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Government Big Data Institute
สถาบันส่งเสริมการวิเคราะห์และบริหารข้อมูลขนาดใหญ่ภาครัฐ (สวข.)

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Introduction to Machine Learning: Machine Learning Process and Model Evaluation

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Original materials developed by Patipan Prasertsom and Asst. Prof. Duangjai Jitkongchuen

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Notebooks and Data

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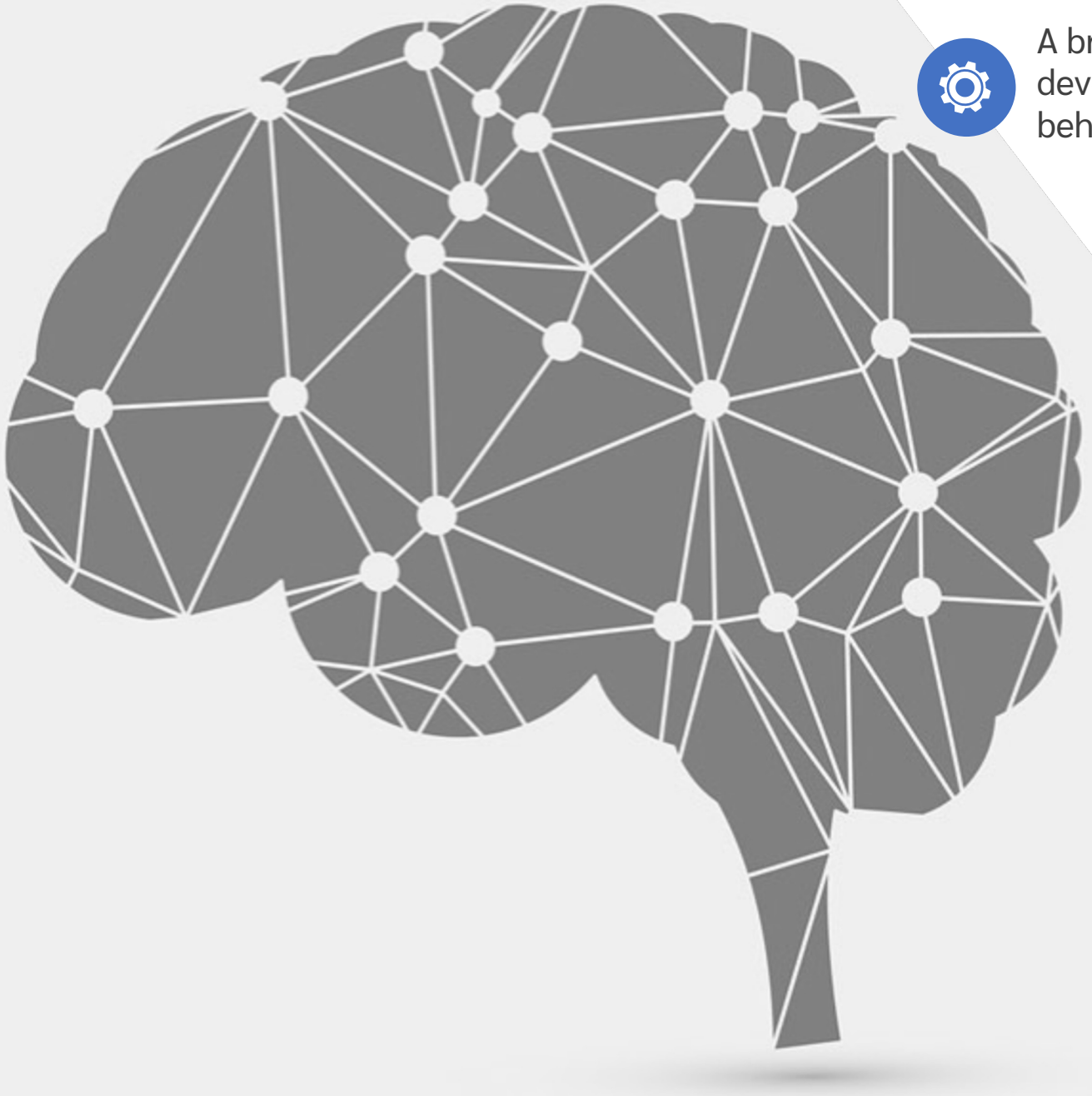


A branch of artificial intelligence, concerned with the design and development of algorithms that allow computers to evolve behaviors based on empirical data.

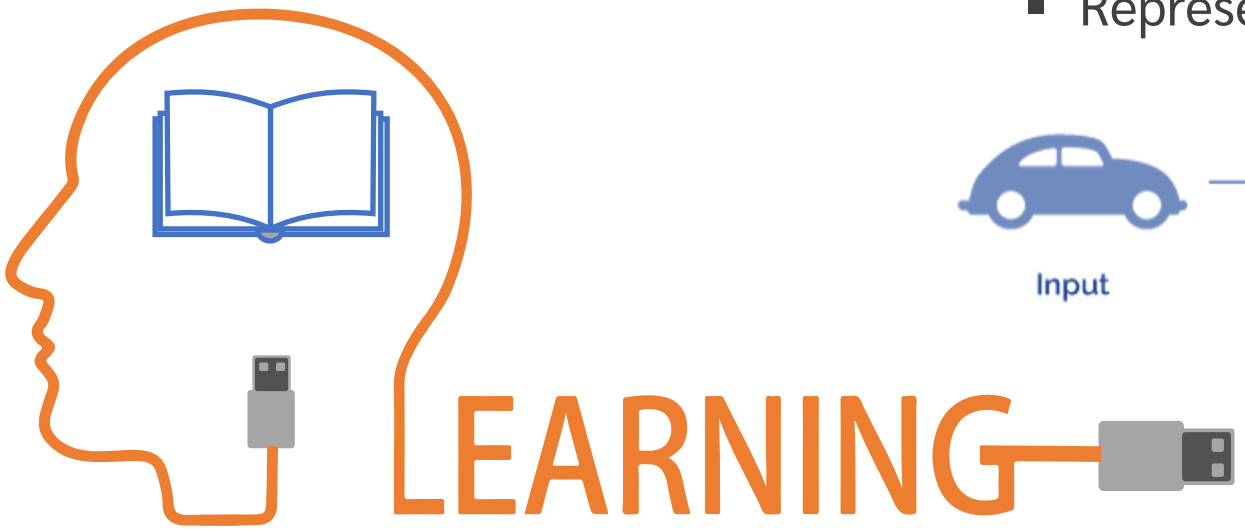
The goal of machine learning is to develop methods that can automatically detect patterns in data and then to use the uncovered patterns to predict future data or other outcomes of interest. -- Kevin P. Murphy

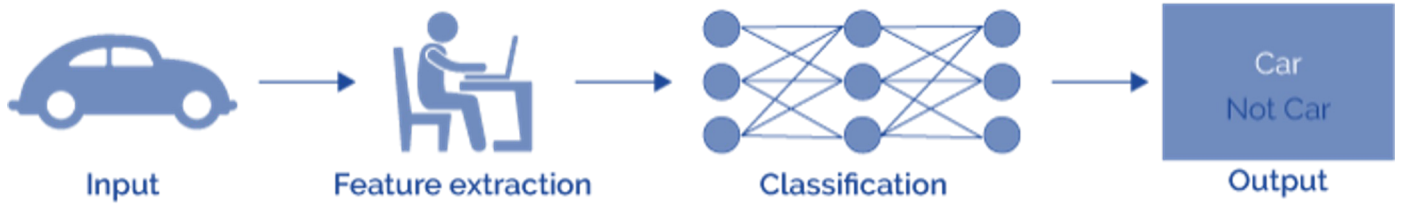
A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at the tasks improves with the experiences. -- Tom Mitchell

Machine Learning

What is Machine Learning?

- Study of algorithms that improve their performance at some task with experience
- Optimize a performance criterion using example data or past experience.
- **Role of Statistics**: Inference from a sample
- **Role of Computer science**: Efficient algorithms to
  - Solve the optimization problem
  - Representing and evaluating the model for inference





Types of Learning

2. Unsupervised learning

3. Semi-supervised learning

1. Supervised (inductive) learning

4. Reinforcement learning

Types of Learning

1. Supervised (inductive) learning

- Learn through examples of which we know the desired output (what we want to predict).
- Is this a cat or a dog?
- Are these emails spam or not?
- Predict the market value of houses, given the square meters, number of rooms, neighborhood, etc.

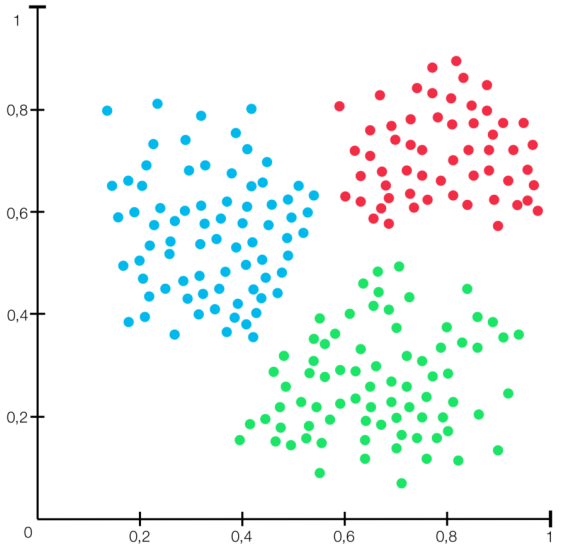
Classification

Output is a discrete variable (e.g., cat/dog)

Regression

Output is continuous (e.g., price, temperature)

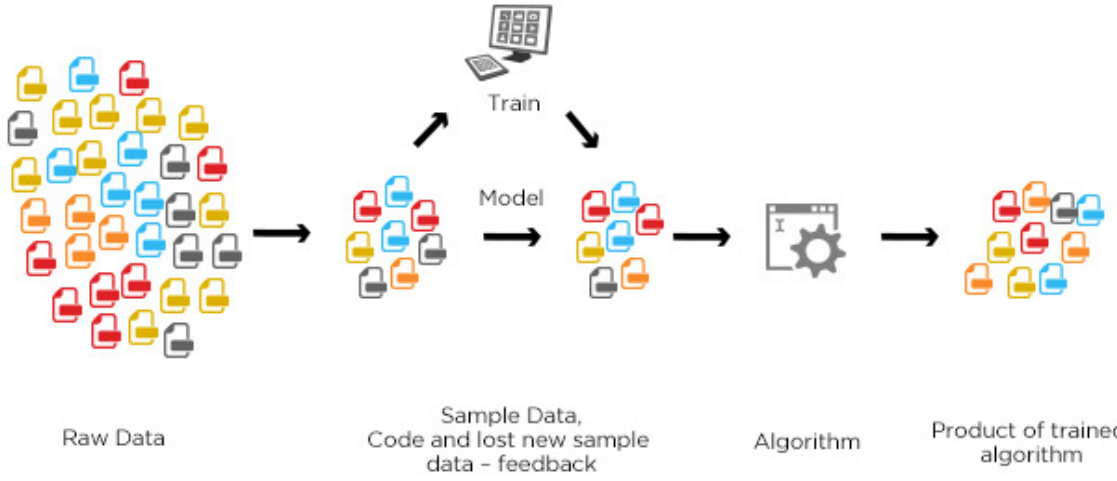
Types of Learning

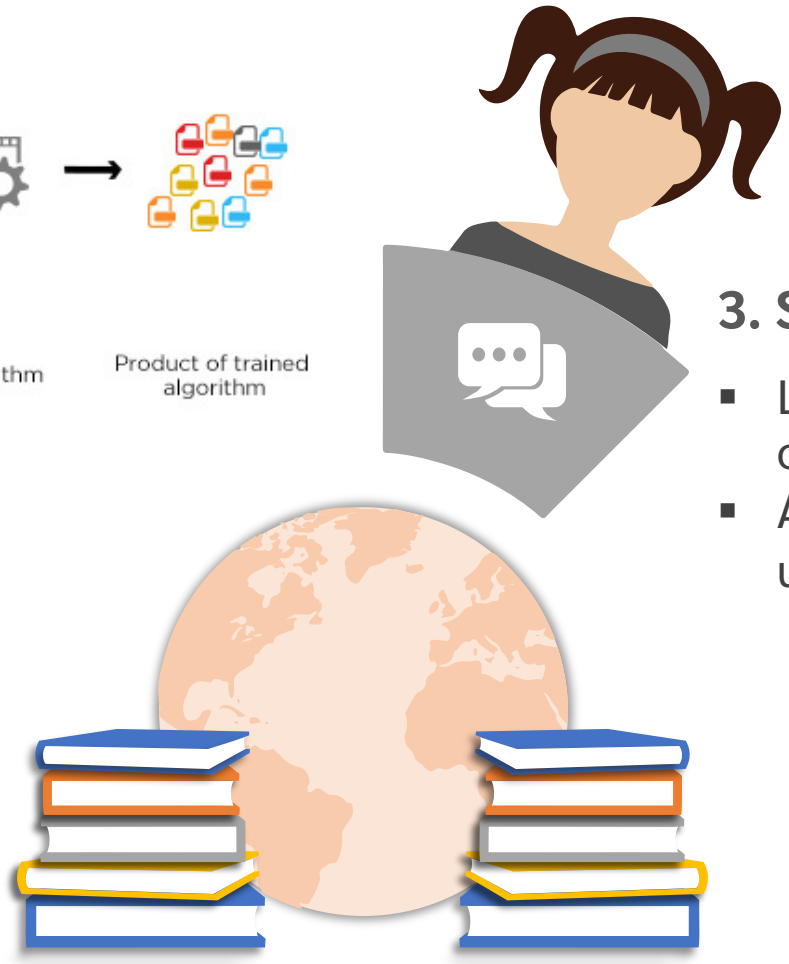


2. Unsupervised learning

- There is no desired output. Learn something about the data. Latent relationships.
- I have photos and want to put them in 20 groups.
- I want to find anomalies in the credit card usage patterns of my customers.
- Useful for learning structure in the data (clustering), hidden correlations, reduce dimensionality, etc.

Types of Learning





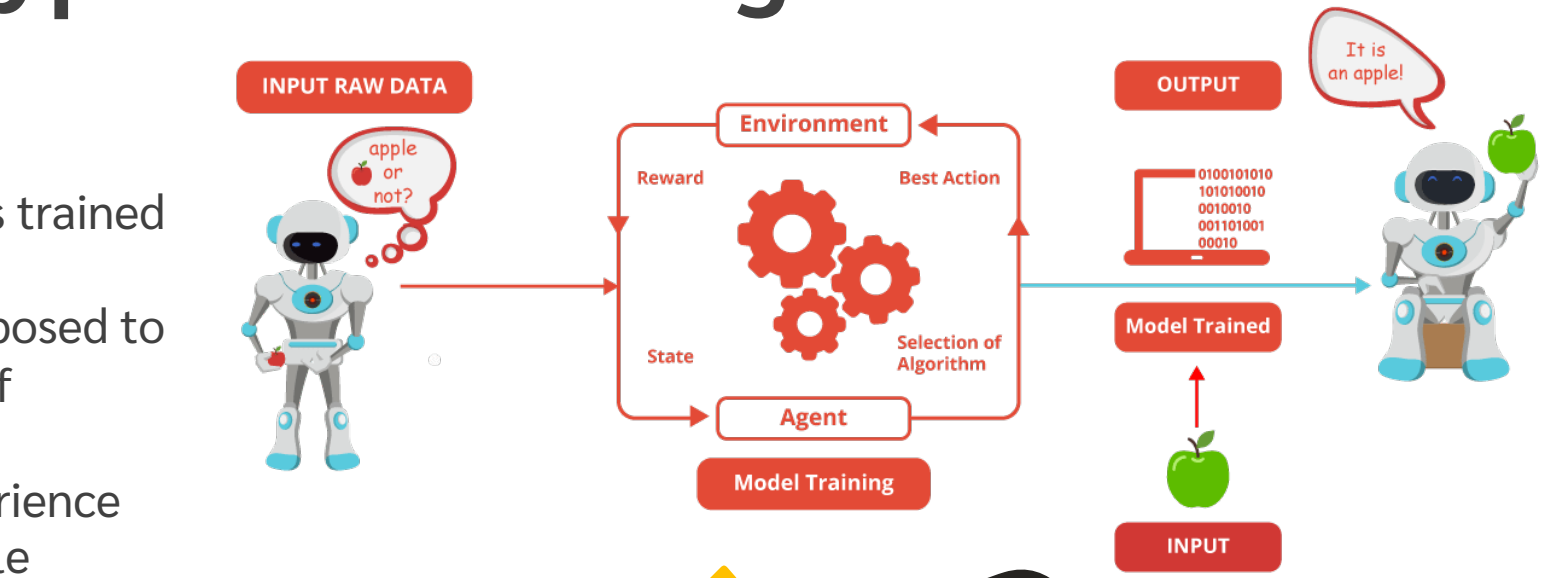
3. Semi-supervised learning

- Labels or output known for a subset of data
- A blend of supervised and unsupervised learning

Types of Learning

4. Reinforcement learning

- Using this algorithm, the machine is trained to make specific decisions.
- It works this way: the machine is exposed to an environment where it trains itself continually using trial and error.
- This machine learns from past experience and tries to capture the best possible knowledge to make accurate business decisions.



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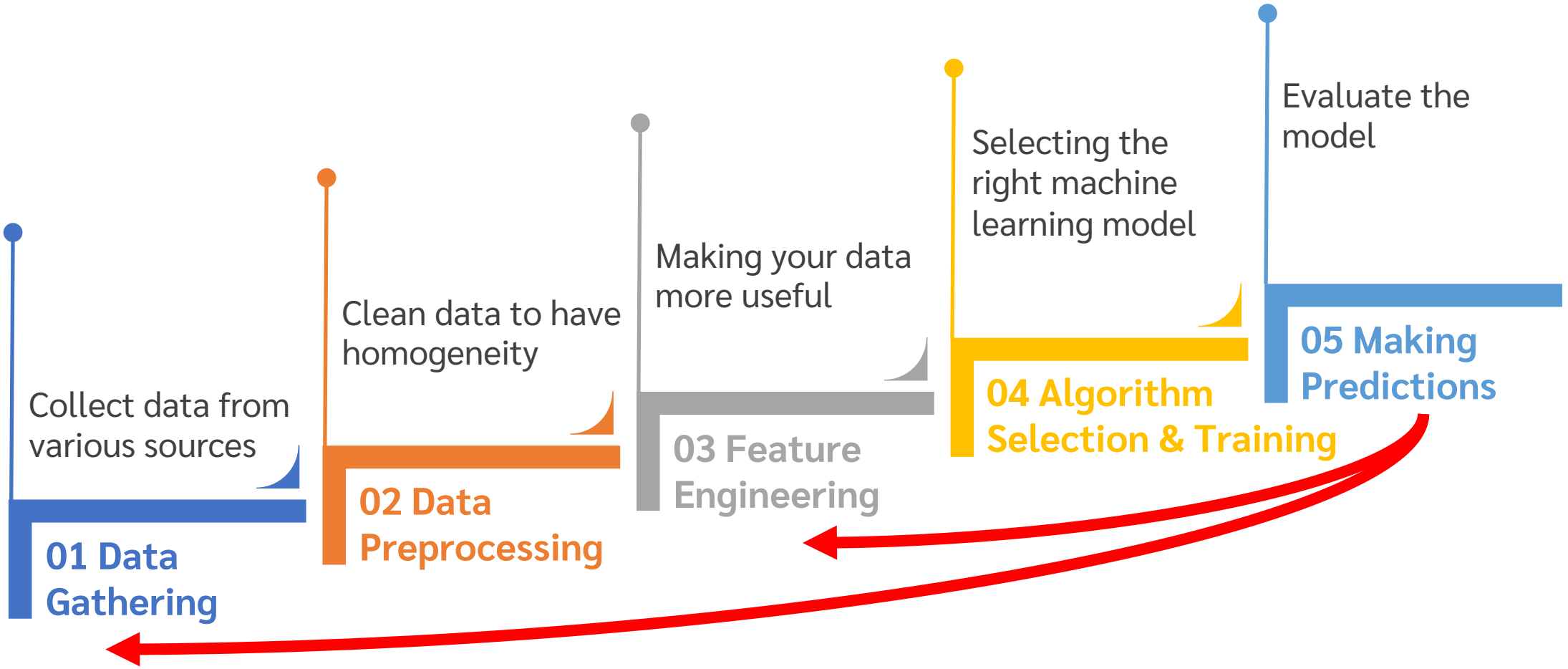
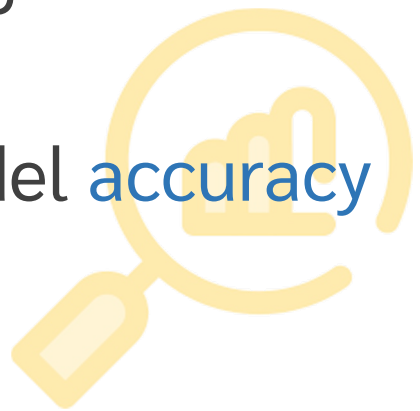
Steps to Solve a Machine Learning Problem



01 Data Gathering

- Might depend on human work
  - Manual labeling for supervised learning.
  - Domain knowledge. Maybe even experts.
- May come for free, or "sort of“
  - E.g., Machine Translation.
- The more the better : Some algorithms need large amounts of data to be useful (e.g., neural networks).
- The quantity and quality of data dictate the model accuracy



02 Data Preprocessing

- Perform **Exploratory Data Analysis (EDA)**
  - Essentially, **study the data**
  - This is arguably the most important step
- Is there anything wrong with the data?
  - Missing values
  - Outliers
  - Bad encoding (for text)
  - Wrongly labeled examples
  - Biased data
- Need to fix/remove data?

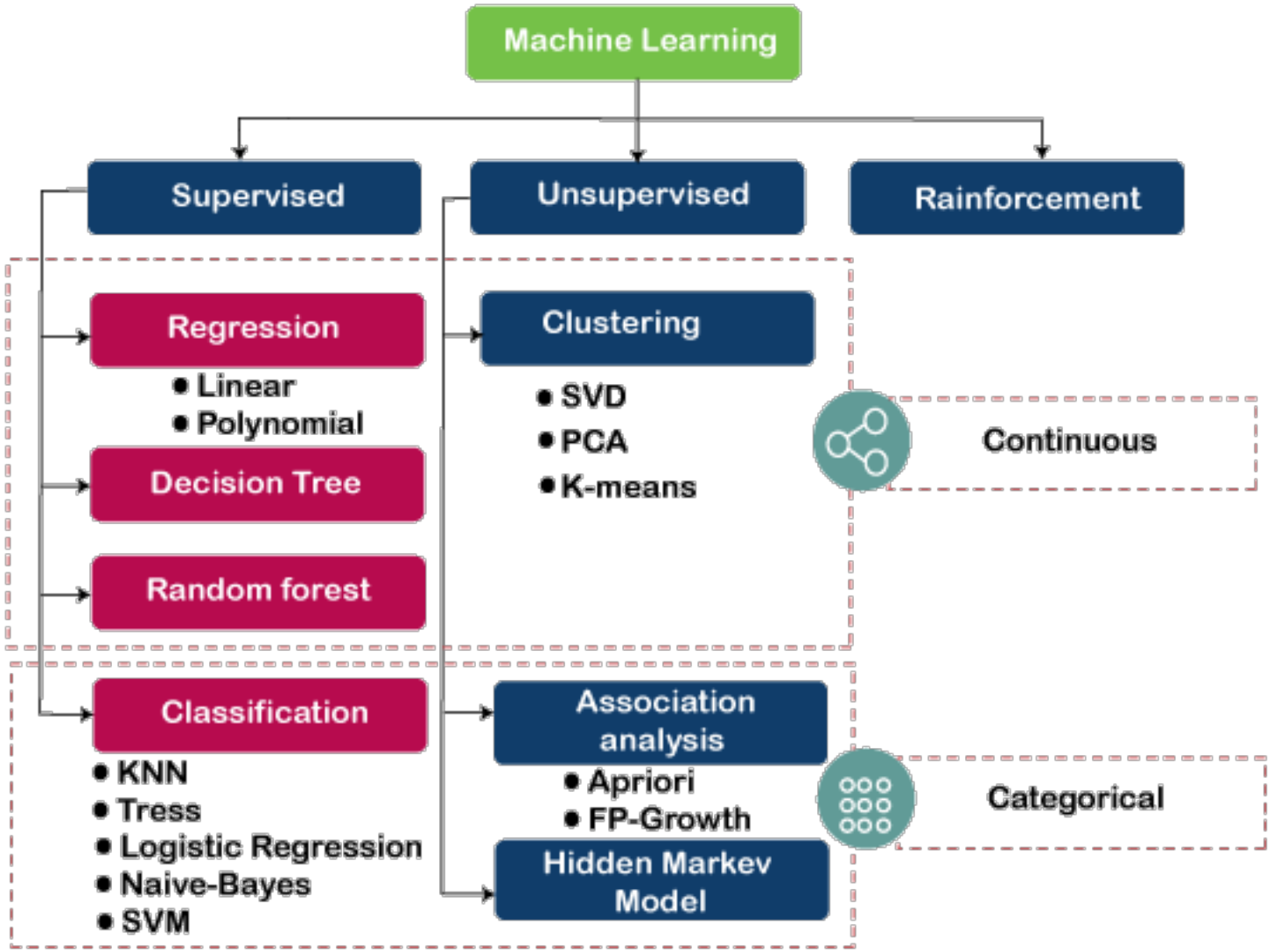
03 Feature Engineering

- What is a **feature**?
  - A feature is an individual measurable property of a phenomenon being observed
- Our inputs are represented by a set of features.
- To classify spam email, features could be:
  - Number of words that have been ch4ng3d like this.
  - Language of the email (0=English,1=Spanish)
  - Number of emojis

03 Feature Engineering

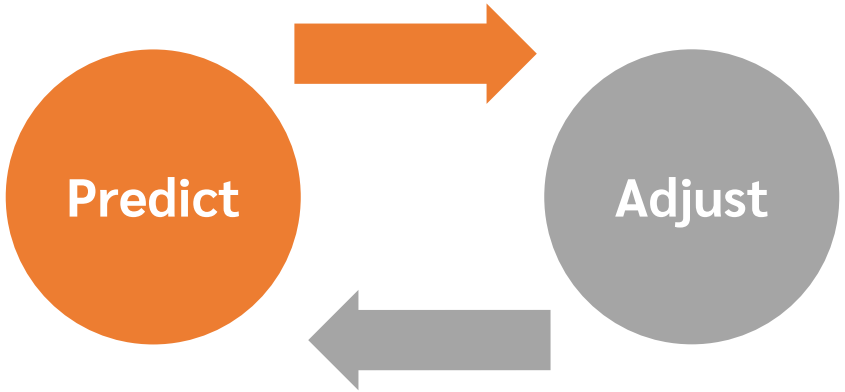
- Extract more information from existing data, not adding "new" data
  - Making it more useful
  - With good features, most algorithms can learn faster
- It can be an art
  - Requires thought and knowledge of the data
- Two steps:
  - Variable transformation (e.g., dates into weekdays, normalizing)
  - Feature creation (e.g., n grams for texts, if word is capitalized to detect names, etc.)

04 Algorithm Selection & Training



04 Algorithm Selection & Training

- Goal of training : making the correct prediction as often as possible
  - Incremental improvement:



  - Use of metrics for evaluating performance and comparing solutions
  - Hyperparameter tuning : more an art than a science

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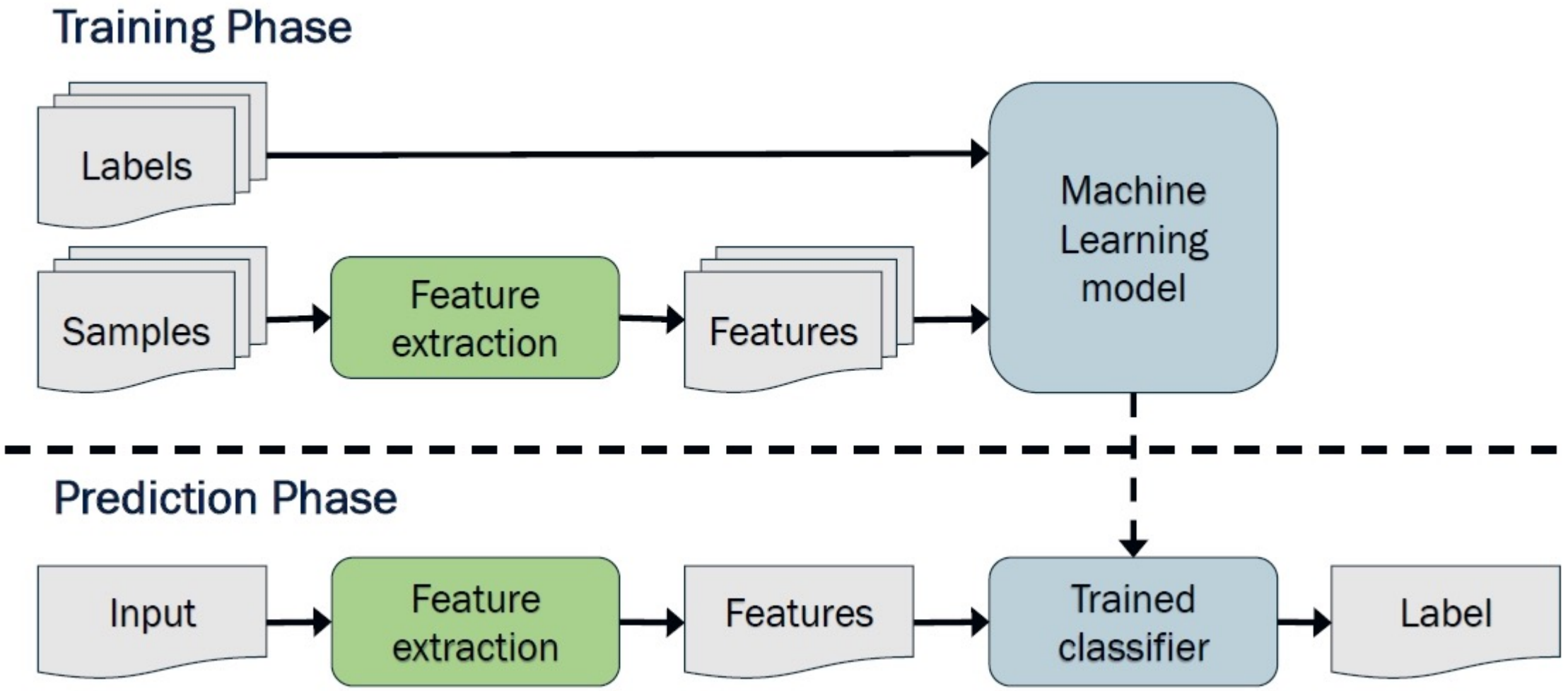
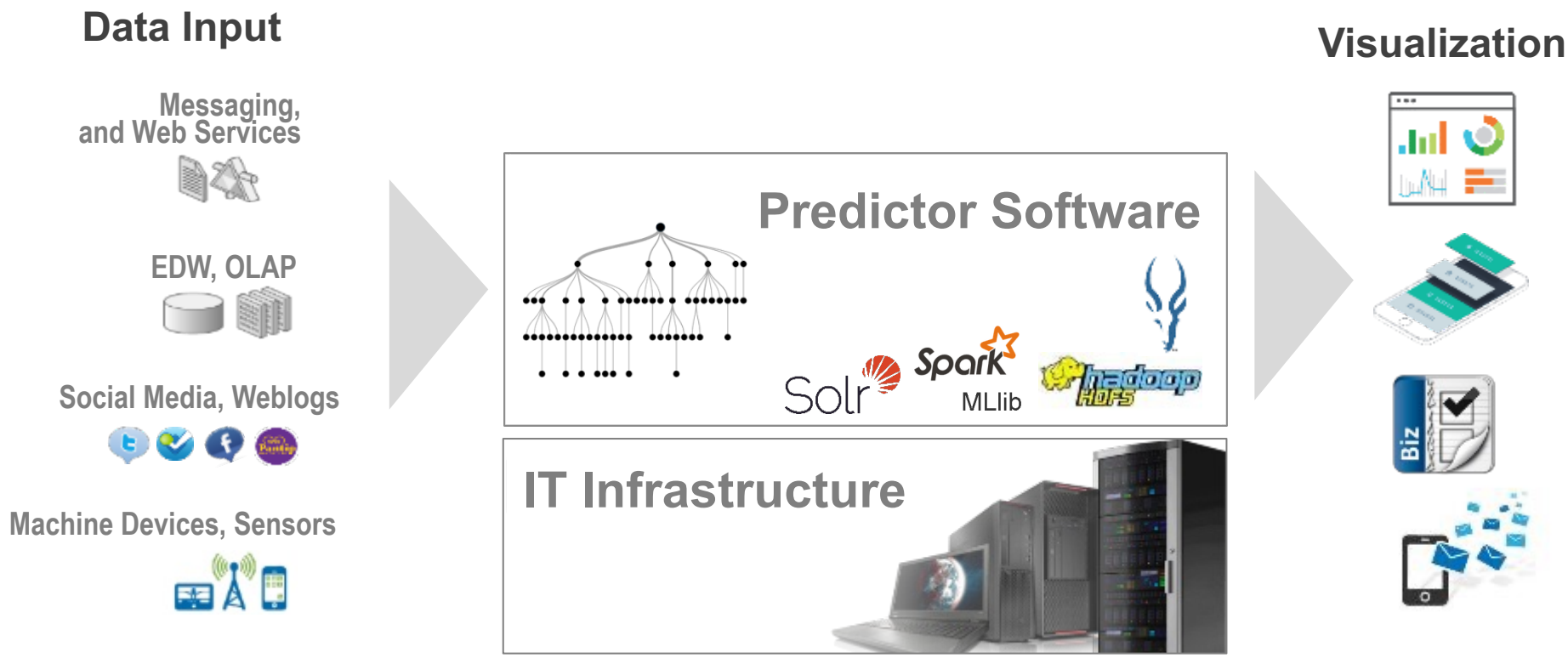
05 Making Predictions

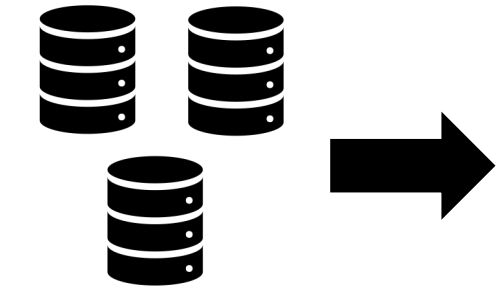


Implementation and Deployment



Model Evaluation

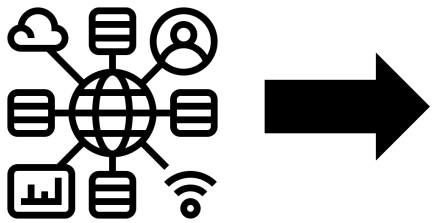
Machine Learning Model



Training data

(Should be) Good performance

The model is optimized toward training data



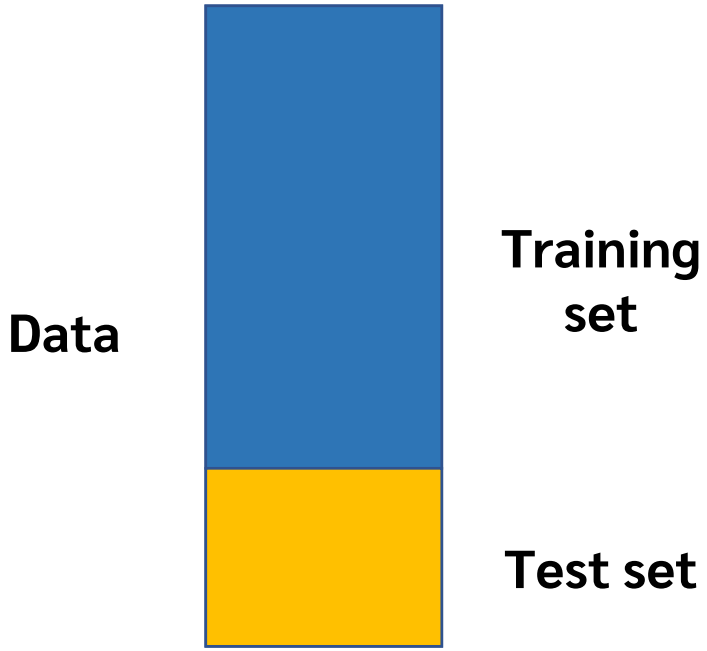
Real world data

(Hopefully) Good performance

Ideally the model should perform well on unseen data as well

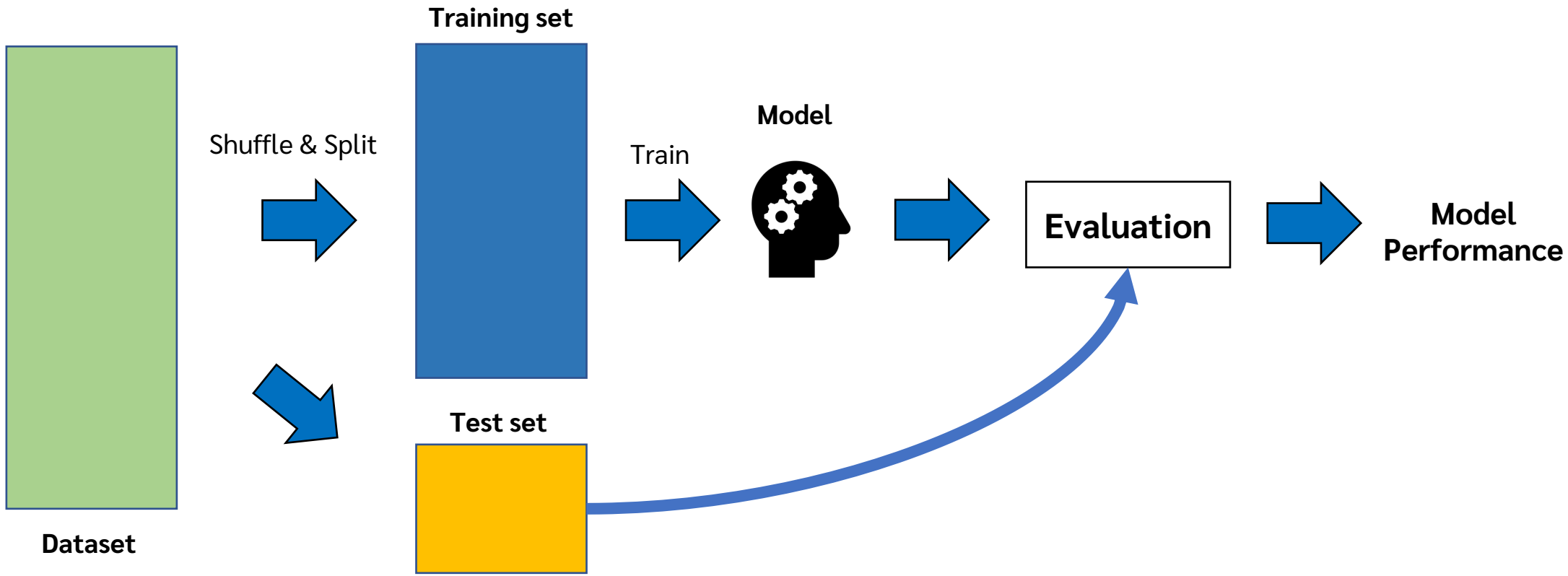
Evaluating a Model: Training Data and Test Data

- In the most basic machine learning project, we shuffle the data and split them into a training set and a test set
- A training set is used to **train** the model – creating a mathematical equations and/or adjusting the model's parameters so that it can best predict
- A test set is used to represent **unknown** data



Basic Model Evaluation

- The model is trained with training data set and evaluated with test dataset



Hands-on Example: kNN Classification Model

k-Nearest Neighbors classifier (kNN)

- **The idea**: similar data points are likely to be of the same type.
- We infer a class of a data point from its ***k* most similar** data
- How do we find the "most similar" (nearest) data points?
  - There are many way of measuring the distance between data point. One frequently discussed method is the Euclidean distance.
  - Euclidean distance – a distance between 2 points in cartesian coordinates

$$Euclidean\ Distance = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

- Basically asking, "**By looking at k data points that are most similar to me, which class am I most likely to be in?**"

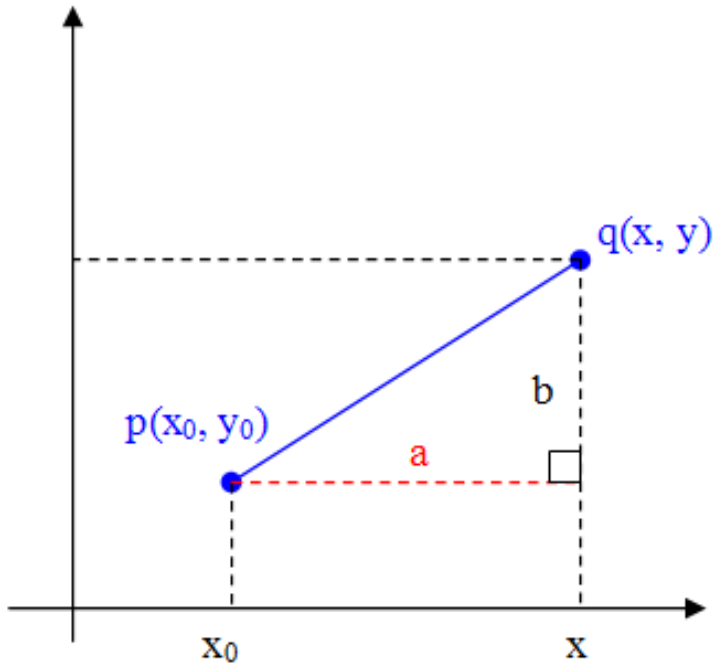


Figure from Illuyanka (https://commons.wikimedia.org/wiki/File:Dot_Product.svg)

k-Nearest Neighbors classifier (kNN)

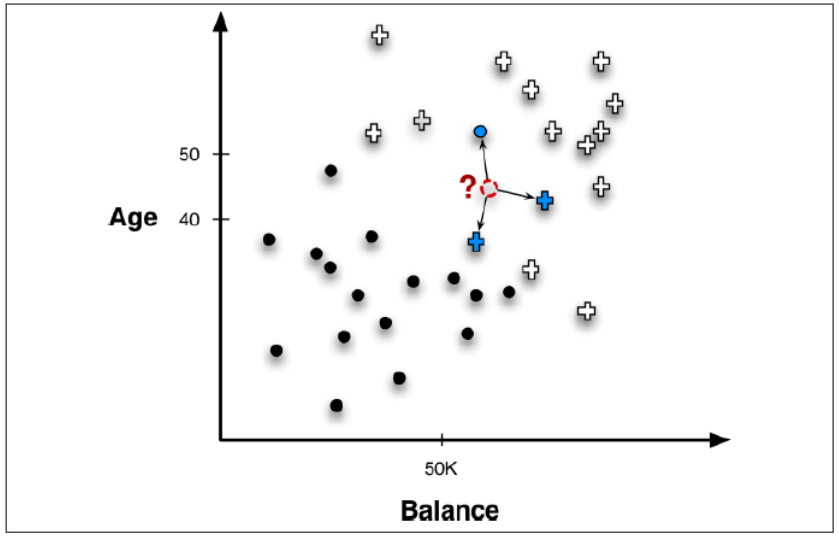
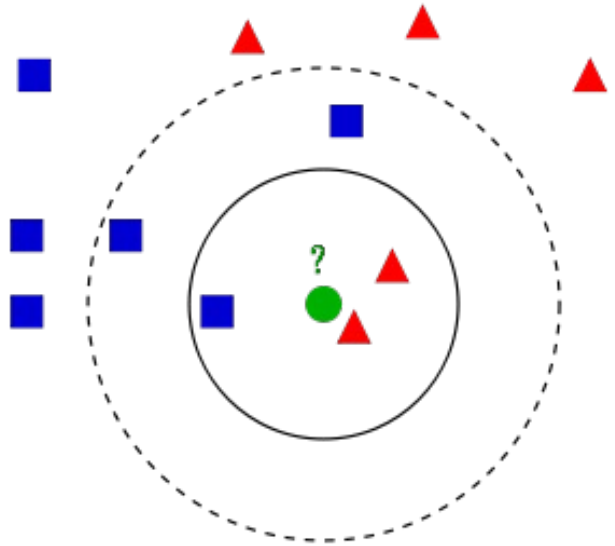


Figure 6-2. Nearest neighbor classification. The point to be classified, labeled with a question mark, would be classified + because the majority of its nearest (three) neighbors are +.

- Observes k closest data point and decide the class of data points by voting.
- Usually, k is chosen as an odd number (why?)



- The choice of ***k*** matters!
- Different number of k can result in different predictions
- Feature scale matters!

Figures from Data Science for Business by Foster Provost & Tom Fawcett and Antti Ajanki AnAj (https://commons.wikimedia.org/wiki/File:Dot_Product.svg)

k-Nearest Neighbors classifier (kNN)

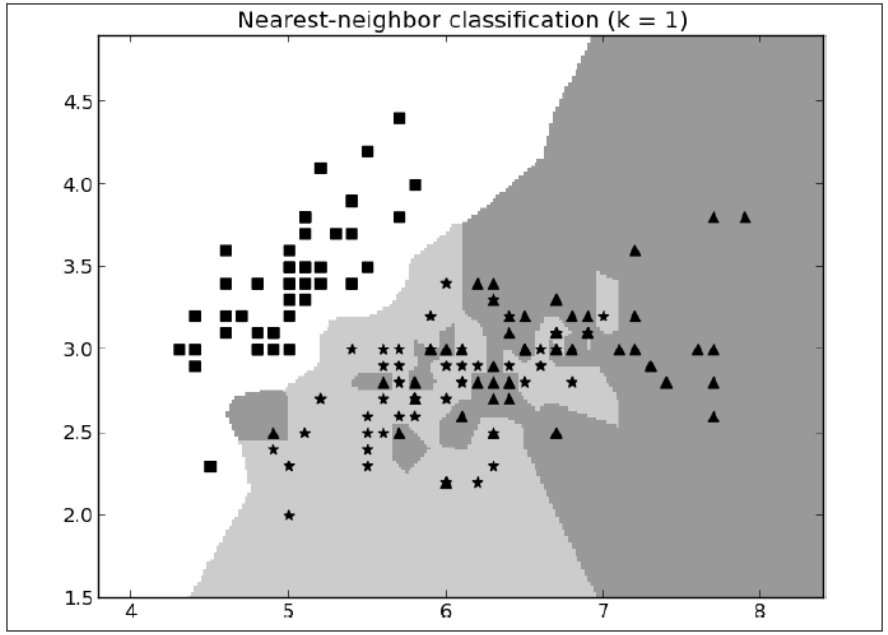


Figure 6-4. Classification boundaries created on a three-class problem created by 1-NN (single nearest neighbor).

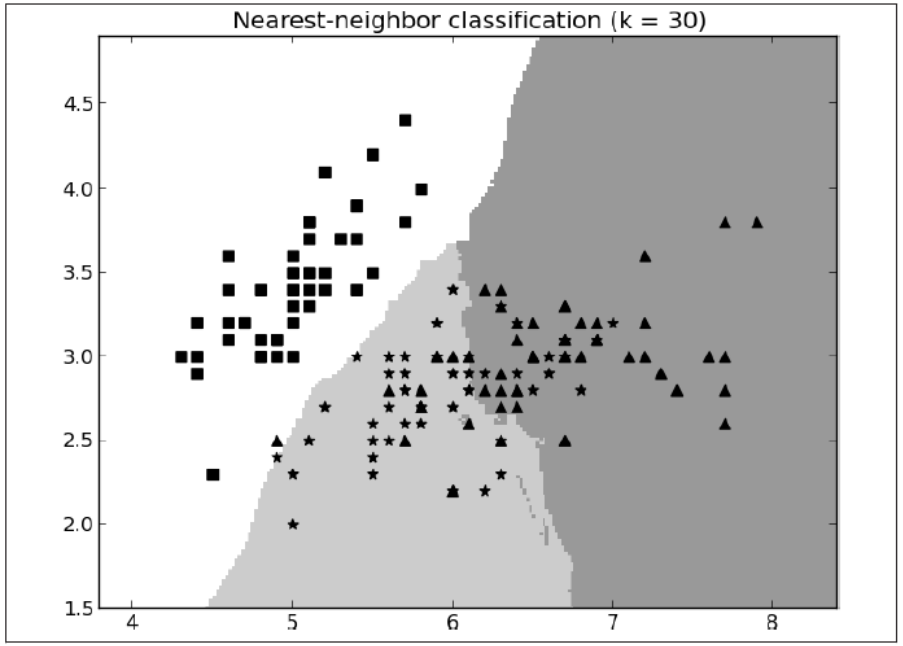


Figure 6-5. Classification boundaries created on a three-class problem created by 30-NN (averaging 30 nearest neighbors).

kNN models with a small *k*

- A finer granularity separation boundaries
- More susceptible to the presents of outlier.

kNN models with a large *k*

- More tolerant to noise
- Smooth but coarser separation boundaries

Figures from Data Science for Business by Foster Provost & Tom Fawcett

kNN Example

- Colab!
- Tutorial – kNN
- Short Exercise: K-Nearest Neighbors (K-NN)

Break
See You around 10:50am

Model Evaluation (Cont.)

Making Adjustment: Hyperparameters Tuning

- Aside from selecting appropriate models for a problem, a data scientist will also need to properly configure and adjust their model to be most suitable for tasks assigned.
- Each machine learning model has their own parameters that need to be set before prior to the start of the model training (can think of it as we configure the “settings” of the model)
  - These parameters values are called **hyperparameters**
- Think of a model as a food. Even if using the same ingredient (data) but the difference in seasoning (parameters adjustment) can affect how good it taste.
  - Hyperparameter tuning can sometimes provide a noticeable improvement in a model performance.
- The process of tuning hyper parameters allows us to obtain the most optimal setting for a model that can maximize our model’s target.

A Situation: Tuning the Hyperparameters

- For this example, let's say we are developing a classification model (or any model) and we are trying to adjust the parameters to maximize the model's performance in real scenario.
- How do we select appropriate values for hyperparameters?

Method 1:

- Try multiple different values for hyperparameters and pick the one that performs the best for the training data
- How is this method?
  - Overly simple and probably not generalizable

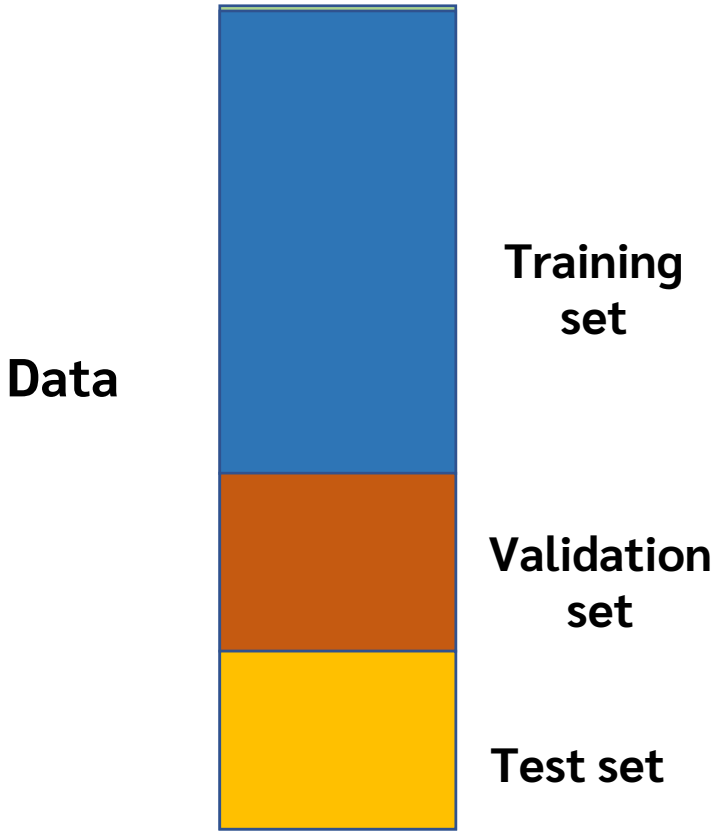
Let’s change the method

Method 2:

- Alternatively, we can try to adjust the model parameters in a way that they maximize the model’s performance on the test data
- How is this method?
  - It’s wrong! … but why?
- By doing so, data in the test dataset is no longer representing “**unknown**” data
  - In fact, the test set now also becomes part of the training data
- This may result in an unfair evaluation of the model performance and can cause the model to *overfit* to the test dataset.

The Correct Way: Holdout Method

- To properly perform hyperparameter tuning and model evaluation, we need to hold an additional portion of data out for final evaluation
- Hence, the data is split into 3 sets instead of 2
  - The training set is used to train the model.
  - The validation set is then used to tune the parameters
  - Finally, the test set (holdout set) is used to perform final evaluation of the model performance



The Holdout Method

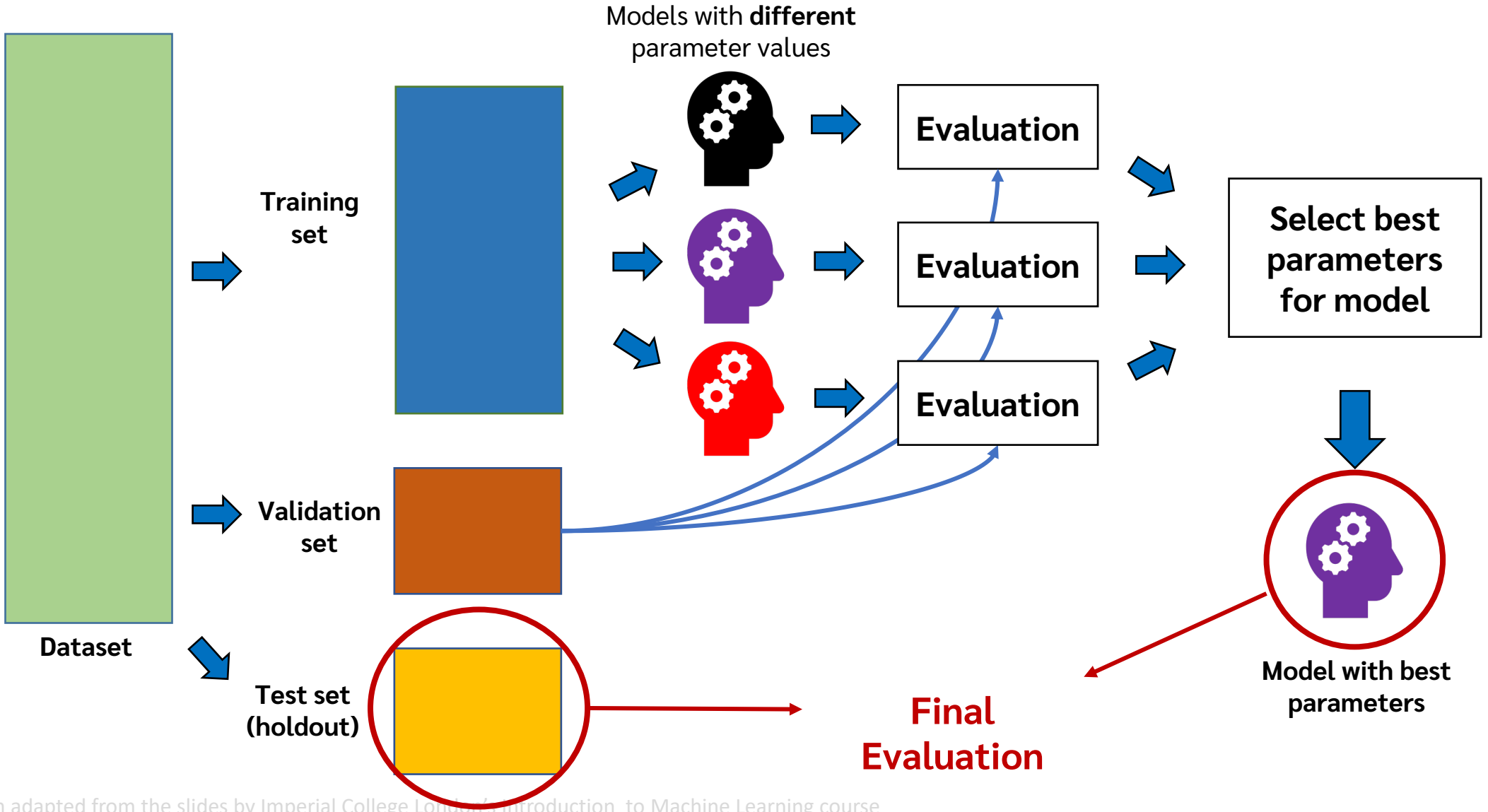


Diagram adapted from the slides by Imperial College London's Introduction to Machine Learning course

The Holdout Method (Cont.)

- Once the model with the best parameters is obtained, we can either
  - Use test set to evaluate it right away
  - Or, combine training and validation set and use them to retrain the model before evaluating with the test set

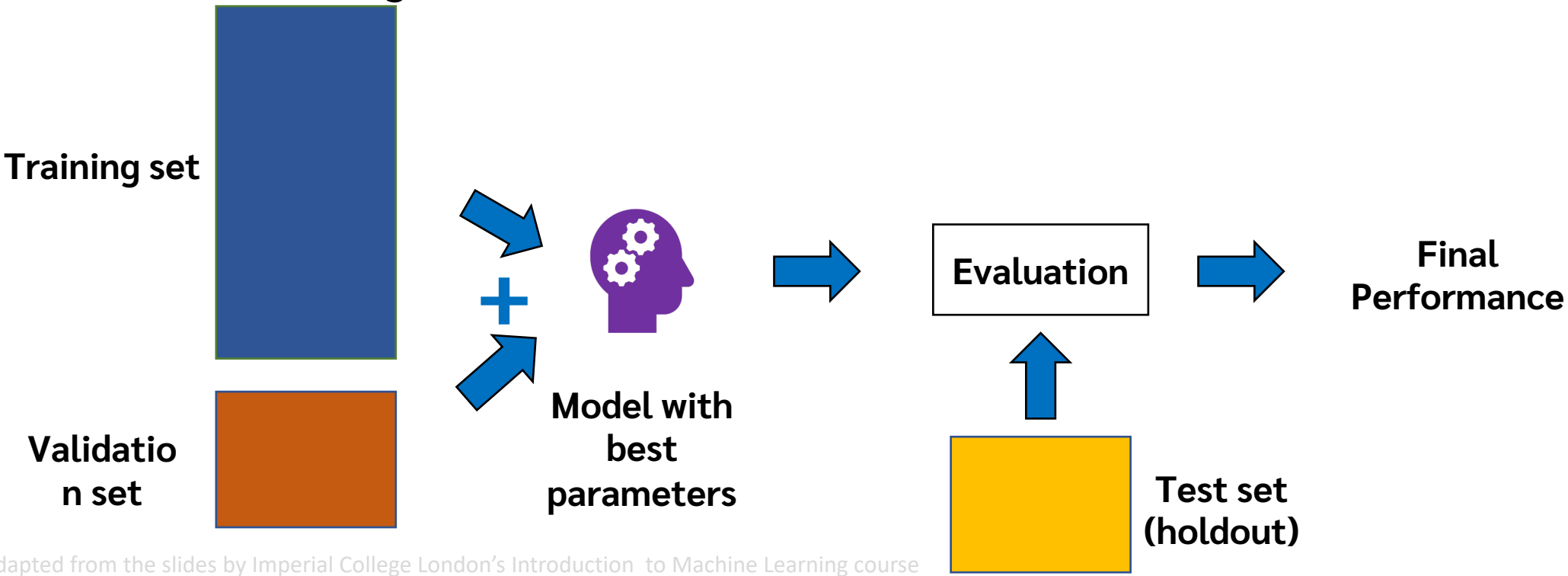
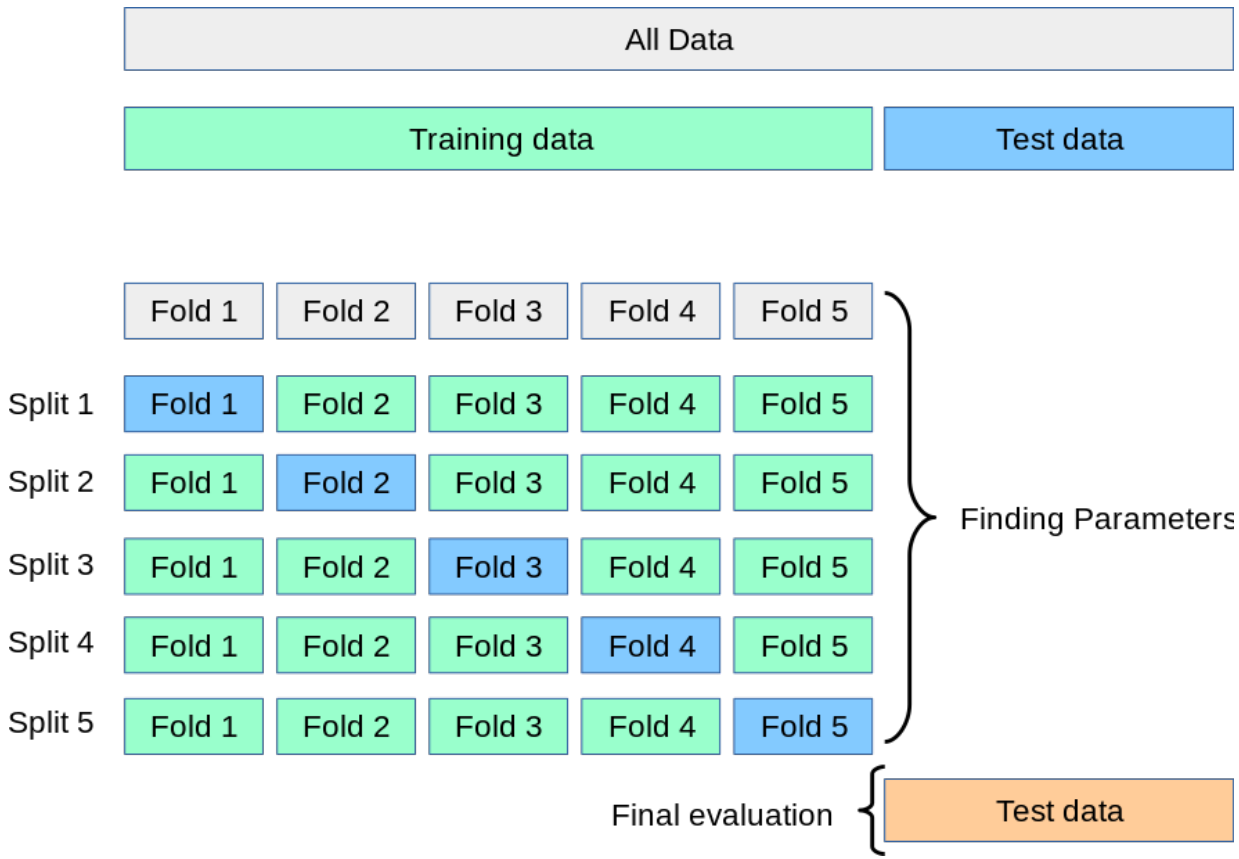


Diagram adapted from the slides by Imperial College London's Introduction to Machine Learning course

Alternative: Cross-validation

- K-fold cross validation splits data into **K folds** (without overlap)
- In each iteration, one of the folds is used as test data and the rest as training + validation data
- Provide us with average accuracy of the model and parameters that perform the best on average

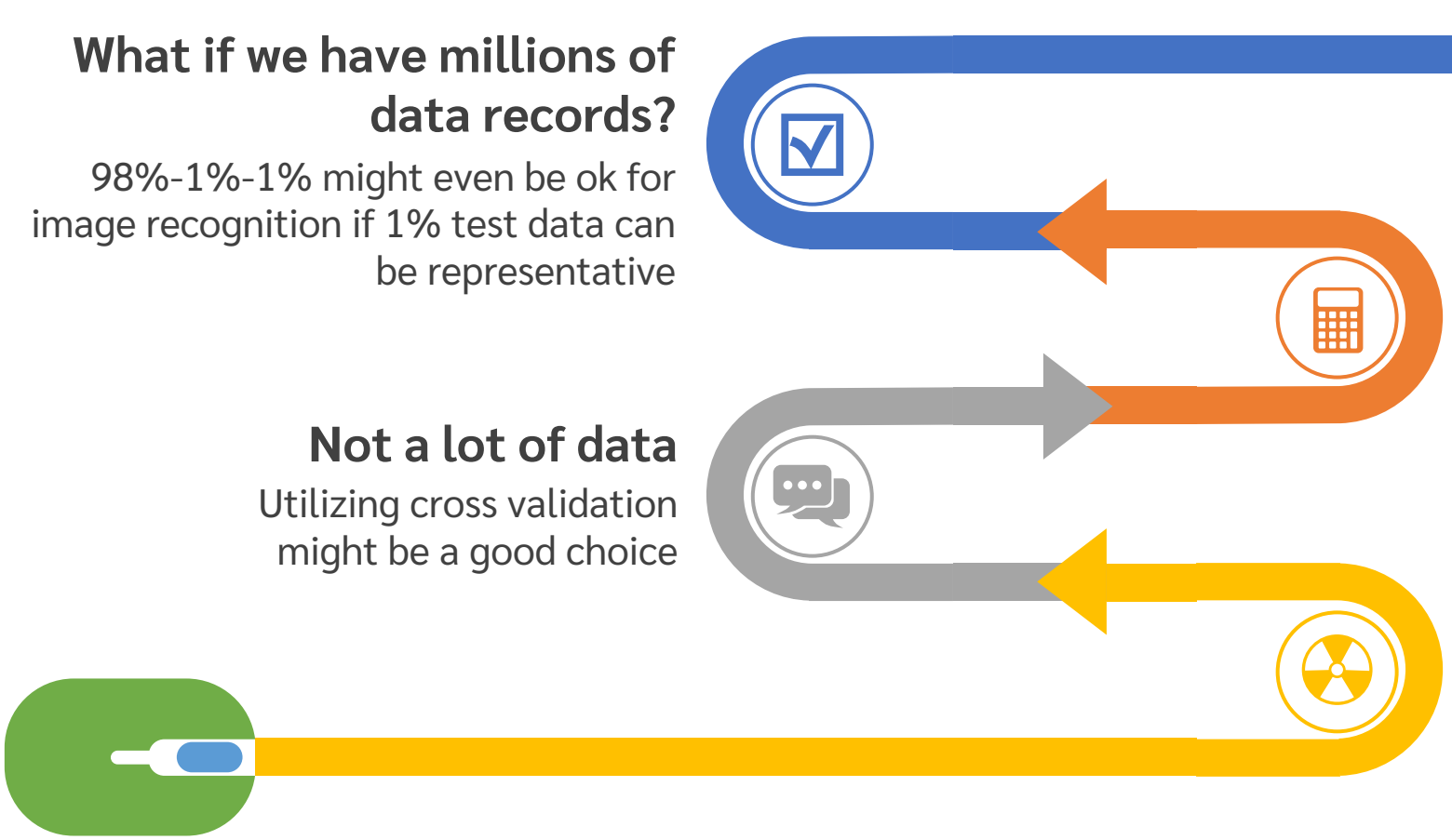


When should you use each method?

What if we have millions of data records?

98%-1%-1% might even be ok for image recognition if 1% test data can be representative

That being said, the ratio also depends on data size and types of applications



How much should be in a training net and test set?

Normally, Train-Validation-Test ratio is 70%-15%-15% or 60%-20%-20% or 80%-10%-10%

Not a lot of data

Utilizing cross validation might be a good choice

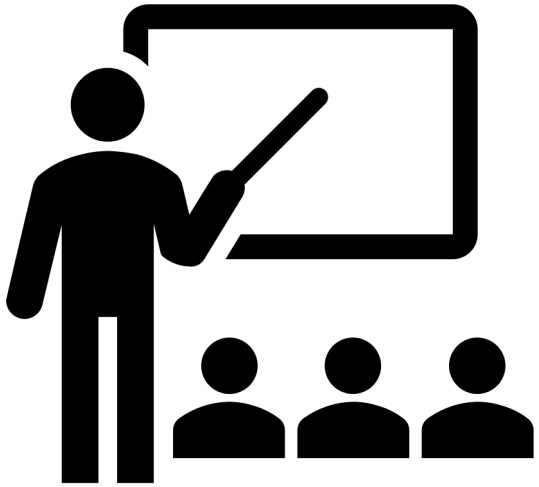
If we have a lot of data available

Hold out method might be appropriate

Model Evaluation Metrics

The Situation

- You're hiring a 3rd party contractor to develop a machine learning model for your organizations (for this purpose, let's say it's a classification problem).
- The contractor go and develop model for a while, then come back and claim their model can achieve a **95%** accuracy on the problem assigned.



Is this model good?

Their Confusion Matrix: What's Wrong?

	True 1	True 0
Predicted 1	0%	2%
Predicted 0	3%	95%

What if

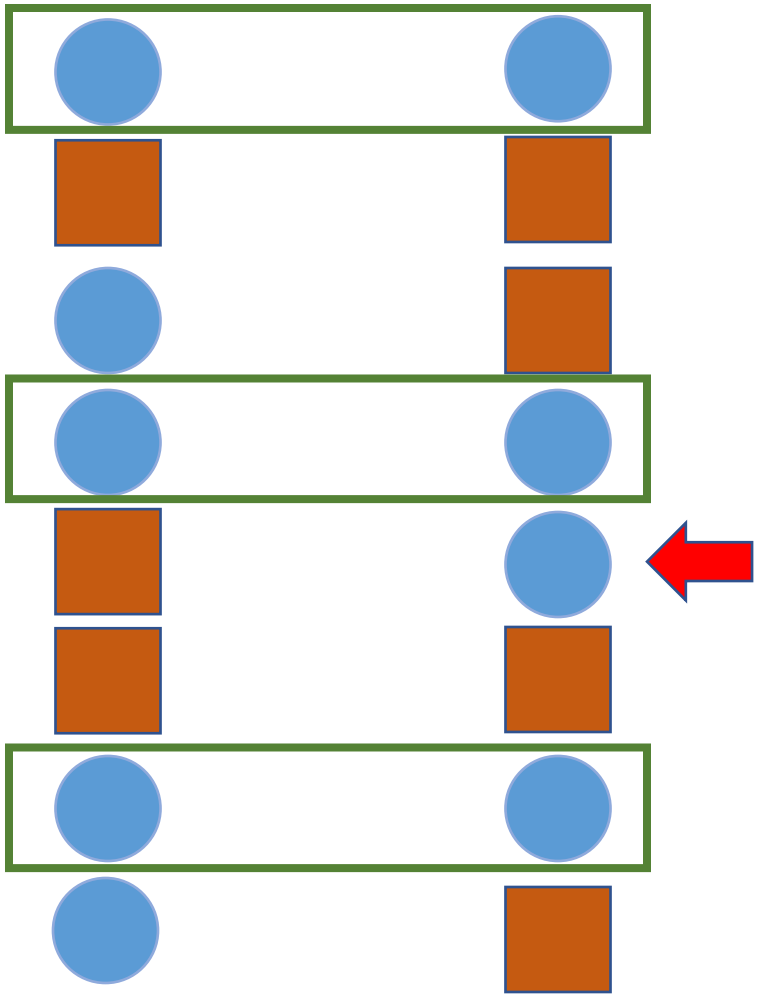
- The data is skewed (majority of people is in one class)
  - Ex. Fraud detection – very small fraction of people commits fraud
- We only care about one type of prediction
  - Ex. Advertisement target – the main concern is whether we can advertise successfully or not
- Is accuracy an appropriate metric?
- How do we evaluate the model?

Getting a Clearer Picture: Confusion Matrix

- For a binary classification problem, there are 4 possible outcomes for a prediction.

		True Label: Positive	True Label: Negative
Predicted Label	**Positive**	True Positive	False Positive
	Negative	False Negative	True Negative

Getting a Clearer Picture: Confusion Matrix



- For a binary classification problem, there are 4 possible outcomes for a prediction.

Target of Interest (True)

Predicted Label \ True Label	Positive	Negative
Positive	3	1
Negative	2	2

Precision

- Precision a fraction of positive target class predicted correctly out of all available target classes.
- In other words, “how many of **target** class did we manage to predict correctly”
- $\boldsymbol{Precision} = \frac{TP}{TP+FP}$

$$\mathbf{Accuracy} = ?$$
$$\mathbf{Precision} = ?$$

Predicted Label \ True Label	Positive	Negative
Positive	3	1
Negative	2	2

Precision

- Precision a fraction of positive target class predicted correctly out of all available target classes.
- In other words, “how many of **target** class did we manage to predict correctly”
- $\boldsymbol{Precision = \frac{TP}{TP+FP}}$

$$\mathbf{Accuracy} = \frac{\mathbf{3+2}}{\mathbf{8}} = \frac{\mathbf{5}}{\mathbf{8}} = \mathbf{62.5\%}$$

$$\mathbf{Precision} = \frac{\mathbf{3}}{\mathbf{3+1}} = \frac{\mathbf{3}}{\mathbf{4}} = \mathbf{75\%}$$

Predicted Label \ True Label	Positive	Negative
Positive	3	1
Negative	2	2

Recall

- Recall is a fraction of positive target classes predicted correctly within all predictions.
- In other words, “how many of our **target** prediction is correct?”
- $Recall = \frac{TP}{TP+FN}$

$$\mathbf{Recall} = ?$$

Predicted Label \ True Label	Positive	Negative
Positive	3	1
Negative	2	2

Recall

- Recall is a fraction of positive target classes predicted correctly within all predictions.
- In other words, “how many of our **target** prediction is correct?”
- $Recall = \frac{TP}{TP+FN}$

$$\textbf{Recall} = \frac{\mathbf{3}}{\mathbf{3+2}} = \frac{\mathbf{3}}{\mathbf{5}} = \mathbf{60\%}$$

Predicted Label \ True Label	Positive	Negative
Positive	3	1
Negative	2	2

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Precision vs. Recall

- Should we focus on precision or recall?
- Case 1: We're building a model to detect cancer?
  - If we focus on precision, are we taking a chance of letting cancer patients go untreated?
  - If we focus on recall, are we wasting people money and scaring them unnecessarily?
- Case 2: We're building a model to predict the likelihood that a loan applicant will pay back the loan on time?
  - If we focus on precision, are we missing out on income opportunities?
  - If we focus on recall, are we making poor decisions?
- A lot of times, this kind of decision is hard to judge

F1 (and F-Beta)

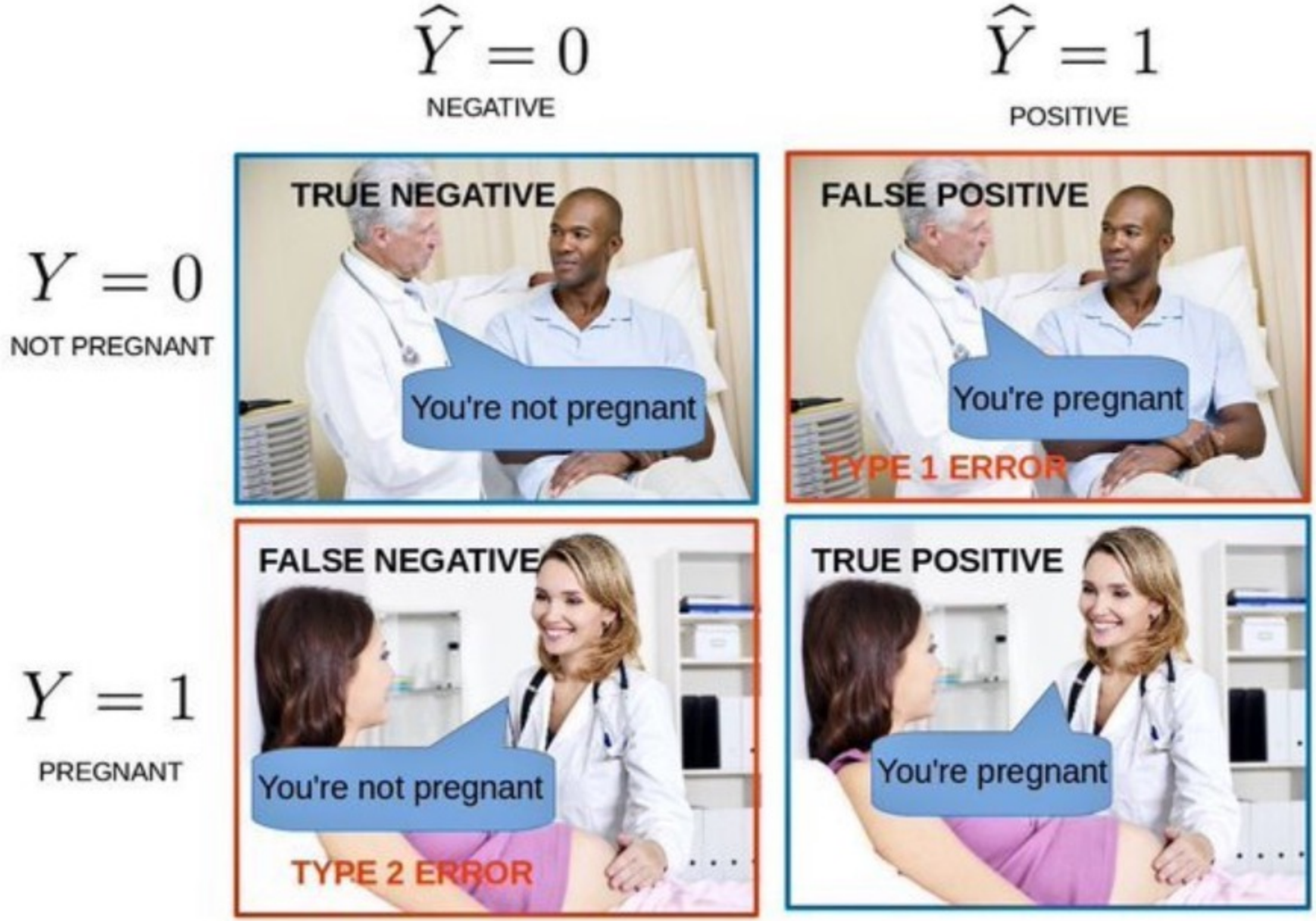
- F1 score is computed as a harmonic mean of precision and recall

$$F1 = 2 \times \frac{Precision \times Recall}{Precision + Recall}$$

  - It gives precision and recall equal importance.
- What if we don't weight each precision and recall equally?

$$F_\beta = (1 + \beta^2) \frac{Precision \times Recall}{\beta^2 Precision + Recall}$$

  - β is a measure specifying that Recall is β times as important as Precision
- Getting the right weight for β is hard.


$\widehat{Y} = 0$
NEGATIVE
$\widehat{Y} = 1$
POSITIVE
$Y = 0$
NOT PREGNANT
$Y = 1$
PREGNANT
TRUE NEGATIVE
You're not pregnant
FALSE POSITIVE
You're pregnant
TYPE 1 ERROR
FALSE NEGATIVE
You're not pregnant
TYPE 2 ERROR
TRUE POSITIVE
You're pregnant

Evaluating cost-benefit: Expected Value

- The **expected value (EV)** is the anticipated outcome value of a situations.
- EV is computed by calculated a weighted average of all possible outcome value, i.e. it is a sum of outcome values weighted by their respective probability

$$EV = prob(o_1) \times value(o_1) + prob(o_2) \times value(o_2) + \cdots$$

  - where $o_1, o_2, \ldots$ are possible outcomes of a situation
- The probability of each outcome can usually be approximated from data
- The values of outcomes are often harder to estimate and may require specific business domain knowledge
- Expected value can be a useful tool for choose appropriate model for the job.

Example: Target Marketing

- A company is trying to perform targeted marketing and offer a product to consumers. If a customer buys a product, the company will gain $100 of profits. However, each product offer made to a customer will cost the company $1.
- The company then builds a model to predict if a customer will buy the product.
- In this situation, the 4 possible outcomes of the predictions are as follow.
  - True Positive – a product is offered to a customer who will buy it. Profit = $100-$1 = $99
  - False Positive – a product is offered to a customer who will not buy it. Profit (loss) = -$1
  - True Negative – a product is not offered to a customer who will not buy it. Profit = $0
  - False Negative – a product is not offered to a customer who will buy it. Profit = $0
    - This is a case of a missed opportunity, but for simplicity, we will not consider that here.

Example from Data Science for Business by Foster Provost and Tom Fawcett

Example: Target Marketing (Cont.)

- Assuming the prediction result is as shown.

Predicted Label \ True Label	Positive	Negative
Positive	56	7
Negative	5	42

- Using $EV = prob(o_1) \times value(o_1) + prob(o_2) \times value(o_2) + \cdots$

Note that the result differs from the book as the number here is not rounded until the end

Example: Target Marketing (Cont.)

- Assuming the prediction result is as shown.

Predicted Label \ True Label	Positive	Negative
Positive	56	7
Negative	5	42

Total # of test data = 56+7+5+42= 110

- Using $EV = prob(o_1) \times value(o_1) + prob(o_2) \times value(o_2) + \cdots$
- The expected value of the model (on this test data) is then

$$EV = \frac{56}{110}(99) + \frac{7}{110}(-1) + \frac{42}{110}(0) + \frac{5}{110}(0) = \$50.34$$

Note that the result differs from the book as the number here is not rounded until the end

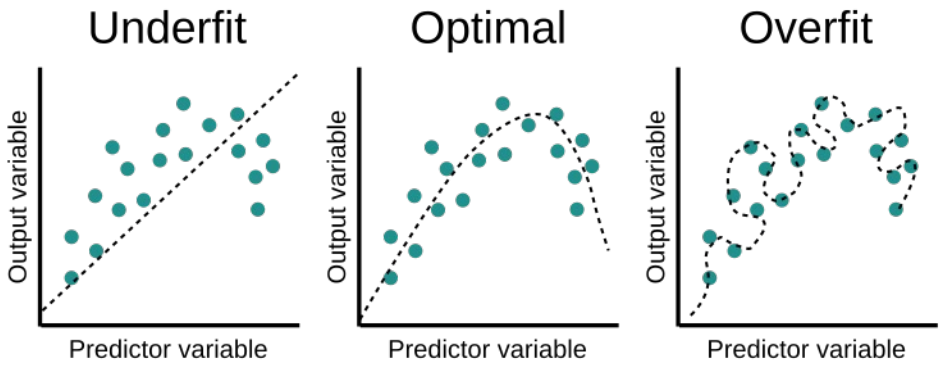
Overfitting vs. Underfitting

Overfitting

Overfitting occurs when the trained model adjust its parameters to fit the training data too well and became unable to generalize well. This behavior is observed when the model performs well with during the development with training data but performs poorly on the unseen data.

Underfitting

Underfitting happens when the trained model is unable to adjust itself to sufficiently fit the training data, resulting in poor performances overall. This behavior is observed when the model is unable to perform well even during the development with training data.



Overfitting vs. Underfitting

Possible Solution for Overfitting	Possible Solution for Underfitting
Collects more data	Increase the model complexity
Reduce number of features	Add more features
Adjust parameters to increase regularization effect	Adjust parameters to reduce regularization effect
etc.	etc.

How can we know if the model works?

- If we deploy a model and observe the improvement in our target performance, how confident can we be that the improvement is caused by the model and not just coincidence?
- We study the distribution of the model's target before and after model deployment. Then, statistical tests can be performed to show whether our target data has a change in distributions as we desired.

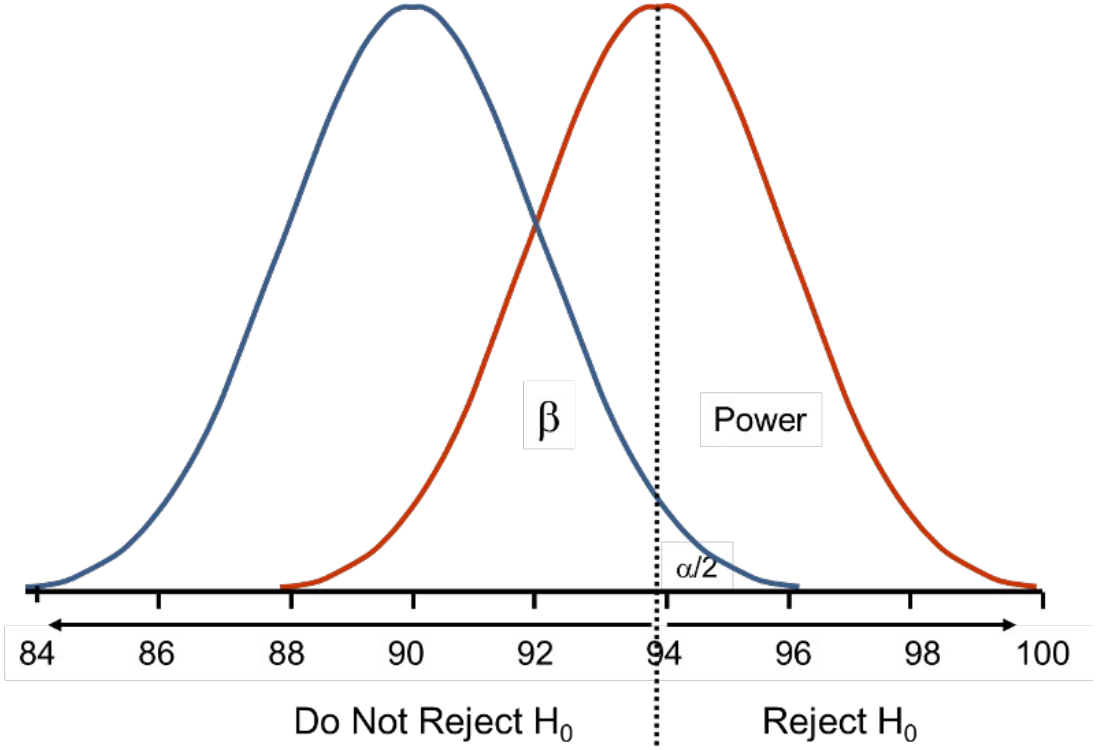


Figure from https://sphweb.bumc.bu.edu/otlt/MPH-Modules/BS/BS704_Power/BS704_Power_print.html

Thank You

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