regression or Classification problems depend target variable (y)
- No Free Lunch: bias vs. variance tradeoff
- Algorithms can be tuned via <mark>hyperparameter</mark>
- K-Fold cross validation is popular resampling technique
- Our model passes the test if training vs. testing performances are similar (not overfit)

ALGORITHMS YOU SHOULD KNOW

We cover 8 algorithms

Linear Regression	Regression		
Logistic Regression	Classification		
Decision Tree	Regression & Classification		
Random Forest	(mainly) Classification		
KNN	(mainly) Classification		
Support Vector Machine	(mainly) Classification		
Neural Networks	Regression & Classification		
K-Means	Unsupervised Learning NN is		

Supervised Learning

NN is special algorithm, it works like reinforcement learning

LINEAR REGRESSION -

Hello World in Machine Learning

Recall these steps

Data Preparation

Algorithms Selection

Parameter Tuning

Evaluating Results

Clean data
Missing Values
Feature selection
Feature engineering

No Free Lunch

- Bias Variance
- Time Money Accuracy

Hyperparameter Tuning For The Best Results

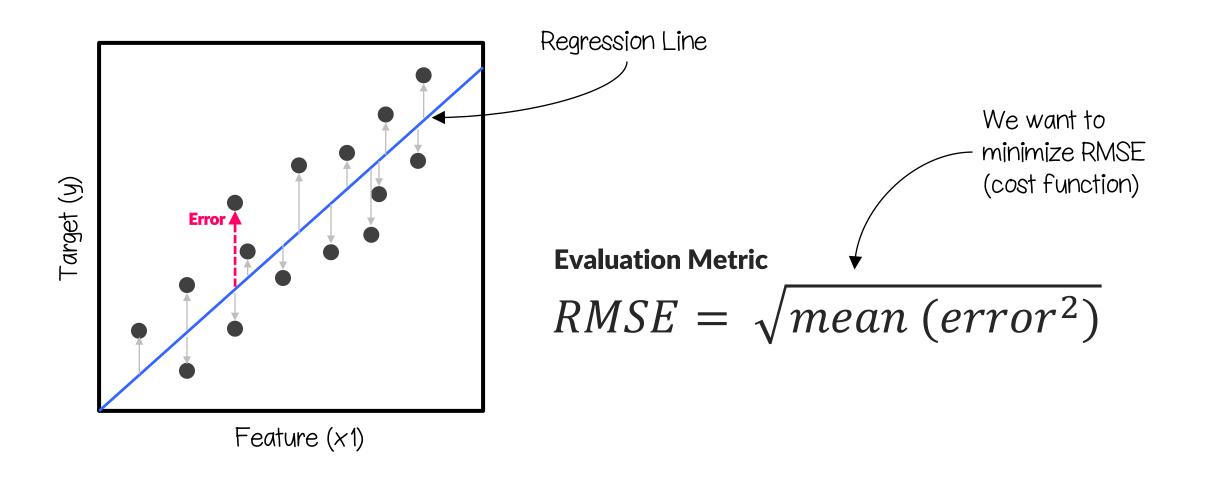
AvoidingOverfitting

Resampling Methods Performance Metrics

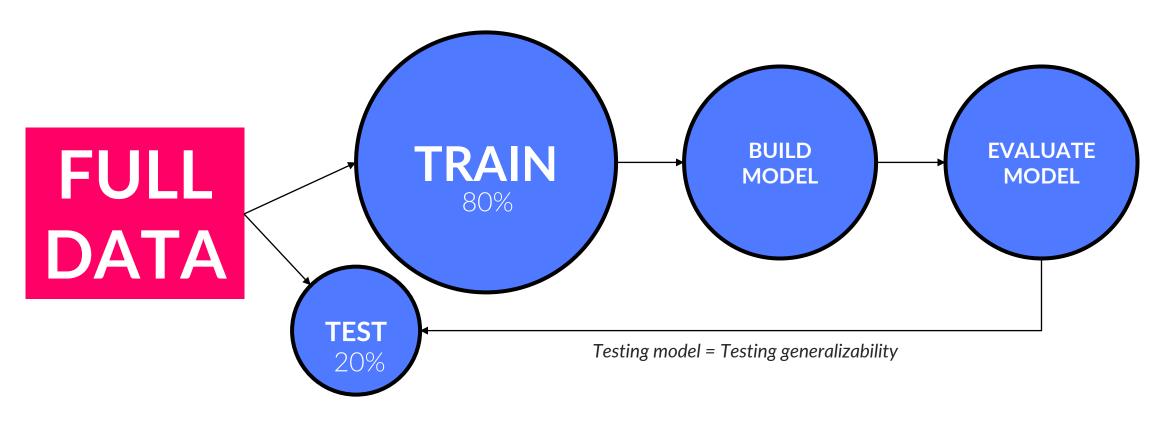
- Accuracy
- AUC
- RMSE

Algorithm explained:

How to draw a single straight line that fit best with given data points



Let's do a train-test split for linear regression problem



Advantages:

- Easy to train
- Always find the optimum solutions (least squared)
- Foundation of advanced algorithms like neural nets

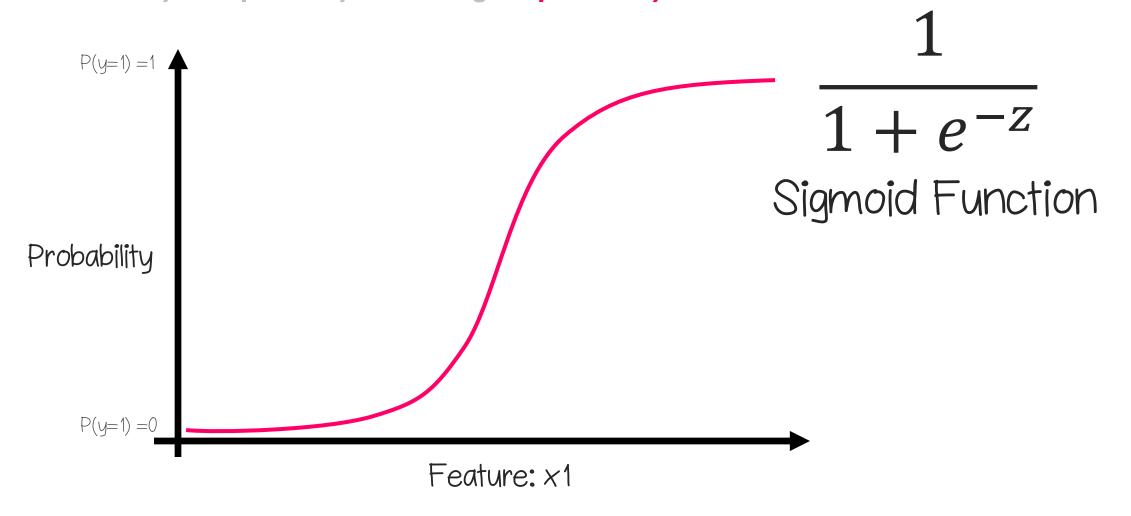
Disadvantages:

- Only work for regression problems (continuous y)
- Full of assumptions (high bias algorithms)

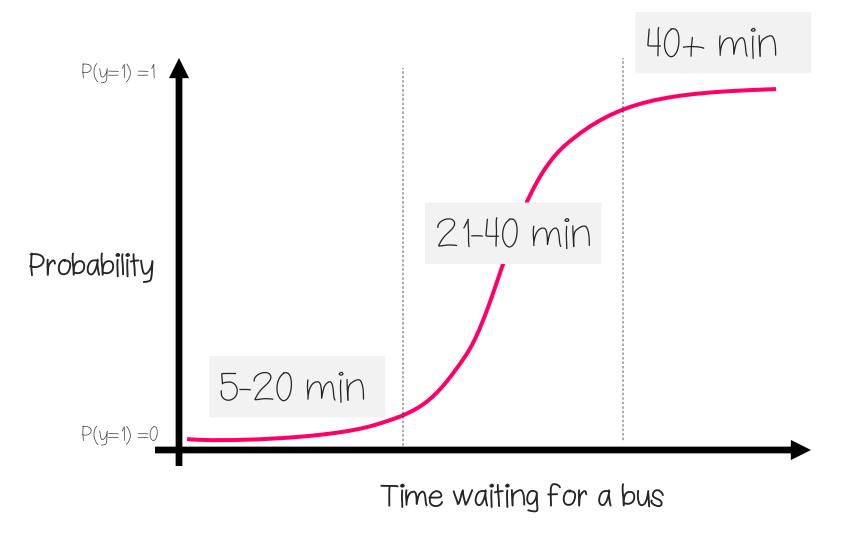
LOGISTIC REGRESSION

Algorithm explained:

Classify data points by calculating the probability that Y=1



Should I get taxi or a bus?





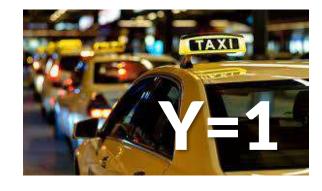


The model is very similar to linear regression

(assuming linear relationship between x and y)

z = bo + b1x1 + b2x2 + b3x3 + b4x4 \rightarrow then 1 / 1+ e^{-z} to get probability scores

ID	X1 (minute)	X2 (crowd)	X3 (time)	X4 (weather)	P(Y=1) (get Taxi)	Prediction
1	50	Many	Friday	Good	.95	Yes
2	20	Many	Saturday	ОК	.32	No
3	20	Few	Monday	ОК	.31	No
4	25	Few	Friday	Bad	.85	Yes
5	30	Many	Friday	Good	.68	Yes
6	35	Few	Saturday	OK	.25	No
7	12	Many	Monday	Good	.52	Yes
8	5	Few	Saturday	OK	.12	No
9	10	Many	Friday	Bad	.20	No
10	65	Few	Friday	Good	.98	Yes



We set threshold = 0.5If p(y=1) >= 0.5, then we predicted YES get taxi!

Advantages:

- One of the most powerful algorithms to date
- Easy to train
- Can be developed to create complex decision boundaries (e.g. x^2 y^2)

Disadvantages:

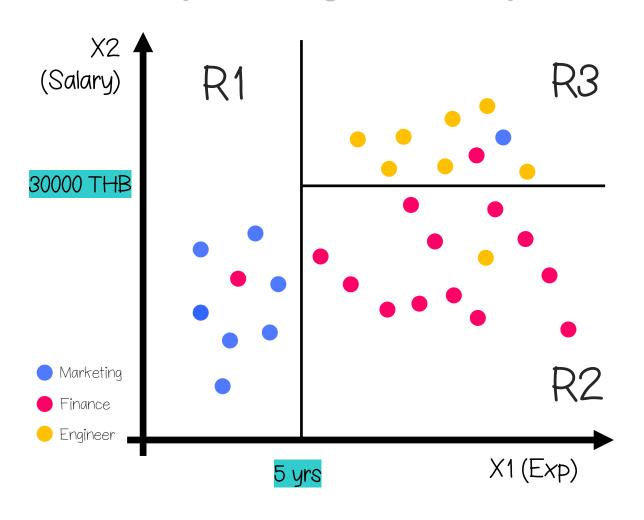
- Also a lot of assumption e.g. no outlier, no noise
- Logistic regression is also a linear algorithm
- Prone to multicollinearity (check correlation first)

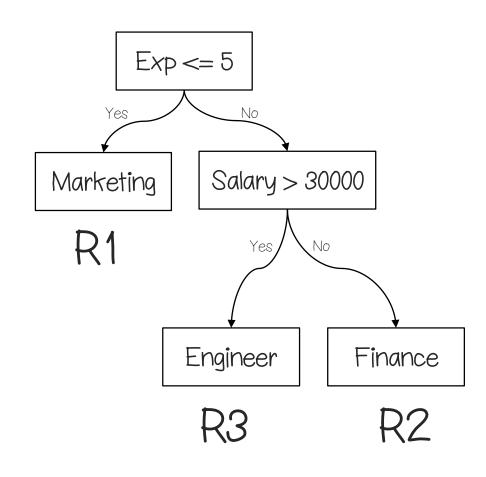
(sigmoid function transform an output into non-linear)

DECISION TREE

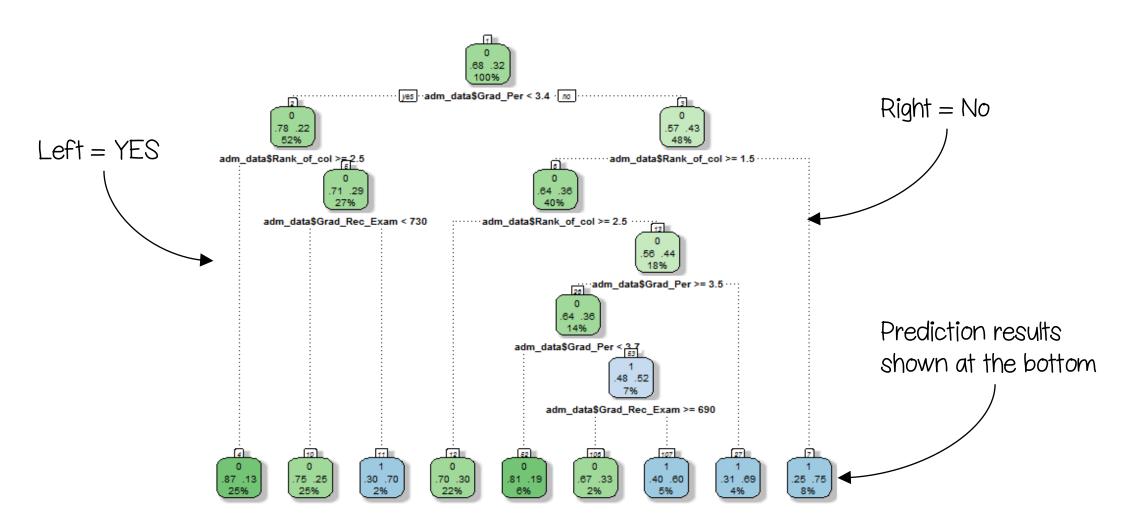
Algorithm explained:

Divide space into regions that best predict data points (classes)





Decision Tree is easily presented using diagram



Advantages:

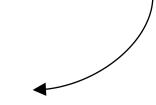
- Easy to train
- Easy to interpret results
- Widely used in many disciplines

Disadvantages:

- Prone to overfitting: Greedy algorithms

The main reason why people use decision tree

Locally optimal decision are made at each node, but can't guarantee globally optimal decision trees



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

Required Packages:

library(caret) - train & test models

library(caTools) - split data into training & testing sets

library(rpart) — train decision tree (CART): recursive partitioning and

regression tree cart

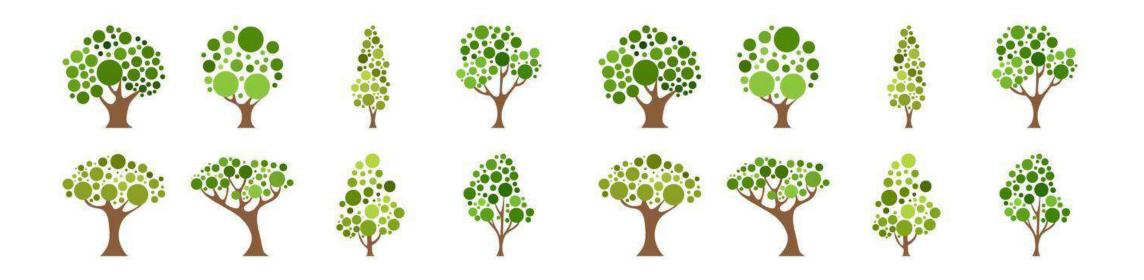


A model-specific variable importance metric is available.

RANDOM FOREST

Algorithm explained:

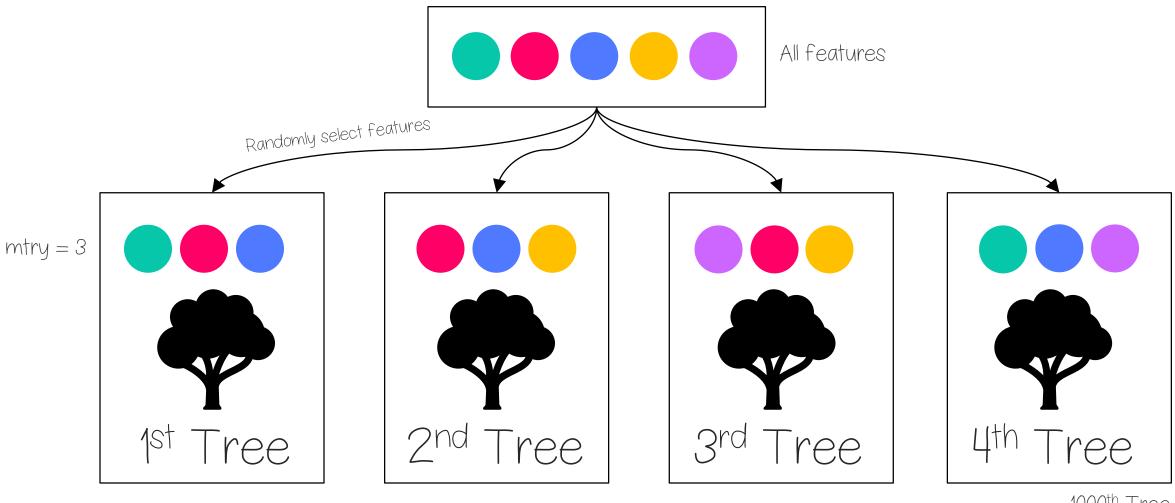
Grow thousand trees and average their prediction results



Grow uncorrelated 1000 trees

How do we grow 1000 trees?

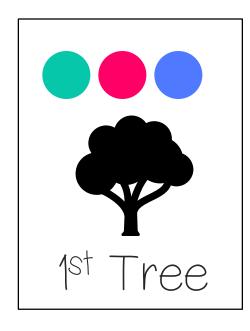
Randomness is your friend, hyperparameter is mtry



... 1000th Tree

Wisdom of the crowds

Find the average prediction results of all grown trees









... 1000th Tree

Advantages:

- Amongst the best learners in the world
- Easy to train (Improvement from Decision Tree)

Disadvantages:

- Can be slow to train for large dataset
- Black Box Algorithm (not easy to explain)

Required Packages:

library(caret) - train & test models

library(caTools) - split data into training & testing sets

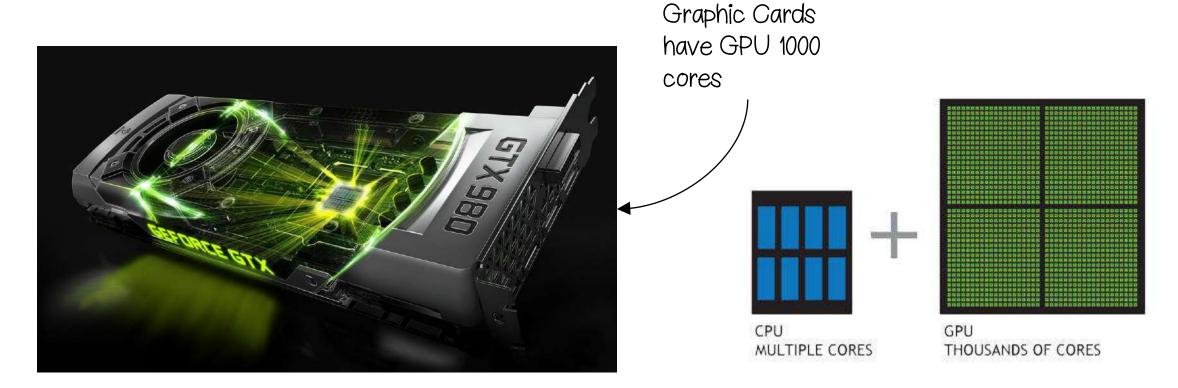
library(randomForest) - train random forest in caret

Random Forest



A model-specific variable importance metric is available.

Let's talk about the hardware side



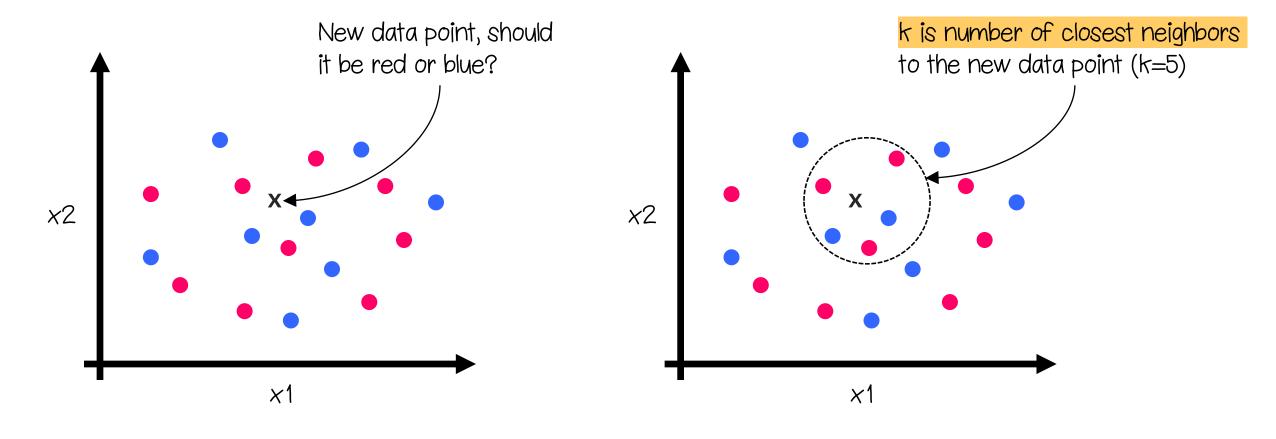
Nvidia has CUDA technology

Read more: https://developer.nvidia.com/about-cuda

KNN (K-NEAREST NEIGHBOR)

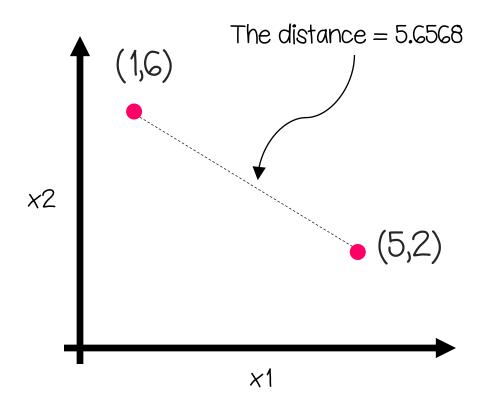
Algorithm explained:

Predict new data according to the distance from its neighbors



Euclidean Distance:

The most popular distance calculation method



$$d = \sqrt{\sum (x_i - y_i)^2}$$

$$d = \sqrt{(1-5)^2 + (6-2)^2}$$

$$d = \sqrt{16 + 16}$$

$$d = 5.656854$$

Very simple to compute

Another Example

Consider the nutrient dataset provided with the flexclust package. The dataset contains measurements on the nutrients of 27 types of meat, fish, and fowl. The first few observations are given by

```
We can calculated
> data(nutrient, package="flexclust")
> head(nutrient, 4)
                                                                 many dimensions
                                                                 (more than two)
             energy protein fat calcium iron
BEEF BRAISED
                              28
                                           2.6
                 340
                          20
                                           2.7
HAMBURGER
                               17
                 245
BEEF ROAST
                 420
                               39
                                           2.0
BEEF STEAK
                 375
                          19
                              32
                                           2.6
```

and the Euclidean distance between the first two (beef braised and hamburger) is

$$d = \sqrt{(340 - 245)^2 + (20 - 21)^2 + (28 - 17)^2 + (9 - 9)^2 + (26 - 27)^2} = 95.64$$

Advantages:

- Very simple
- Easy to train (remember all data)

Disadvantages:

- Worst for large dataset
- Not good with high dimensional data (many features)
- Don't work well with categorical data

Example Code:

```
## load library
    library(caret)
   ## train model
   ## define trControl
   my_trcontrol = trainControl(method = "cv",
                                  number = 3,
                                  verboseIter = TRUE,
                                  search = "random")
14
   knn_model \leftarrow train(Species \sim . , data = m,
                        method = "knn",
16
                        metric = "Accuracy",
18
                        tuneLength = 10,
                        trControl = my_trcontrol)
```

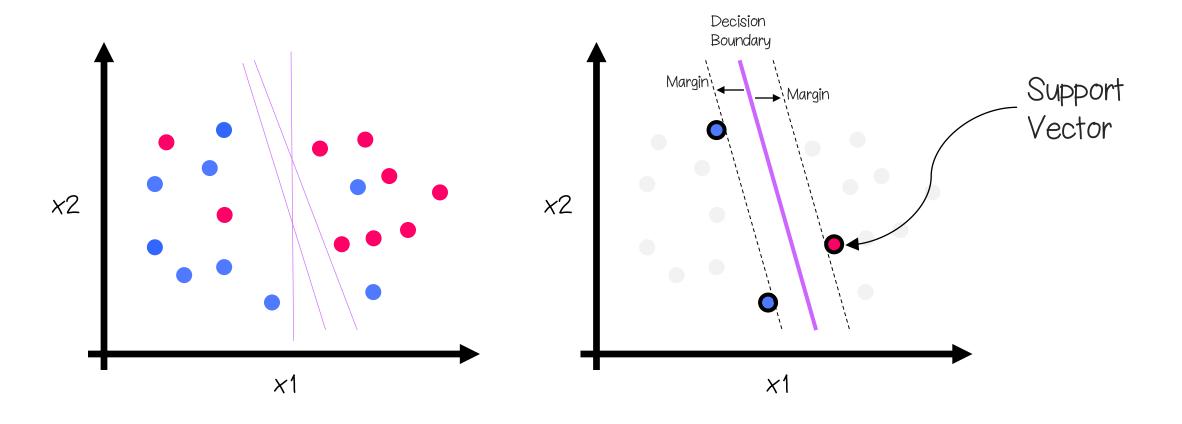
Define our technique (to train the model)

Train the model using random search + tuneLength = 10

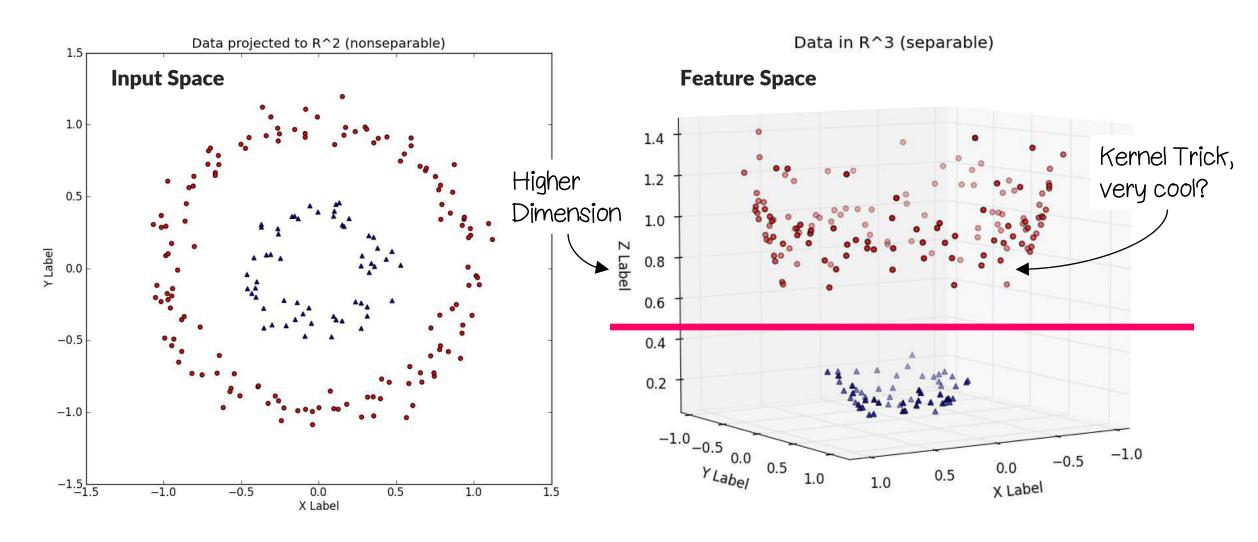
SUPPORT VECTOR MACHINE

Algorithm explained:

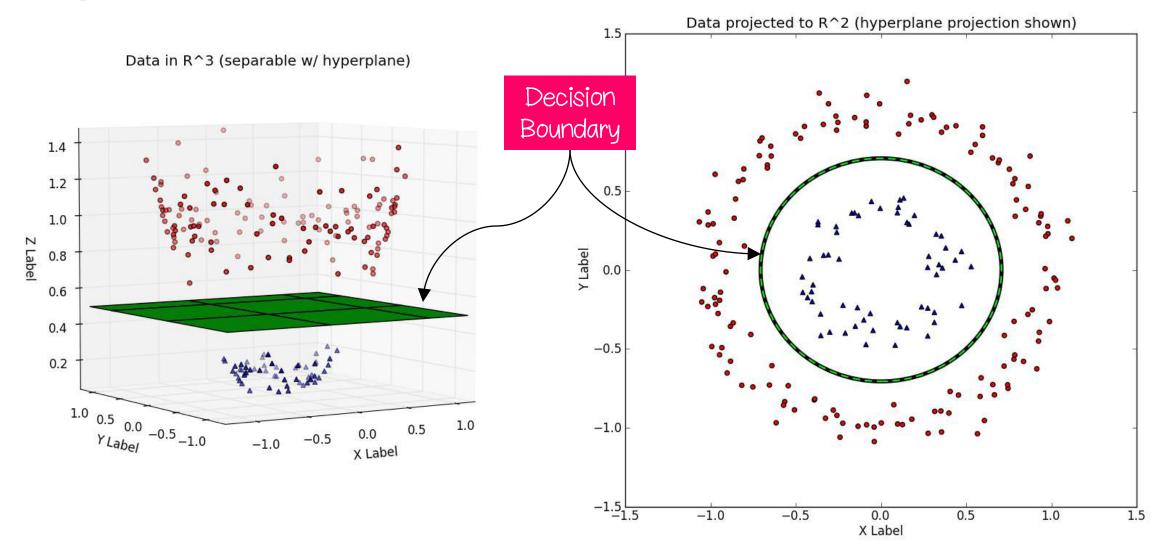
We want to maximize the margin from decision boundary



But can you divide this with a single straight line?



Impressive Result!!

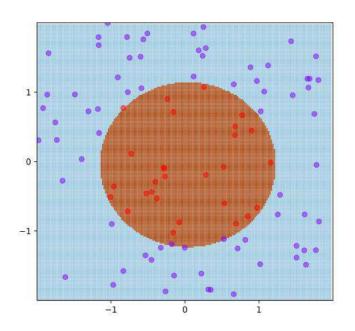


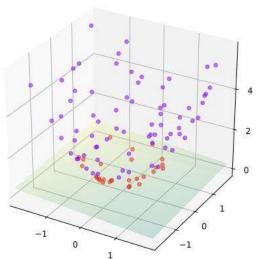
Let's look closely at kernel trick

- we have (x,y) coordinates



3rd dimension





https://en.wikipedia.org/wiki/Kernel method

Advantages:

- Work with Regression | Classification problems
- Superior Performance
- Having lots of available kernel tricks

https://topepo.github.io/caret/train-models-by-tag.html#support-vector-machines

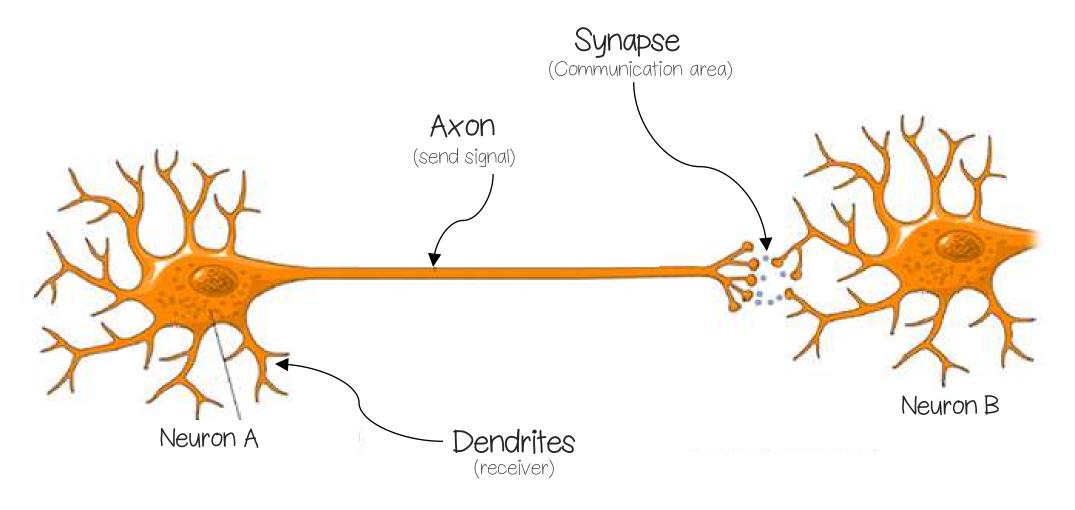
Disadvantages:

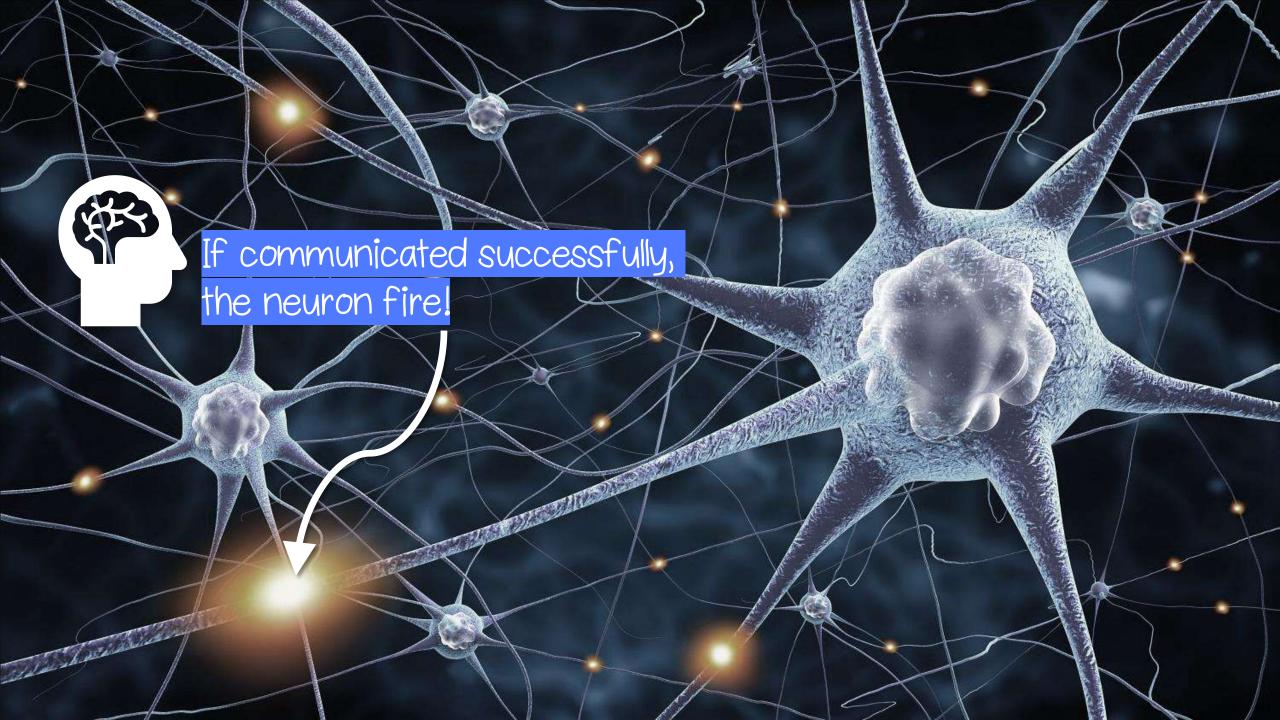
- Expensive
- It's lazy algorithm (remember data like KNN)

NEURAL NETWORK



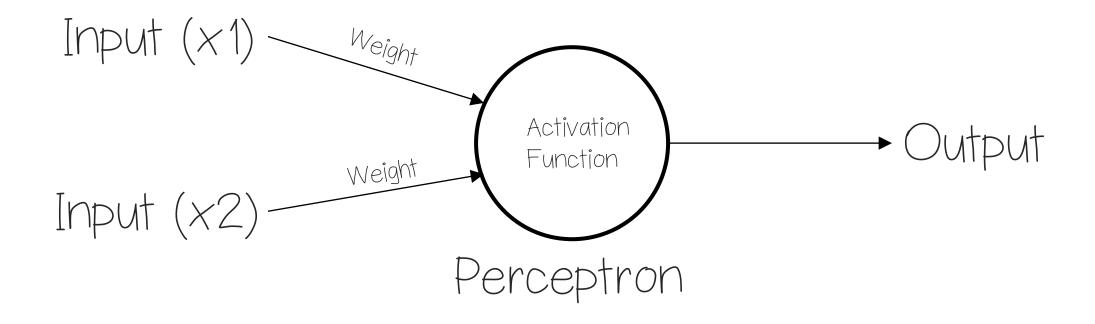
How your brain cells communicate

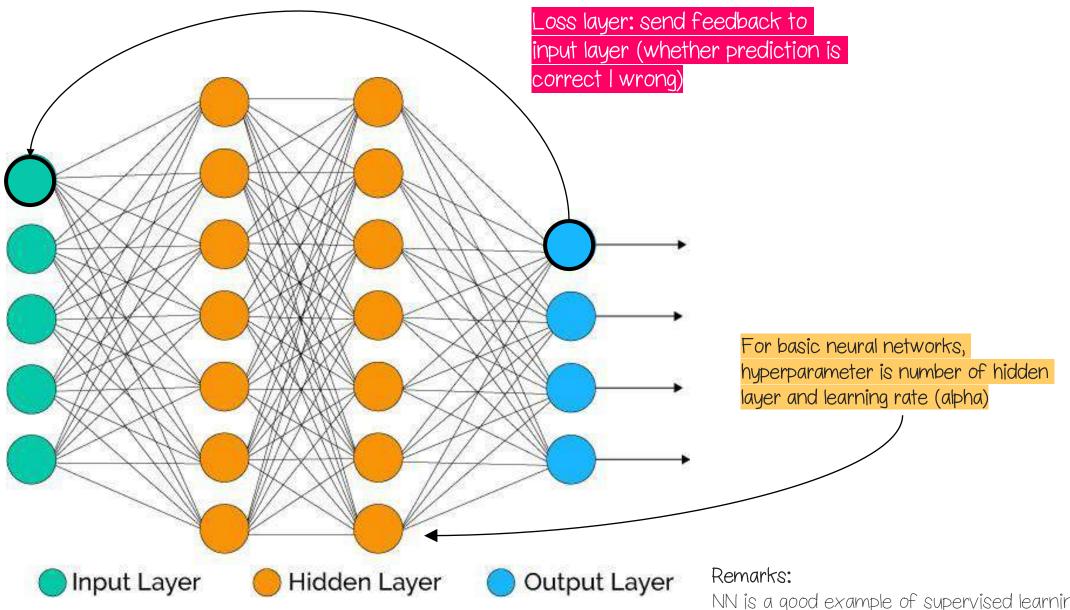




Algorithm Explained:

Neurons fire only when it's the signal strong enough to activate them



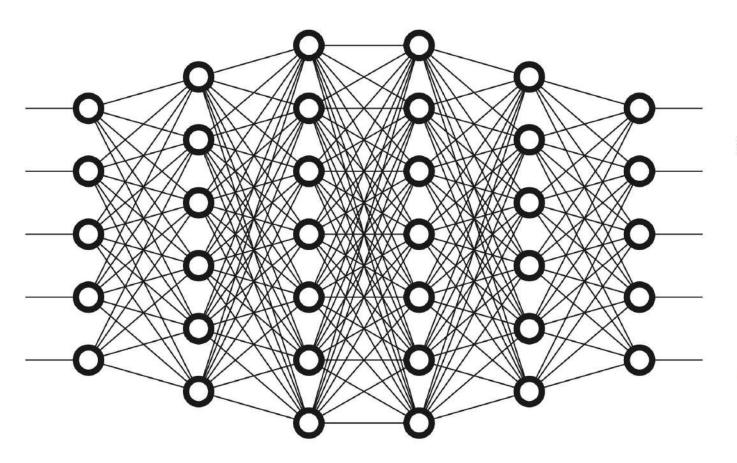


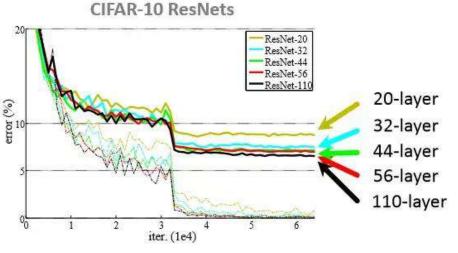
https://medium.com/@xenonstack/overview-of-artificial-neural-networks-and-its-applications-2525c1addff7

NN is a good example of supervised learning that also a reinforcement learning (learn from experience)

Deep Learning

Expands the number of hidden layers







Hieu Pham, Has done some machine learning Updated Apr 29, 2017

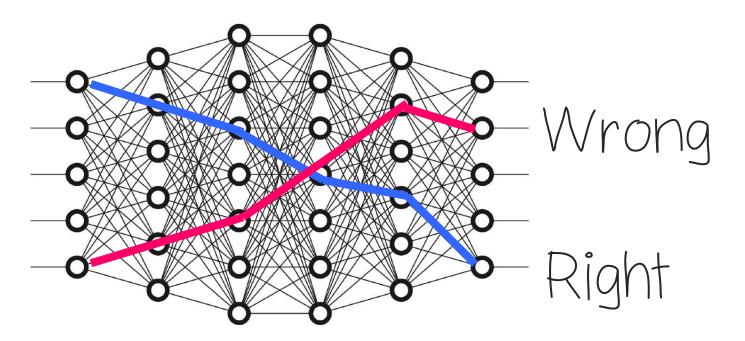


In this paper (Huang et al, 2016), the authors report that they "can increase the depth of residual networks *even beyond 1200 layers* and still yield meaningful improvements in test error (4.91% on CIFAR-10)".

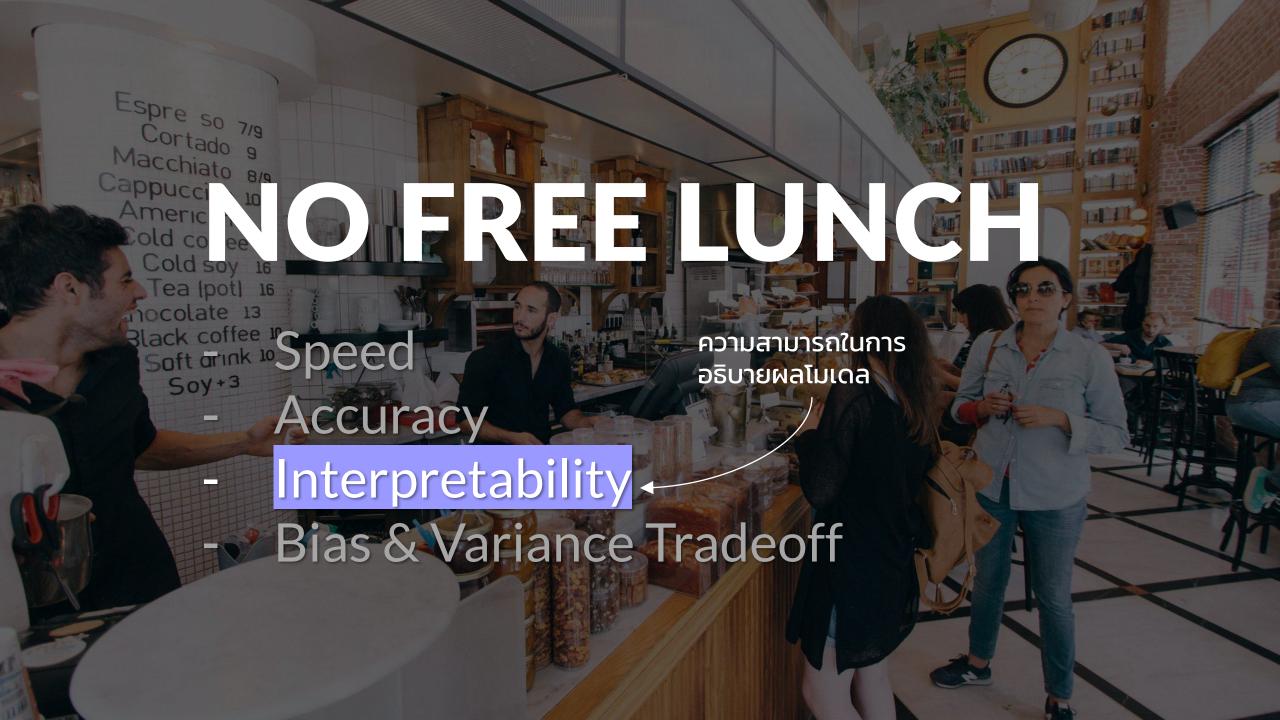
I have never heard of anything deeper than that.

Backpropagation

The backbone of artificial neural networks



Send feedback to input layers and adjust the weights

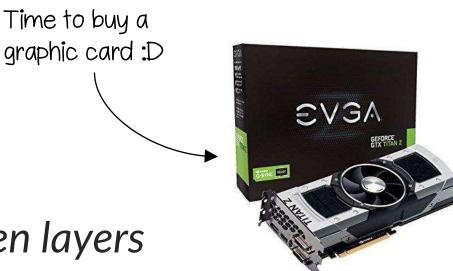


Advantages:

- Amongst the very best performers | learners in the world
- Can be developed into deep learning algorithms
- Work with both regression and classification problems

Disadvantages:

- Requires large data set
- Black Box
- Prone to overfitting problem
- Need more power if more hidden layers



ALGORITHMS ARE NOT CREATED EQUAL

- Neural Nets [Backpropagation]
- **SVM** [Kernel Tricks]
- KNN [Majority Vote]
- Random Forest [Randomness]
- **Decision Tree** [Recursive Partitioning]
- Logistic Regression [Sigmoid Function]
- Linear Regression [Least Squared]



R has powerful package written by Max Kuhn (10 years in development)

```
# CARET
# Classification And Regression Training
# 238 models can be trained using caret
install.packages("caret")
library(caret)
```

For more details, go to this website http://topepo.github.io/caret/index.html