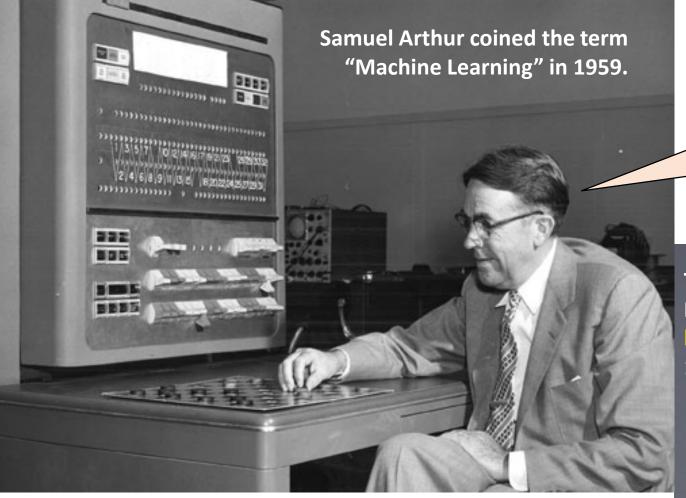
# Introduction to Machine Learning

Hiranmayi Ranganathan, LLNL June 19, 2020

### **Learning Objectives**

- What is Machine Learning?
- Main branches of Machine Learning
- Machine Learning Workflow
  - Data Collection
  - Feature Engineering
  - Training
  - Validation
  - Testing
  - Evaluation, hyperparameter tuning
- Scikit-Learn Examples (independent learning)



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

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.



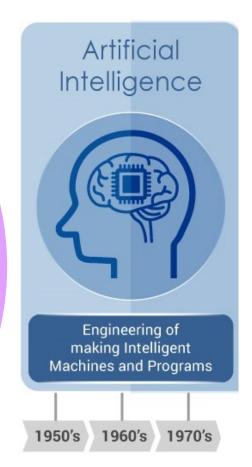
### $AI \supset ML \supset DL$

**Computer Science** 

Artificial Intelligence

Machine Learning

Deep Learning



## ARTIFICIAL INTELLIGENCE

## MACHINE LEARNING

DEEP LEARNING

"This work is really tedious, yet requires a lot of troubleshooting and problem solving. Maybe I can get a machine to do it for me."

"It's really difficult to program this computer to understand what I need it to do. Maybe it can teach itself how to do it, if I can help it along by distilling the data into the meaningful examples and exposing enough of these examples to the computer.

"I don't know the best way to distill the data into meaningful examples.

Maybe if I can give it TONS of data, it can figure out what's important from the data without my help.



50 LAZY...

### ARTIFICIAL INTELLIGENCE

1950 – Alan Turing proposes his Turing Test for intelligence.

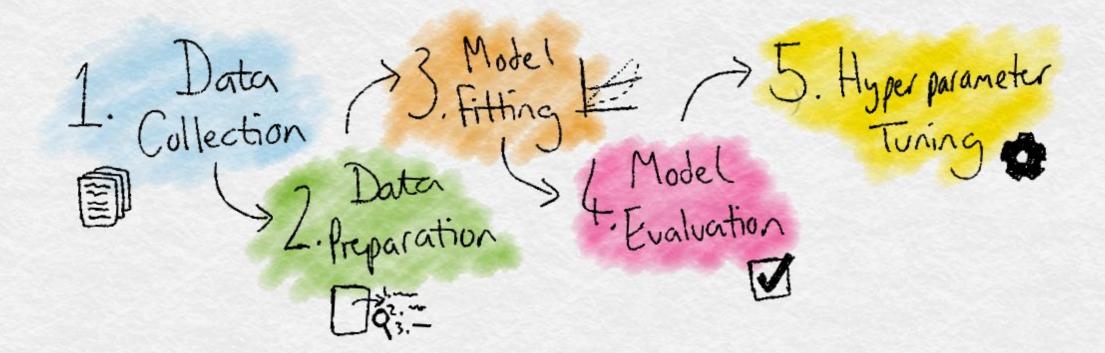
### MACHINE LEARNING

- 1952 Arthur Samuel wrote the first computer learning program.
- 1957 Frank Rosenblatt designed the first neural network.

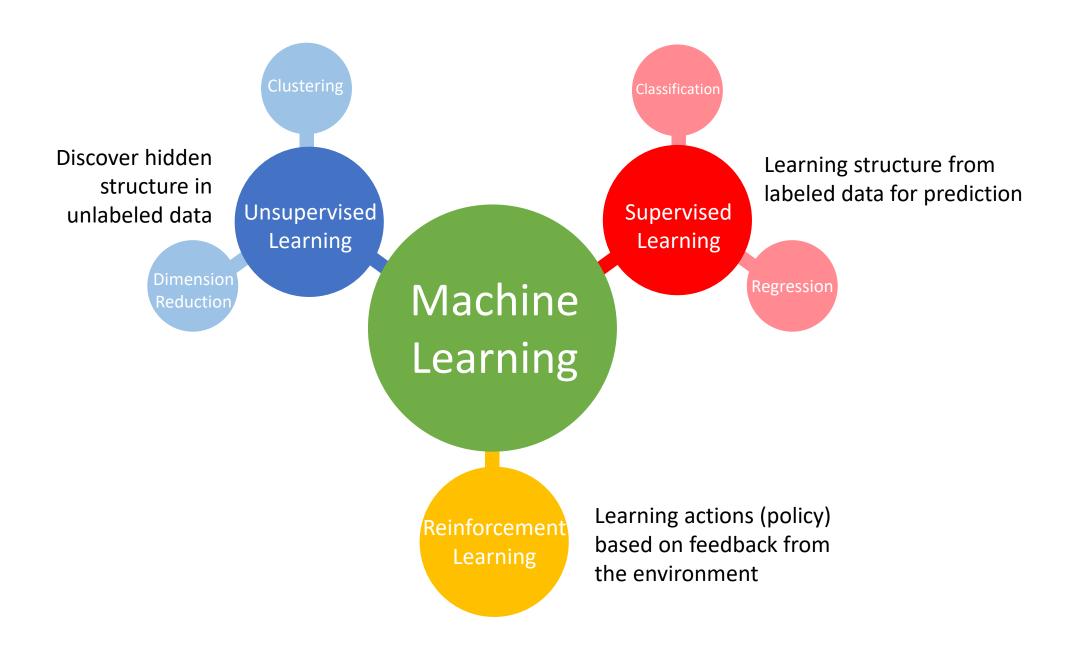
### DEEP LEARNING

- 2006 Geoffrey Hinton coins the term "Deep Learning".
- 2012 Google is able to identify videos that contain cats.
- 2014 Facebook can verify people in photos.
- 2016 Google's AlphaGo beats world champion at Go.

racera A yperparameters 3



### Machine Learning Approaches

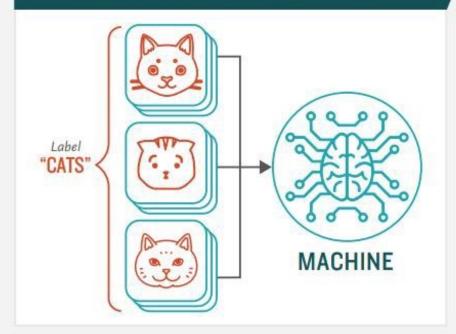


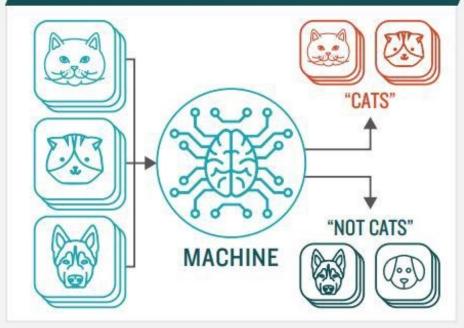
### How **Supervised** Machine Learning Works

STEPI

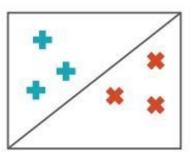
Provide the machine learning algorithm categorized or "labeled" input and output data from to learn STEP 2

Feed the machine new, unlabeled information to see if it tags new data appropriately. If not, continue refining the algorithm



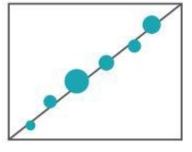


### TYPES OF PROBLEMS TO WHICH IT'S SUITED



### CLASSIFICATION

Sorting items into categories



#### REGRESSION

Identifying real values (dollars, weight, etc.)

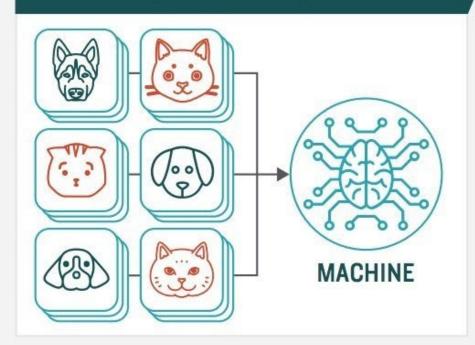
### How **Unsupervised** Machine Learning Works

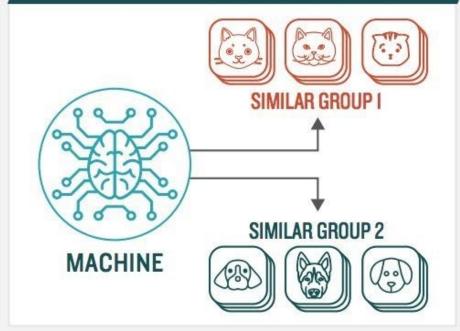
STEP I

Provide the machine learning algorithm uncategorized, unlabeled input data to see what patterns it finds

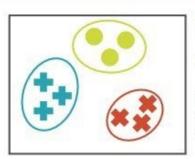
STEP 2

Observe and learn from the patterns the machine identifies





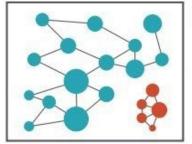
#### TYPES OF PROBLEMS TO WHICH IT'S SUITED



#### **CLUSTERING**

#### Identifying similarities in groups

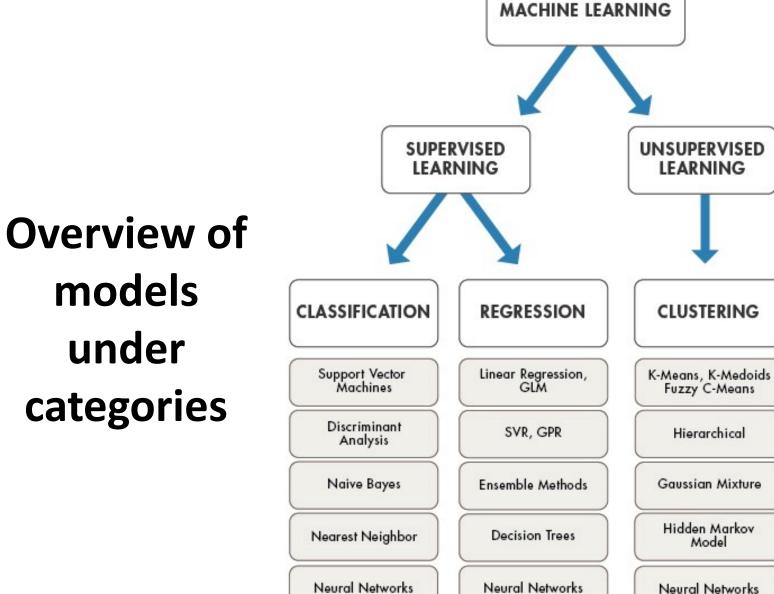
For Example: Are there patterns in the data to indicate certain patients will respond better to this treatment than others?



#### **ANOMALY DETECTION**

#### Identifying abnormalities in data

For Example: Is a hacker intruding in our network?



models

under

### How reinforcement learning works

takes Action changes-The agent's job is to take actions State is into maximize its Agent Environment cumulative rewards.  $S_{t+1}$ is represented by -is received by-State  $R_{t+1}$ is received by-Reward produces new-

The reward is a time-delayed feedback on the optimality of the agent's action.

# The ML workflow

- 1. Define the Problem appropriately
- 2. Collect Data
- 3. Choose a Measure of Success

# The ML workflow

- 1. Define Appropriately the Problem
- 2. Collect Data
- 3. Choose a Measure of Success:
- 4. Preparing The Data

# Methods of Preparing The Data

Dealing with missing data

Handling Caterogical Data

Color		Red	Yellow	Green
Red				
Red		1	0	0
Yellow		1	0	0
Green		0	1	0
Yellow		0	0	1

Feature Scaling

$$X_{changed} = rac{X - X_{min}}{X_{max} - X_{min}}$$

$$z = \frac{x - \mu}{\sigma}$$

$$\mu = Mean$$

$$\sigma =$$
 Standard Deviation

# The ML workflow

- 1. Define Appropriately the Problem
- 2. Collect Data
- 3. Choose a Measure of Success:
- 4. Preparing The Data
- 5. Splitting Data Into Subsets

Input Target  $\chi$ 

Feature engineering

 $\tilde{x} = f(x)$ 

Input Target  $\tilde{\chi}$ 

y

Raw input & target

D=(x,y)

Feature engineering

 $\tilde{x} = f(x)$ 

Processed input & target

Data

partitioning

 $\widetilde{D}=(\widetilde{x},y)$ 

Disjoint data splits

Training data

$$\widetilde{D}_{train} = (\widetilde{x}_{train}, y_{train})$$

Validation data

$$\widetilde{D}_{val} = (\widetilde{x}_{val}, y_{val})$$

Test data

$$\widetilde{D}_{test} = (\widetilde{x}_{test}, y_{test})$$

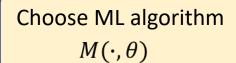
Worked out examples for studying

Practice examples to try on your own

Exam questions

# The ML workflow

- 1. Define Appropriately the Problem
- 2. Collect Data
- 3. Choose a Measure of Success:
- 4. Preparing The Data
- 5. Splitting Data Into Subsets
- 6. Training the Model





Train ML model

 $\hat{y}_{train} = M(\tilde{x}_{train}, \boldsymbol{\theta})$ 

### Disjoint data splits

#### Training data

$$\widetilde{D}_{train} = (\widetilde{x}_{train}, y_{train})$$

#### Validation data

$$\widetilde{D}_{val} = (\widetilde{x}_{val}, y_{val})$$

#### Test data

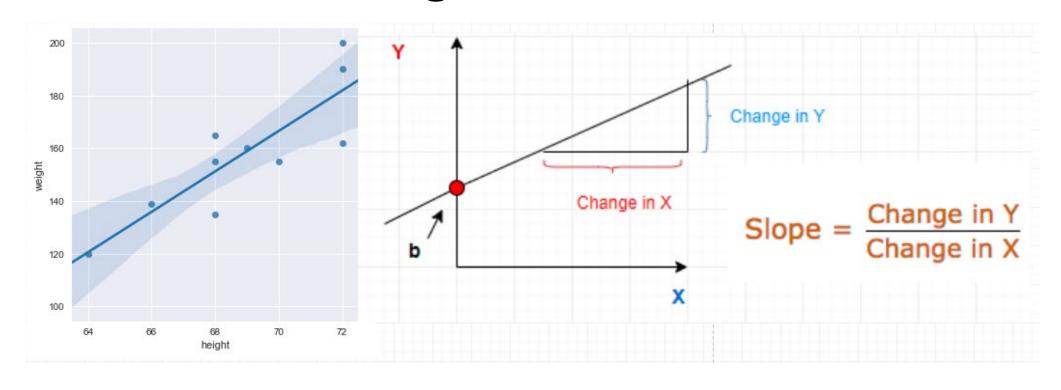
$$\widetilde{D}_{test} = (\widetilde{x}_{test}, y_{test})$$

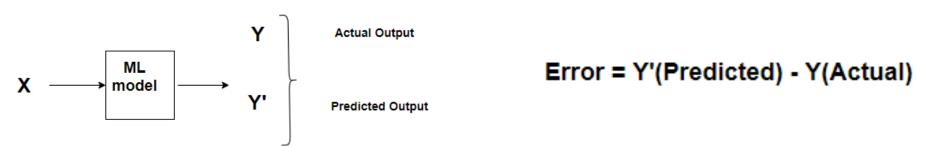
Optimize parameters  $\theta$  to minimize loss function L

$$MSE = \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}$$

$$CrossEntropyLoss = -(y_i log(\hat{y}_i) + (1 - y_i) log(1 - \hat{y}_i))$$

# A Machine Learning Model





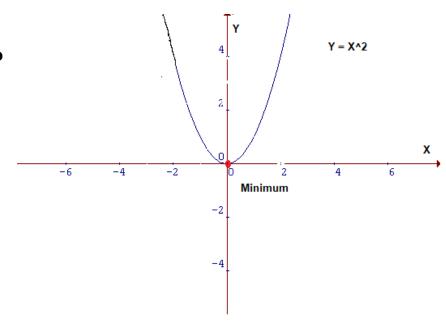
### Cost function

Let's say, there are a total of 'N' points in the dataset and for all those 'N' data points we want to minimize the error. So the Cost function would be the total squared error i.e

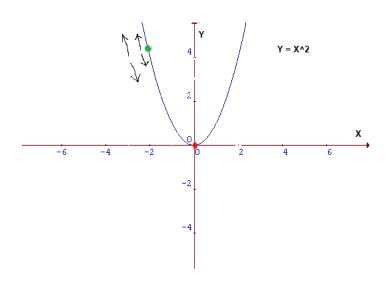
$$Cost = \frac{1}{N} \sum_{i=1}^{N} (Y' - Y)^2$$

How do we actually minimize any function?

**Cost function** is of the form  $Y = X^2$ 



### **Gradient Descent**

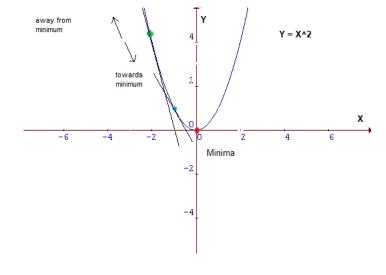


#### Possible actions would be:

- You might go upward or downward
- •If you decide on which way to go, you might take a bigger step or a little step to reach your destination.

Essentially, there are two things that you should know to reach the minima, i.e. which way to go and how big a step to take.





The slope at the blue point is less steep than that at the green point which means it will take much smaller **steps** to reach the minimum from the blue point than from the green point.

### Mathematical Interpretation of Cost Function

#### Parameters with small changes:

$$m = m - \delta m$$
  
 $b = b - \delta b$ 

Given Cost Function for 'N' no of samples

$$Cost = \frac{1}{N} \sum_{i=1}^{N} (Y_i' - Y_i)^2$$

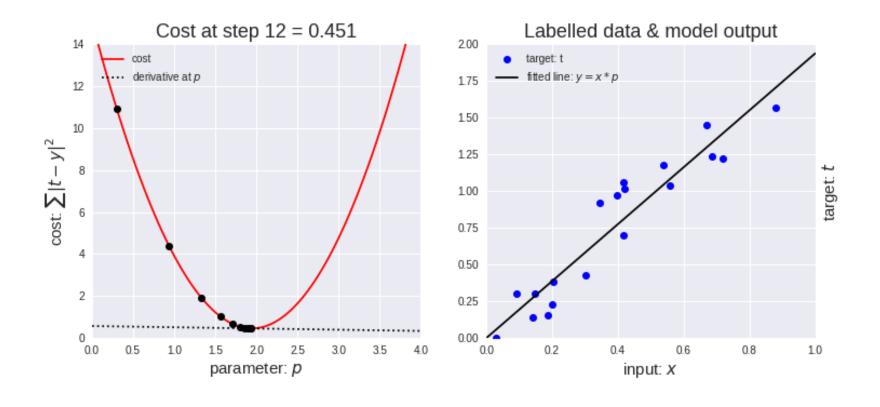
Cost function is denoted by J where J is a function of m and b

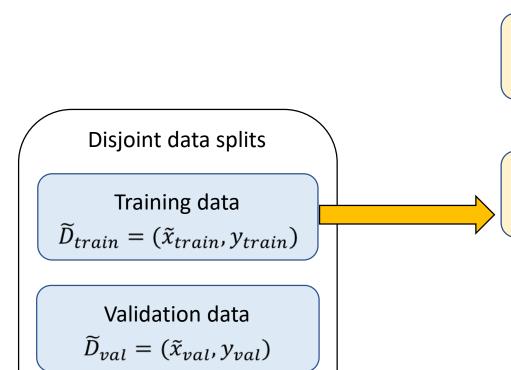
$$J_{m,b} = \frac{1}{N} \sum_{i=1}^{N} (Y_i' - Y_i)^2$$

Substituting the term Y'-Y with error for simplicity

$$J_{m,b} = \frac{1}{N} \sum_{i=1}^{N} (Error_i)^2$$

### **Gradient Descent**





Test data

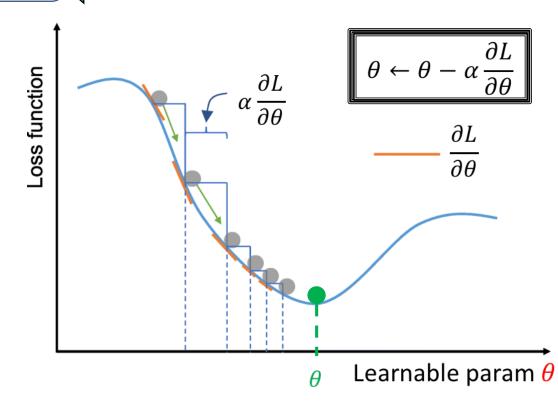
 $\widetilde{D}_{test} = (\widetilde{x}_{test}, y_{test})$ 

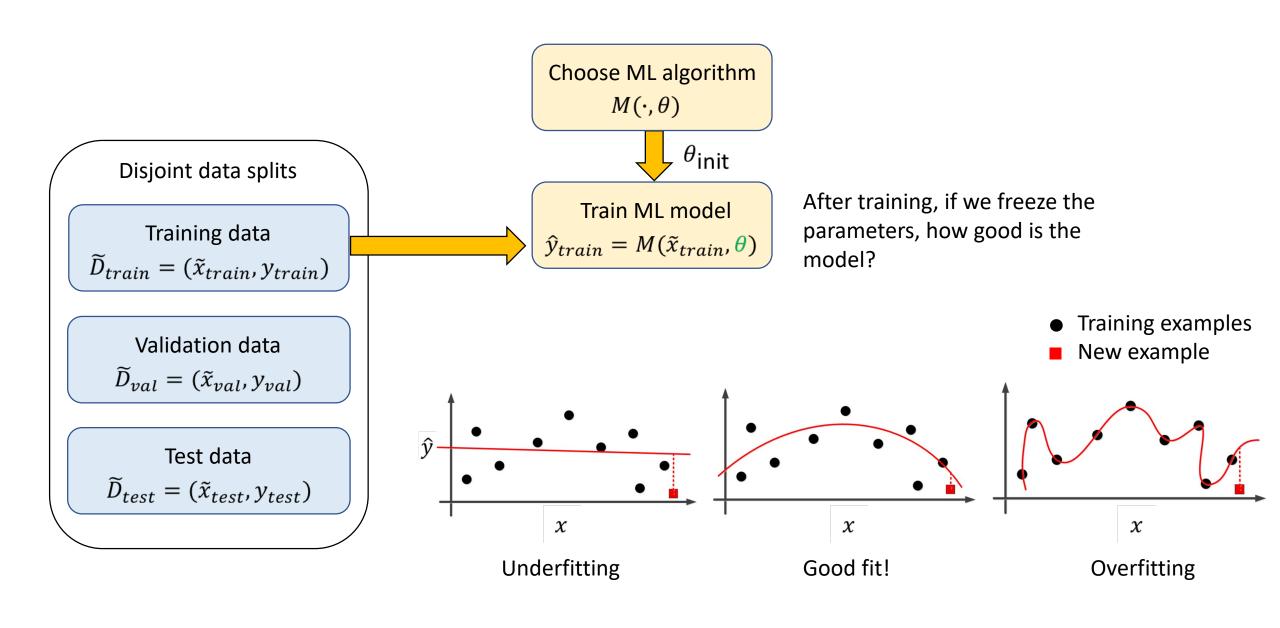
Choose ML algorithm  $M(\cdot, \theta)$ 



Train ML model  $\hat{y}_{train} = M(\tilde{x}_{train}, \theta)$ 

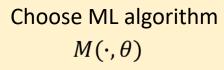
Optimize parameters  $\theta$  to minimize loss function L







Validation set





Loss

Train ML model

$$\hat{y}_{train} = M(\tilde{x}_{train}, \theta)$$



Validate ML model

$$\hat{y}_{val} = M(\tilde{x}_{val}, \theta)$$



Disjoint data splits

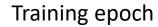
 $\widetilde{D}_{train} = (\widetilde{x}_{train}, y_{train})$ 

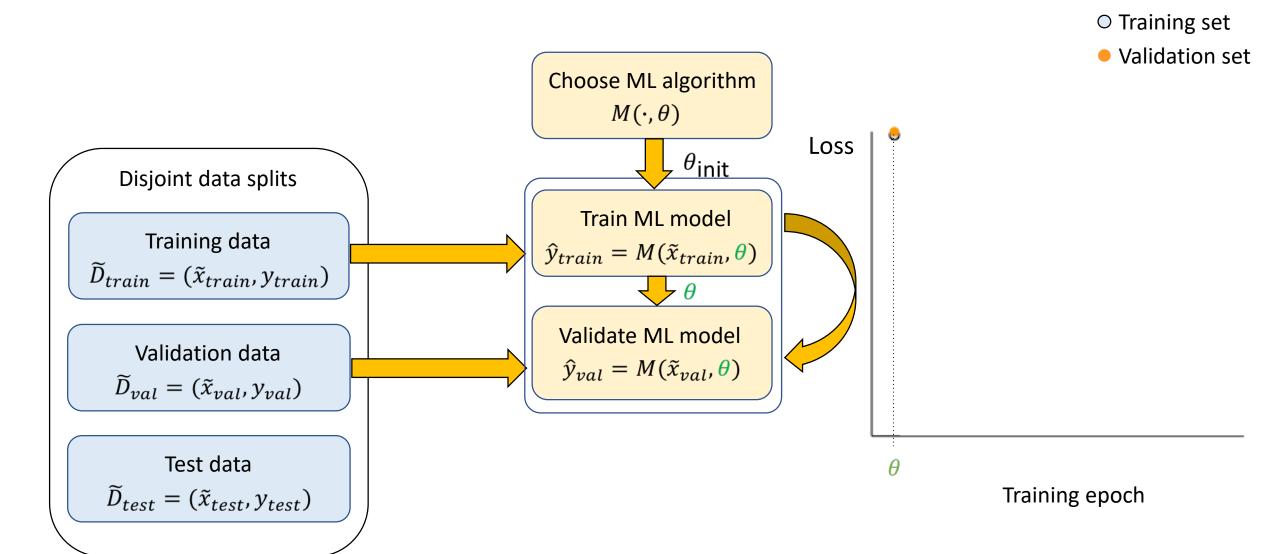
Validation data

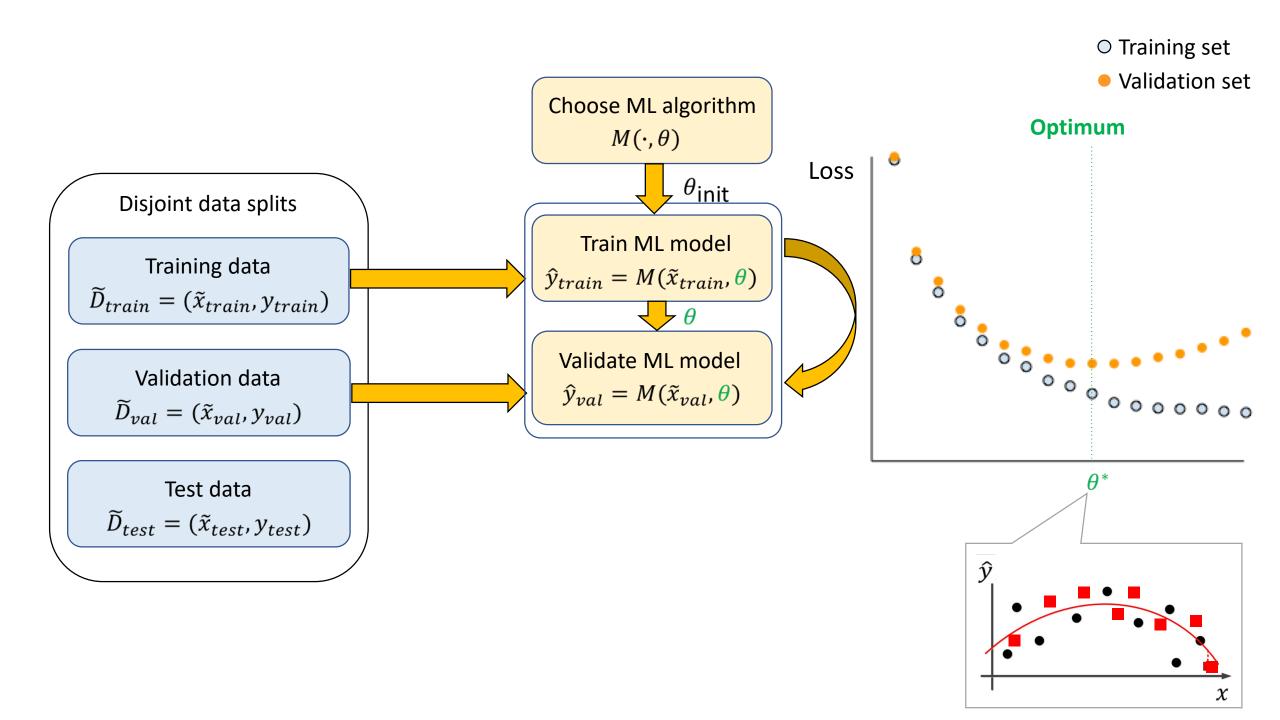
$$\widetilde{D}_{val} = (\widetilde{x}_{val}, y_{val})$$

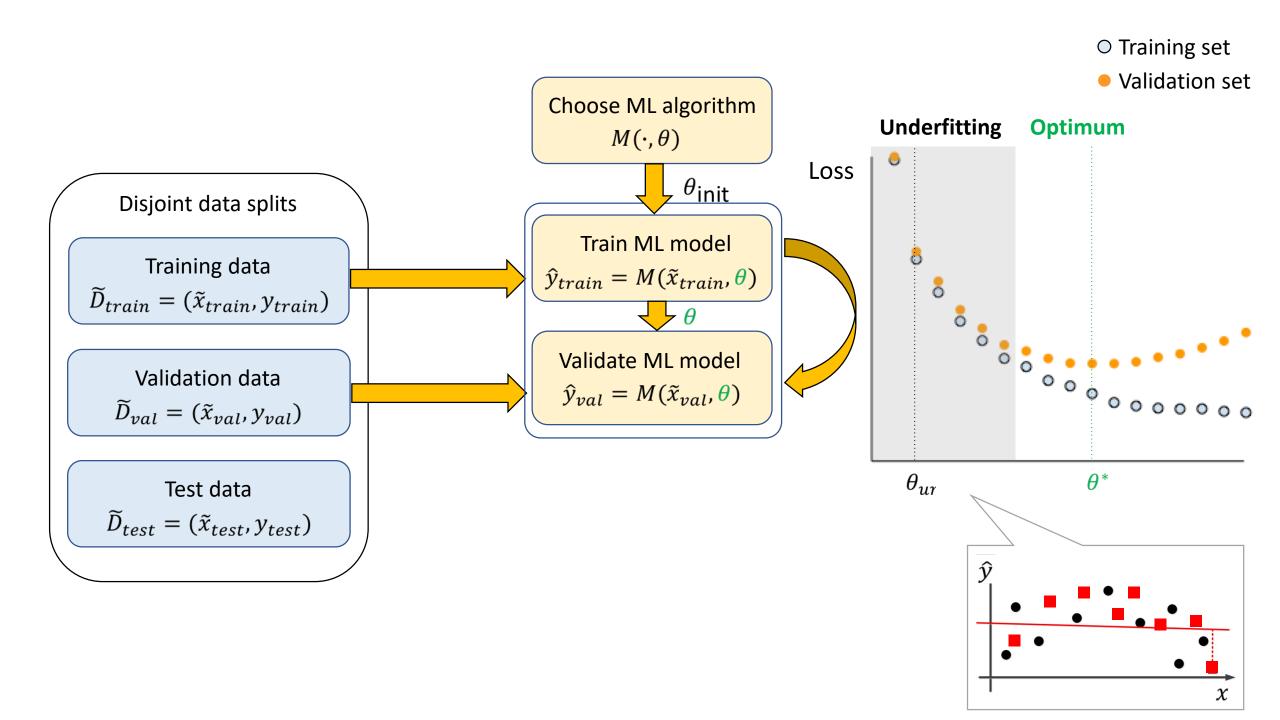
Test data

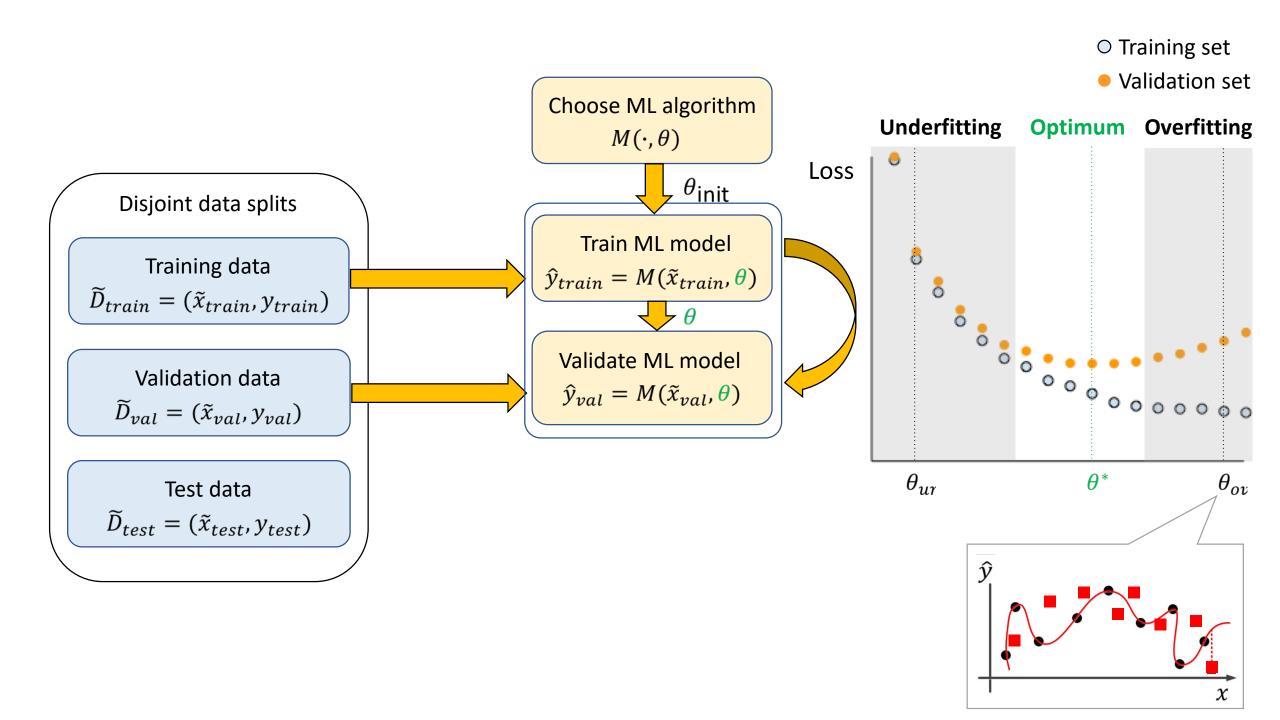
$$\widetilde{D}_{test} = (\widetilde{x}_{test}, y_{test})$$





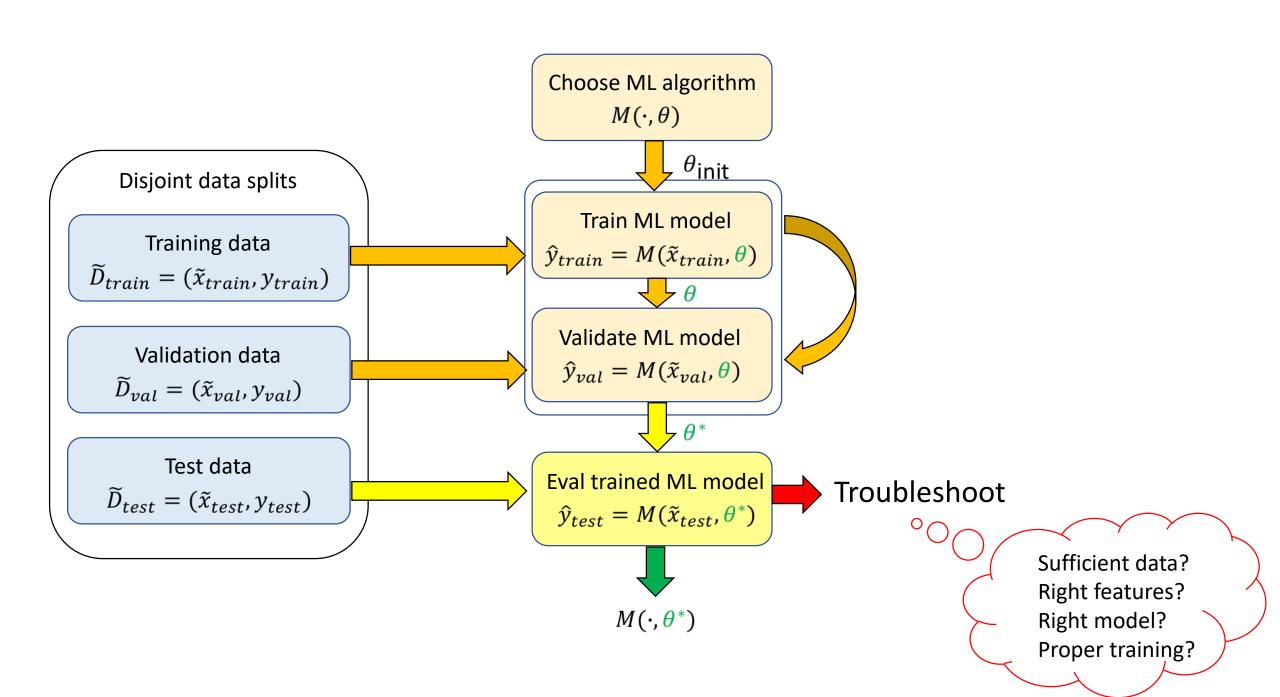






# The ML workflow

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- 6. Training the Model
- 7. Test the the Model



## Evaluate your Machine Learning Algorithm

Evaluating your machine learning algorithm is an essential part of any project.

Classification Accuracy
Logarithmic Loss
Confusion Matrix
Area under Curve
F1 Score
Mean Absolute Error
Mean Squared Error

https://towardsdatascience.com/metrics-to-evaluate-your-machine-learning-algorithm-f10ba6e38234

# The ML workflow

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- 6. Training the Model
- 7. Test the the Model
- 8. Tune Hyperparameters

https://medium.com/criteo-labs/hyper-parameter-optimization-algorithms-2fe447525903

# Introduction to Machine Learning using Scikit-Learn Scikit-learn is probably the most useful library for

machine **learning** in Python. The sklearn library contains

a lot of efficient tools for machine learning and statistical

modeling including classification, regression, clustering

and dimensionality reduction

### **Tutorials**

https://scikit-learn.org/stable/

https://scikit-learn.org/stable/tutorial/basic/tutorial.html

https://www.guru99.com/scikit-learn-tutorial.html

### ML Projects for beginners

https://github.com/jakevdp/sklearn\_tutorial

https://www.guru99.com/scikit-learn-tutorial.html

https://elitedatascience.com/machine-learning-projects-for-beginners