



CHULA ENGINEERING  
Foundation toward Innovation

COMPUTER



## Practical Machine Learning

Assoc. Prof. Peerapon Vateekul, Ph.D.  
Department of Computer Engineering,  
Faculty of Engineering, Chulalongkorn University  
[Peerapon.v@chula.ac.th](mailto:Peerapon.v@chula.ac.th)  
[www.cp.eng.chula.ac.th/~peerapon/](http://www.cp.eng.chula.ac.th/~peerapon/)



# Outlines

- Introduction
- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning
- Special Tasks



## Introduction

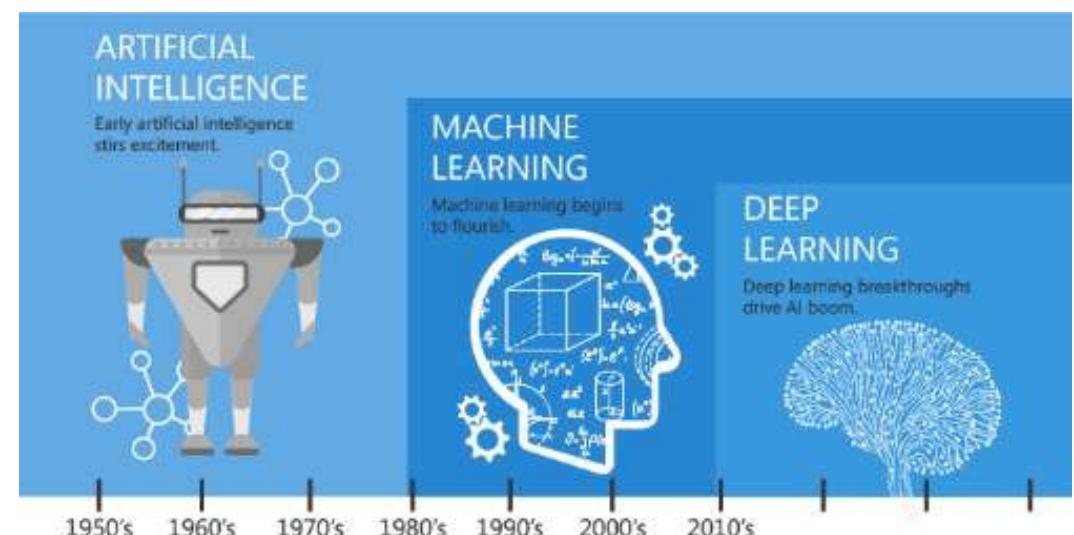
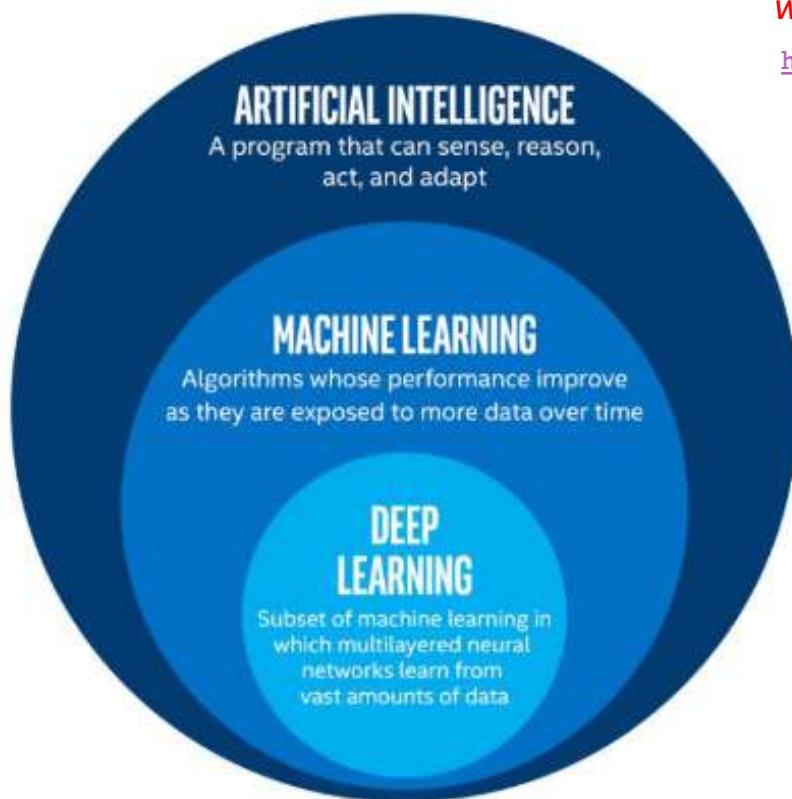


# AI, Machine Learning, and Deep Learning

- Machine Learning (ML) is a subfield in AI focusing on making to learn by itself without human intervention.

*“Machine learning is the science of getting computers to act without being explicitly programmed.” — [Stanford University](#)*

<https://towardsdatascience.com/cousins-of-artificial-intelligence-dda4edc27b55>

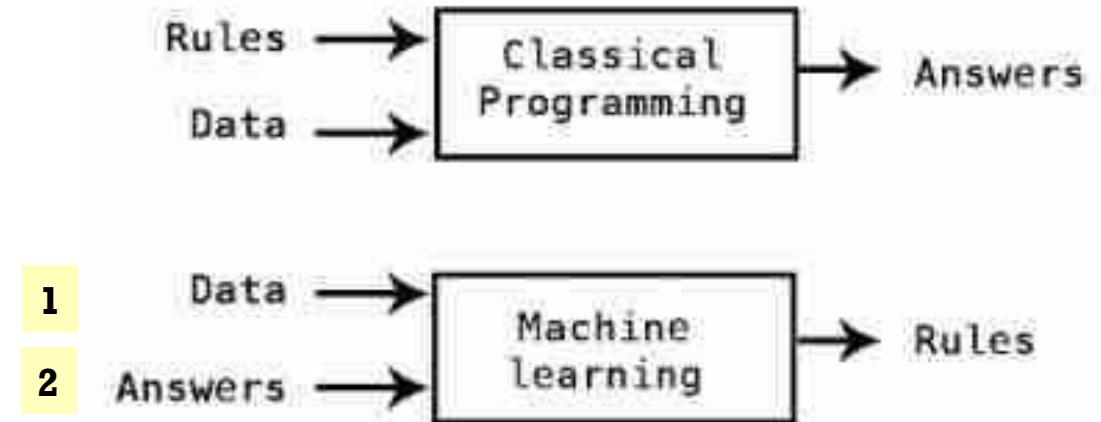
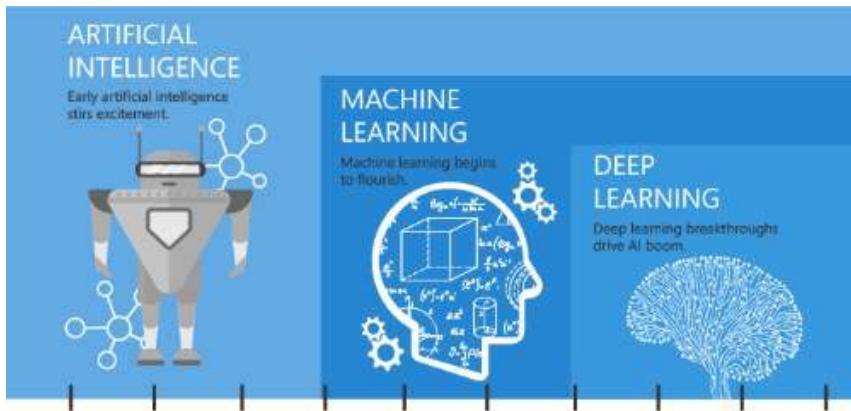


Since an early flush of optimism in the 1950's, smaller subsets of artificial intelligence - first machine learning, then deep learning, a subset of machine learning - have created ever larger disruptions.



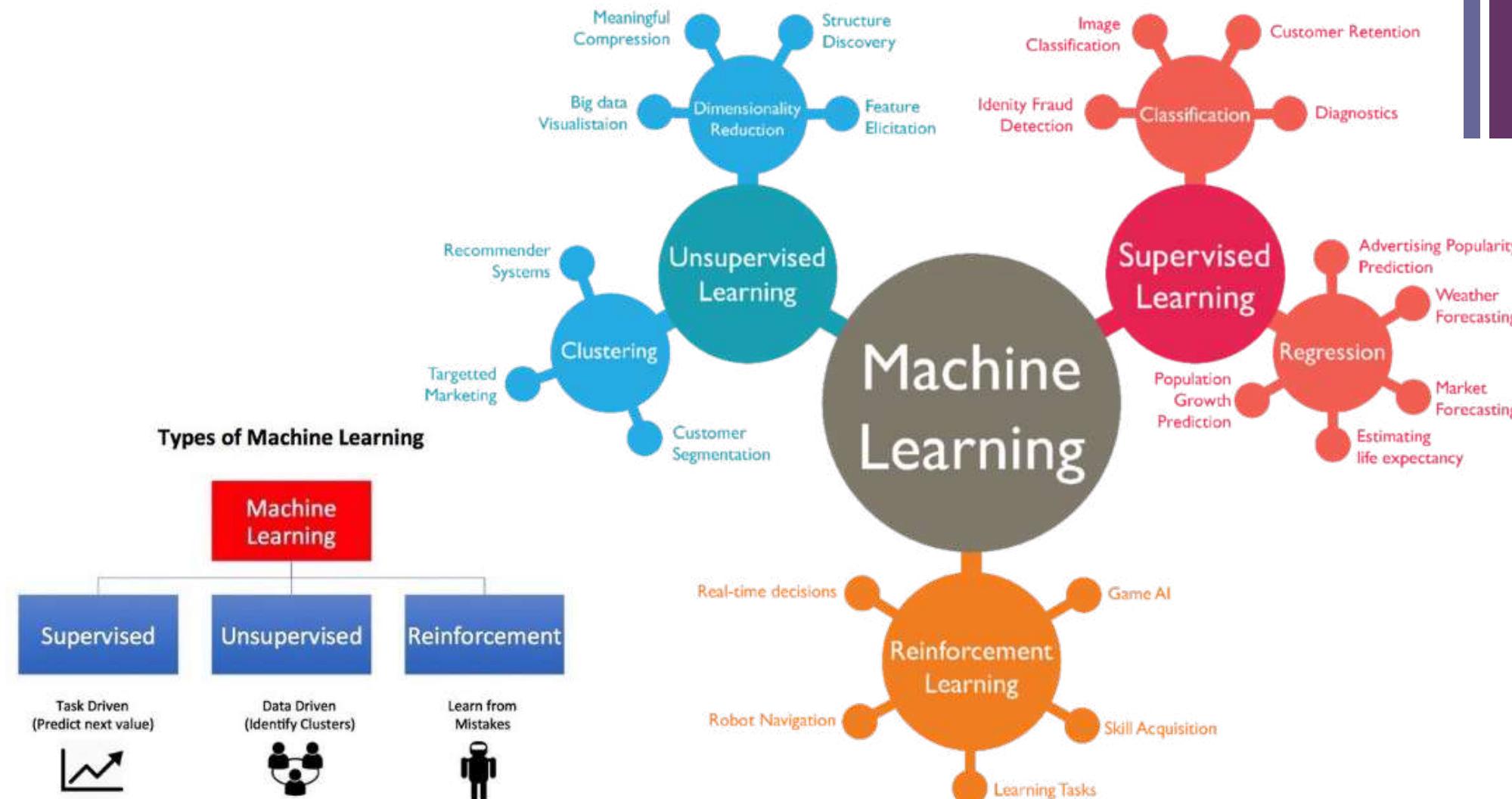
# AI = Automation

- 1) Rule-based AI (Symbolic AI)
- 2) Machine Learning



<https://mc.ai/machine-learning-basics-artificial-intelligence-machine-learning-and-deep-learning/>

# + Machine Learning (cont.)



 [Install](#) [User Guide](#) [API](#) [Examples](#) [More](#)  [Go](#)

# scikit-learn

Machine Learning in Python

[Getting Started](#) [What's New in 0.22.2](#) [GitHub](#)

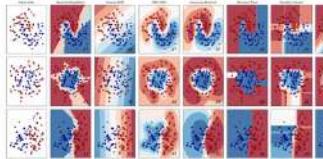
- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

### Classification

Identifying which category an object belongs to.

**Applications:** Spam detection, image recognition.

**Algorithms:** SVM, nearest neighbors, random forest, and more...

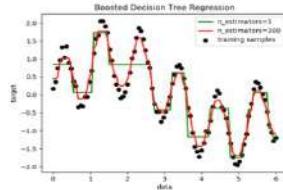


### Regression

Predicting a continuous-valued attribute associated with an object.

**Applications:** Drug response, Stock prices.

**Algorithms:** SVR, nearest neighbors, random forest, and more...



### Clustering

Automatic grouping of similar objects into sets.

**Applications:** Customer segmentation, Grouping experiment outcomes

**Algorithms:** k-Means, spectral clustering, mean-shift, and more...

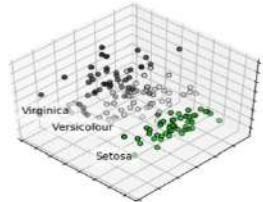


### Dimensionality reduction

Reducing the number of random variables to consider.

**Applications:** Visualization, Increased efficiency

**Algorithms:** k-Means, feature selection, non-negative matrix factorization, and more...

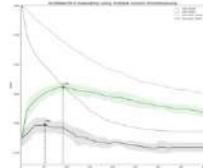


### Model selection

Comparing, validating and choosing parameters and models.

**Applications:** Improved accuracy via parameter tuning

**Algorithms:** grid search, cross validation, metrics, and more...

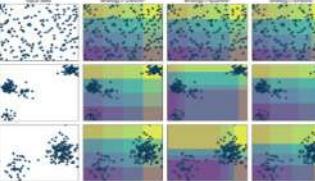


### Preprocessing

Feature extraction and normalization.

**Applications:** Transforming input data such as text for use with machine learning algorithms.

**Algorithms:** preprocessing, feature extraction, and more...



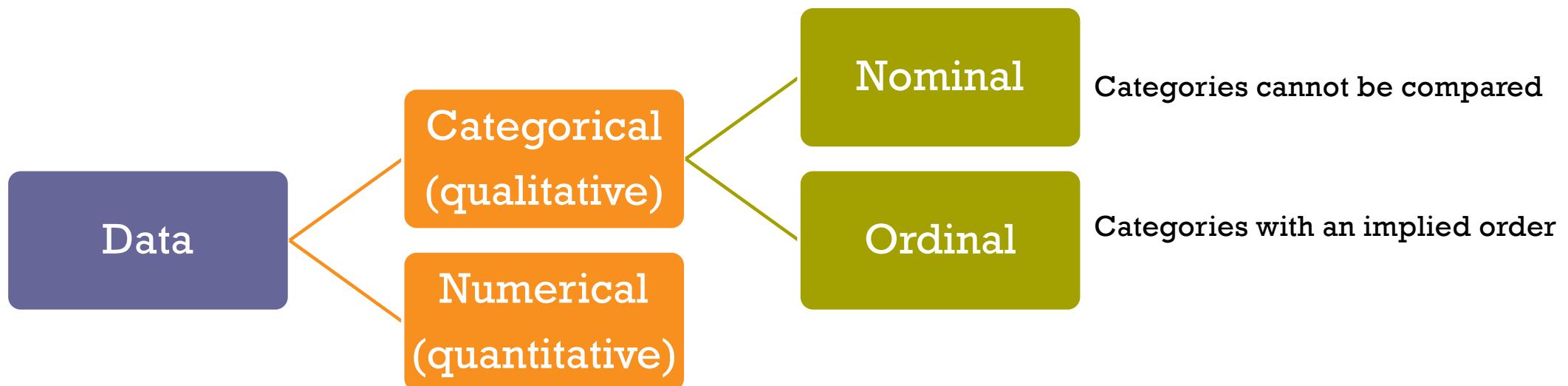


## Terminology: Data table

inputs				target
Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes
32	35,000	Male	Bangkok	No

- Row
  - Example, instance, case, observation, subject
- Column
  - Feature, variable, attribute
- Input
  - Predictor, independent, explanatory variable
- Target
  - Output, outcome, response, dependent variable

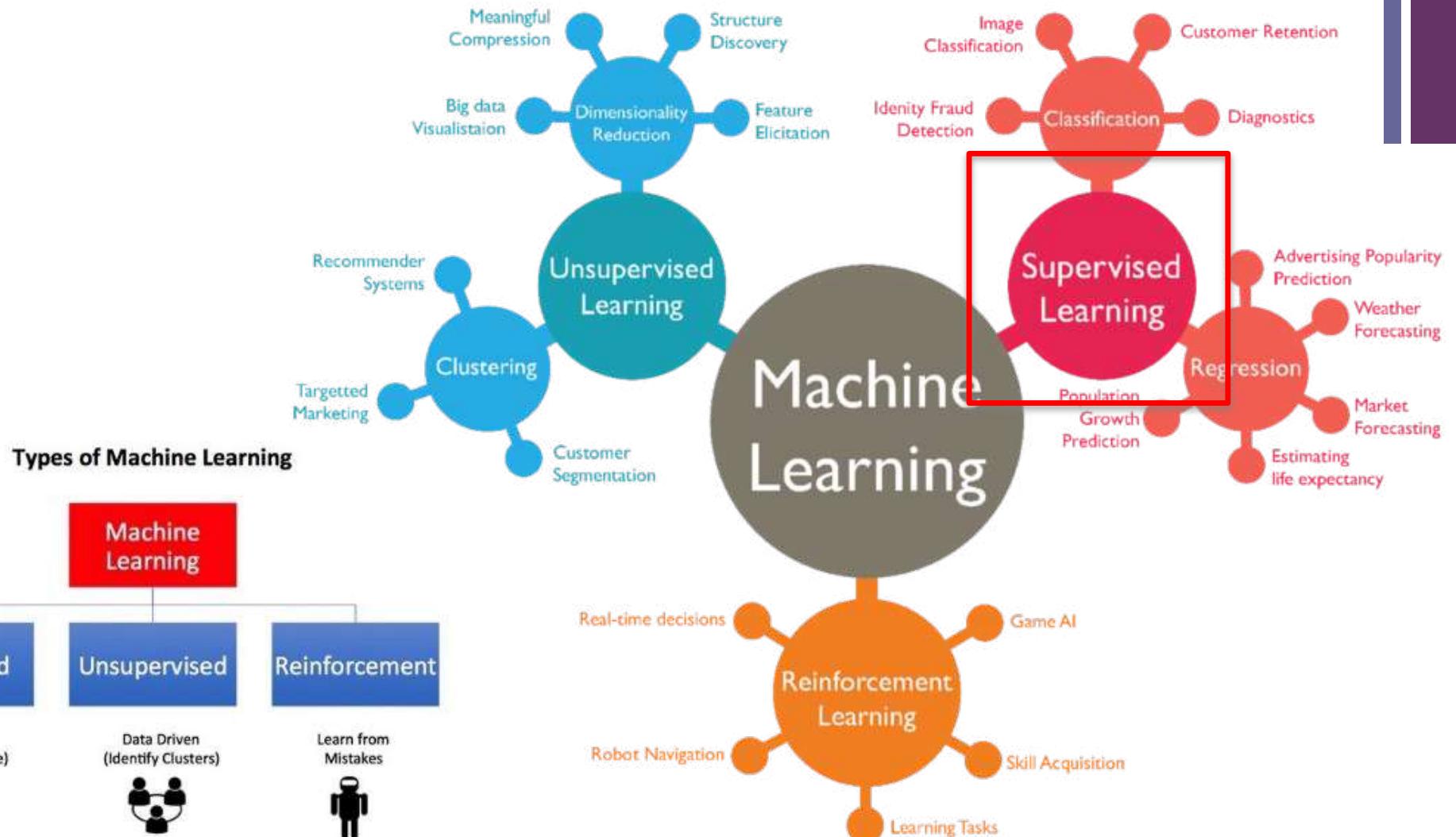
## + Terminology: Kinds of data



+

## Supervised Learning (Predictive Task)

# + Machine Learning (cont.)



## Task1: Supervised learning

### Handcrafted features

Training Data



	inputs				target
	Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes	
35	50,000	Female	Nontaburi	Yes	
32	35,000	Male	Bangkok	No	

Testing Data

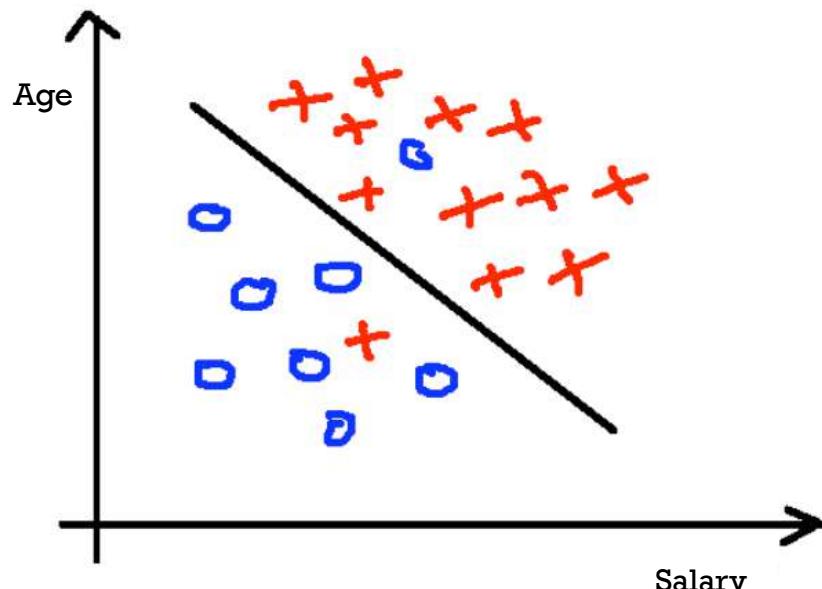


Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	?

Application: Direct Target Marketing

## + Classification: predicting a category

### Logistic Regression



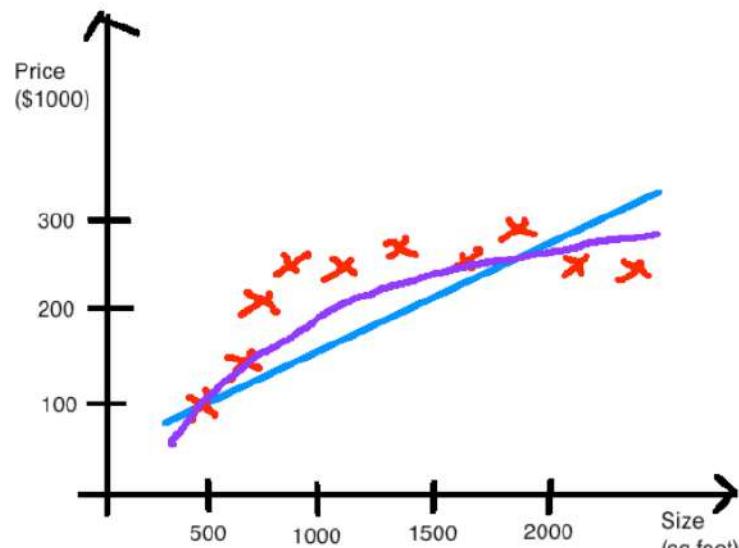
Predict targeted customers who  
tend to buy our product (yes/no)

- Some techniques:
  - Naïve Bayes
  - Decision Tree
  - Logistic Regression
  - Support Vector Machines
  - Neural Network
  - Ensembles
  
- Sample Applications
  - Database marketing
  - Fraud detection
  - Pattern detection
  - Churn customer detection



## Regression: predict a continuous value

### Linear Regression



Predict a sale price of each house

#### ■ Some techniques:

- Linear Regression / GLM
- Decision Trees
- Support vector regression
- Neural Network
- Ensembles

#### ■ Sample Applications

- Financial risk management
- Revenue forecasting





# Scikit-learn: Machine learning library in Python

- Provides many machine learning tools with a common **Estimator interface**
- Built in helpers for common **ML tasks** (e.g., metrics, preprocessing)
- Easily combine algorithms to make **a complex pipeline**
- Relies heavily on numpy and scipy, often used with **pandas**

How do you pronounce the project name?

scikit learn. sci stands for science!

Why scikit?

There are multiple scikits, which are scientific toolboxes built around SciPy. You can find a list at <https://scikit-learn.org/stable/index.html>.

## Classification

Identifying to which category an object belongs to.

**Applications:** Spam detection, Image recognition.

**Algorithms:** SVM, nearest neighbors, random forest, ...

— Examples

## Regression

Predicting a continuous-valued attribute associated with an object.

**Applications:** Drug response, Stock prices.

**Algorithms:** SVR, ridge regression, Lasso, ...

— Examples

## Clustering

Automatic grouping of similar objects into sets.

**Applications:** Customer segmentation, Grouping experiment outcomes

**Algorithms:** k-Means, spectral clustering, mean-shift, ...

— Examples

## Dimensionality reduction

Reducing the number of random variables to consider.

**Applications:** Visualization, Increased efficiency

**Algorithms:** PCA, feature selection, non-negative matrix factorization.

— Examples

## Model selection

Comparing, validating and choosing parameters and models.

**Goal:** Improved accuracy via parameter tuning

**Modules:** grid search, cross validation, metrics.

— Examples

## Preprocessing

Feature extraction and normalization.

**Application:** Transforming input data such as text for use with machine learning algorithms.

**Modules:** preprocessing, feature extraction.

— Examples

<http://scikit-learn.org/stable/index.html>





# Estimator Interface

## Decision Trees

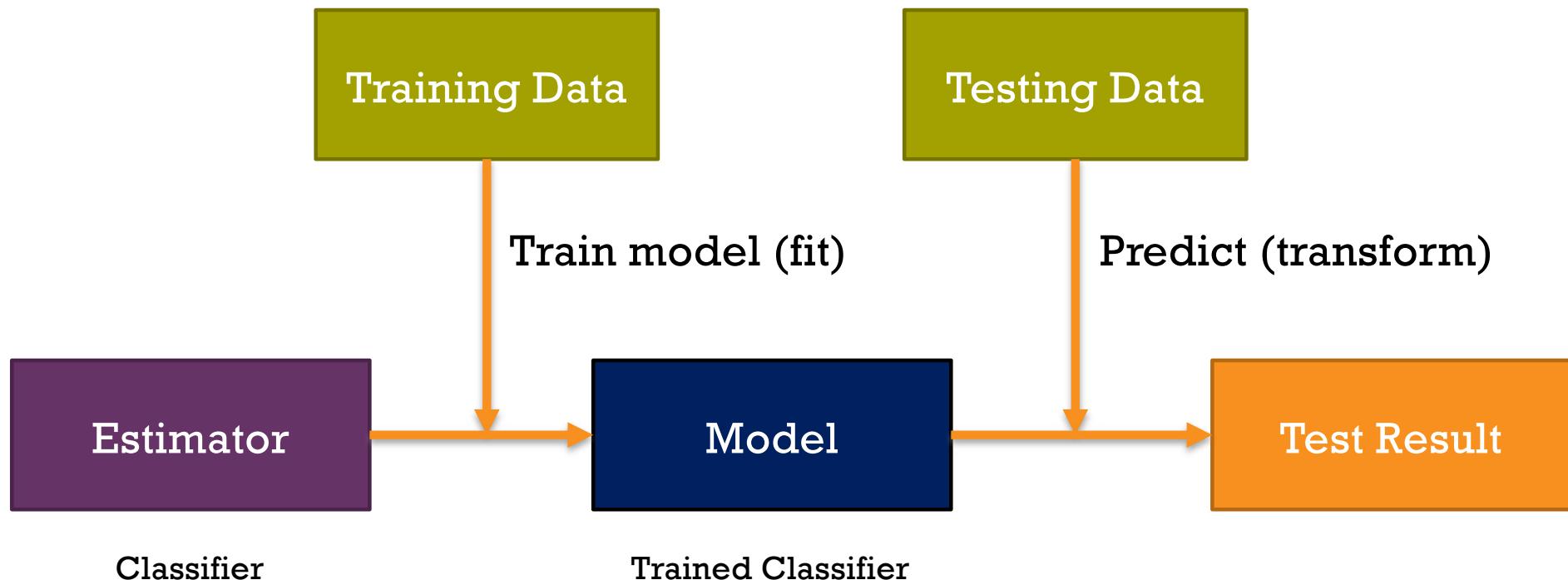
We'll start just by training a single decision tree.

```
In [8]: from sklearn.tree import DecisionTreeClassifier
In [9]: dtree = DecisionTreeClassifier(min_samples_leaf=10, criterion='entropy')
In [10]: dtree.fit(X_train,y_train)
Out[10]: DecisionTreeClassifier(class_weight=None, criterion='entropy', max_depth=None,
                                 max_features=None, max_leaf_nodes=None,
                                 min_impurity_decrease=0.0, min_impurity_split=None,
                                 min_samples_leaf=10, min_samples_split=2,
                                 min_weight_fraction_leaf=0.0, presort=False, random_state=None,
                                 splitter='best')
```

## Prediction and Evaluation

Let's evaluate our decision tree.

```
[11]: predictions = dtree.predict(X_test)
[12]: from sklearn.metrics import classification_report,confusion_matrix
[13]: print(classification_report(y_test,predictions))
          precision    recall  f1-score   support
absent       0.85      0.85      0.85       20
present      0.40      0.40      0.40        5
avg / total   0.76      0.76      0.76       25
```





# Training Phase

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split

cancer = load_breast_cancer()      # Get some data
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target,
    stratify=cancer.target, random_state=1337)

tree = DecisionTreeClassifier(random_state=7331)
tree.fit(X_train, y_train) # Learn a Decision Function
```



## Testing Phase (Prediction)

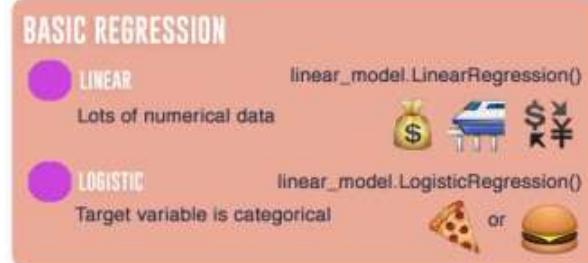
```
y_pred = tree.predict(X_test)
```

```
>>> from sklearn.metrics import classification_report
>>> y_true = [0, 1, 2, 2, 2]
>>> y_pred = [0, 0, 2, 2, 1]
>>> target_names = ['class 0', 'class 1', 'class 2']
>>> print(classification_report(y_true, y_pred, target_names=target_names))
          precision    recall  f1-score   support
class 0       0.50    1.00    0.67      1
class 1       0.00    0.00    0.00      1
class 2       1.00    0.67    0.80      3

  micro avg   0.60    0.60    0.60      5
  macro avg   0.50    0.56    0.49      5
weighted avg   0.70    0.60    0.61      5
```

# + Prediction Algorithms

- Decision Tree
- (Logistic) Regression
- Neural Networks (NN)
- kNN
- Support Vector Machine
- Deep Learning

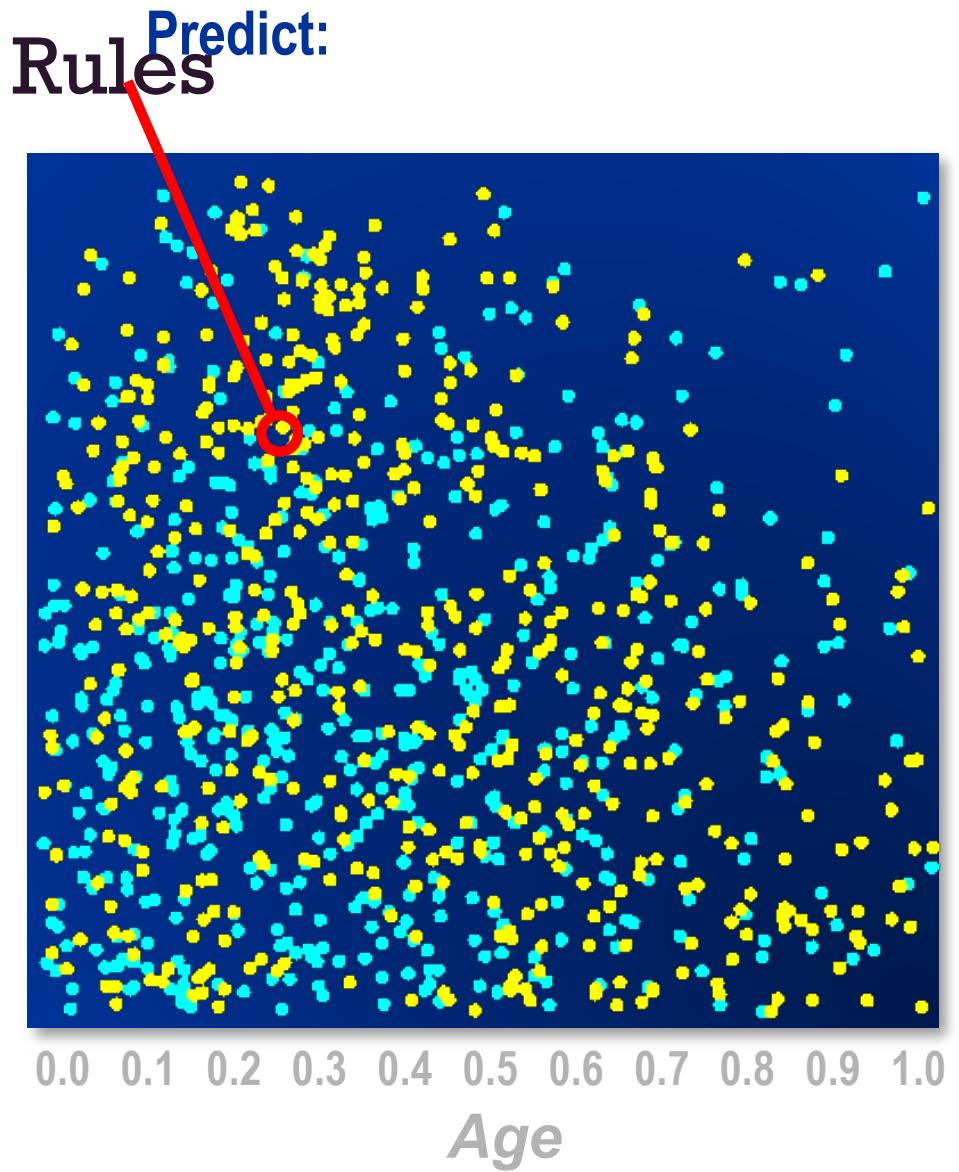
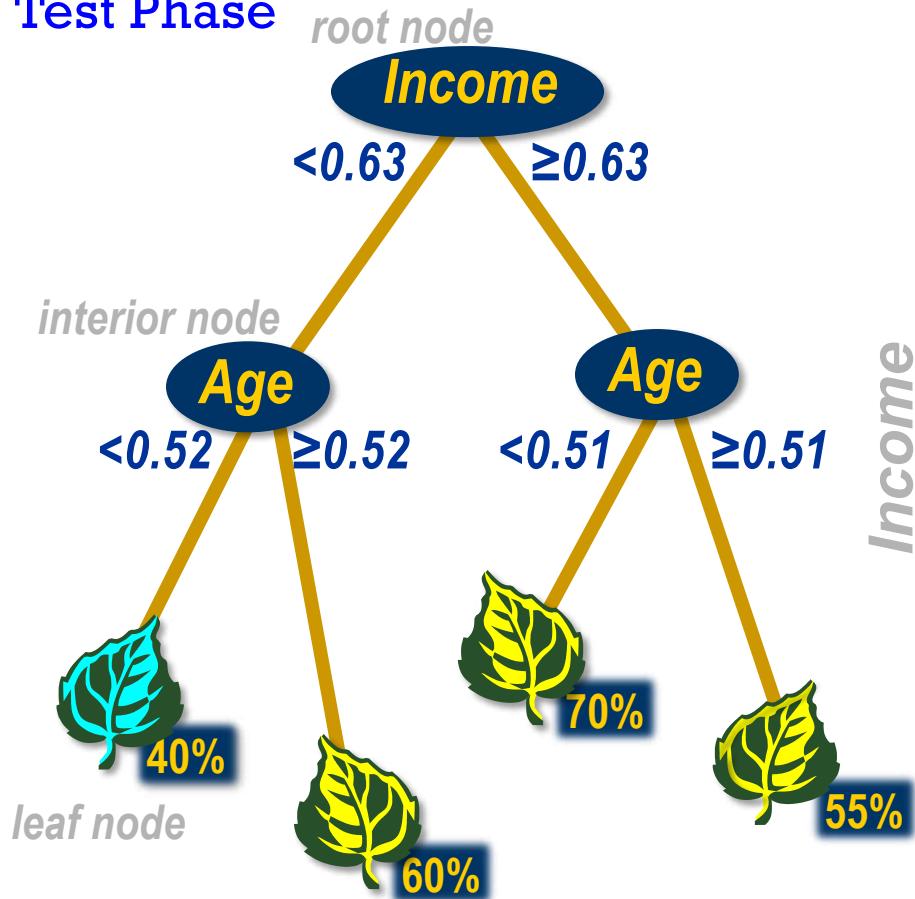


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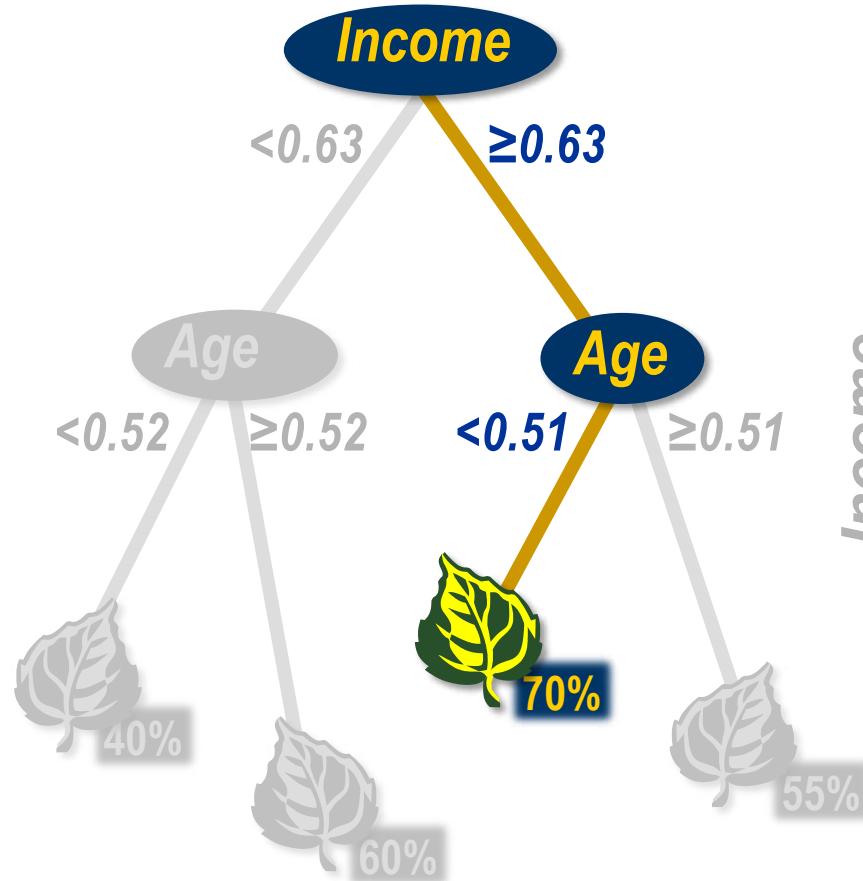
## 1) Decision Tree

# 1) Decision Tree Prediction Rules

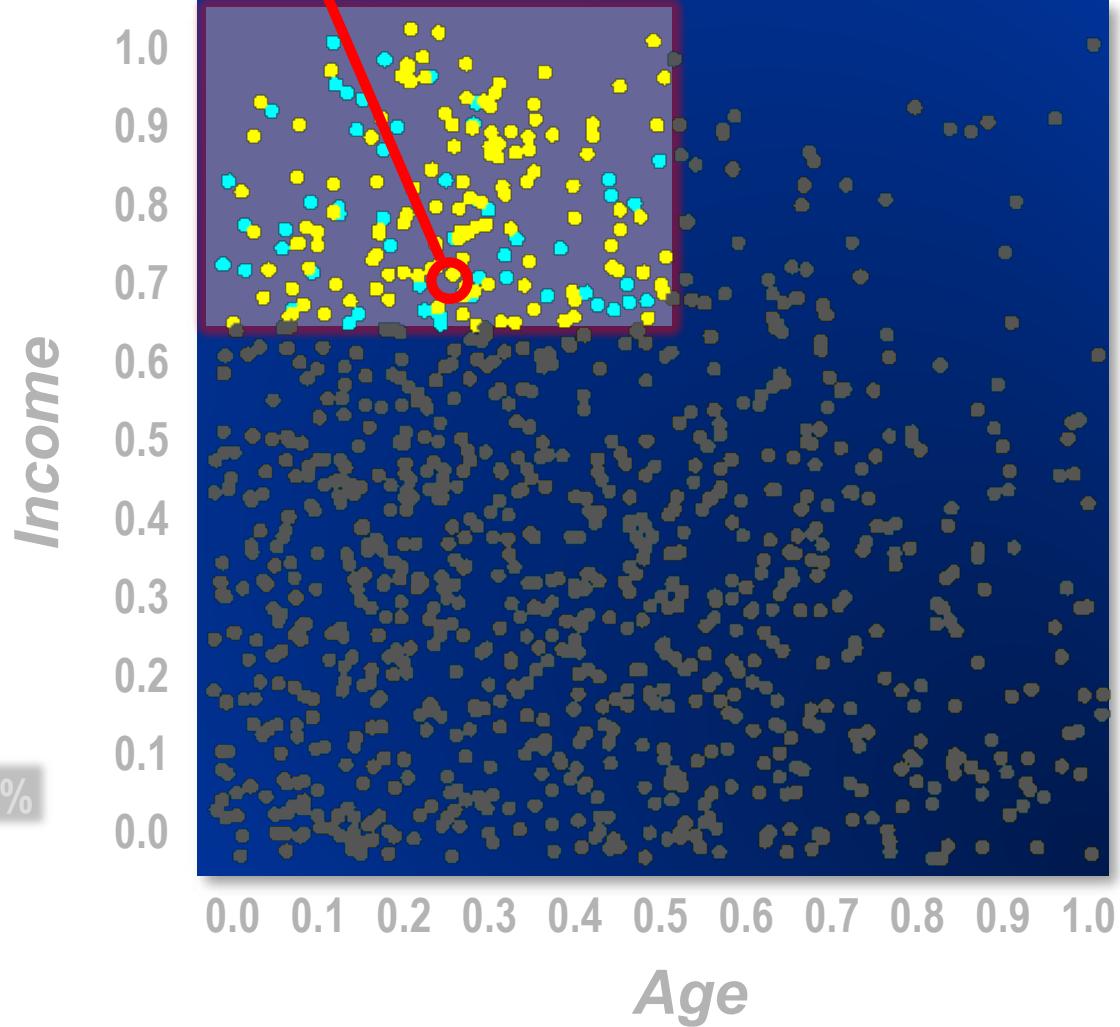
Test Phase



# Decision Tree Prediction Rules



Predict: Decision = ●  
Estimate = 0.70



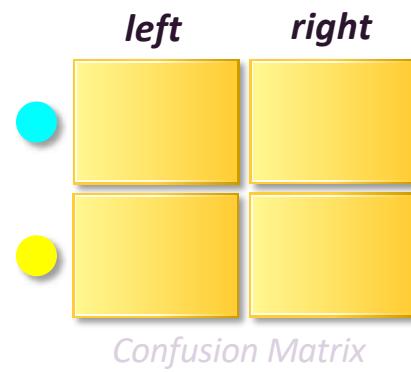
# Model Essentials: Decision Trees

- ▶ Predict cases.
- ▶ Select useful predictors.

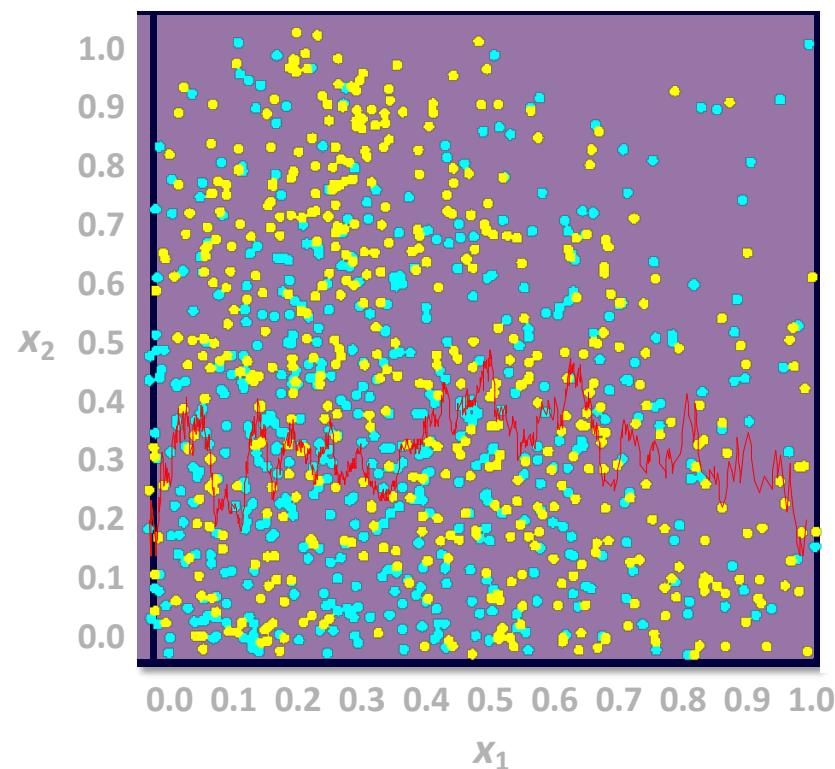
**Prediction rules**

**Split search**

# Decision Tree Split Search

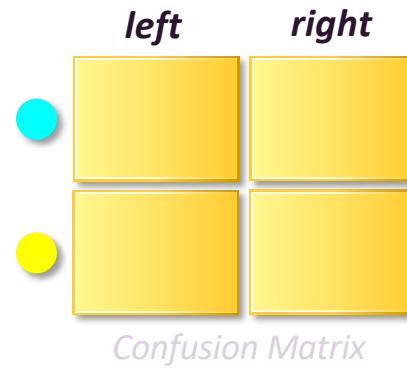


**Calculate information  
gain on partitions  
on input  $x_1$ .**

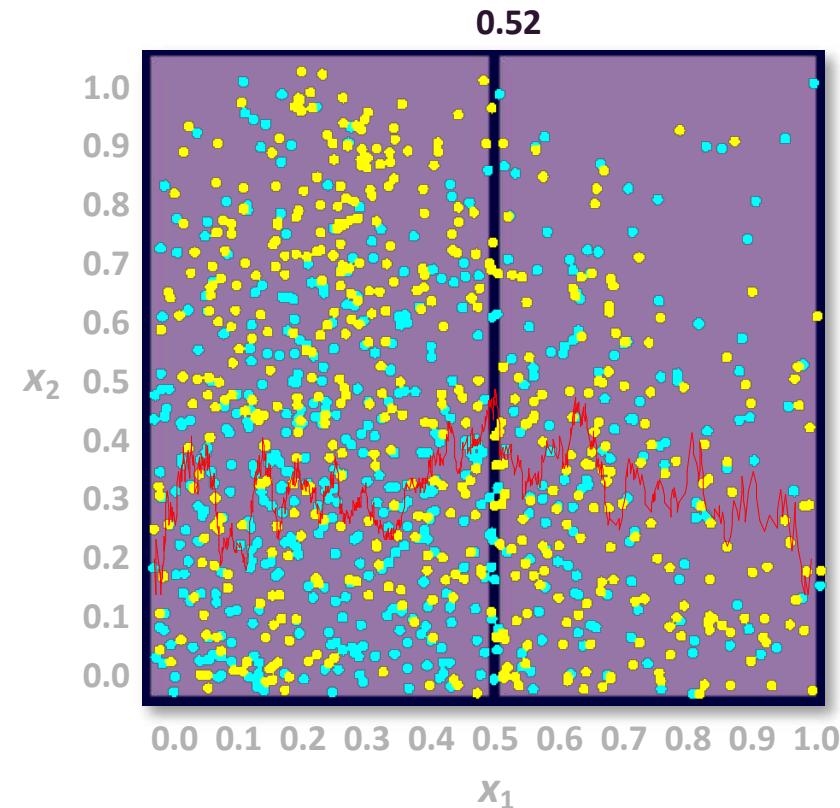


...

# Decision Tree Split Search



**Calculate the gain  
of every partition  
on input  $x_1$ .**



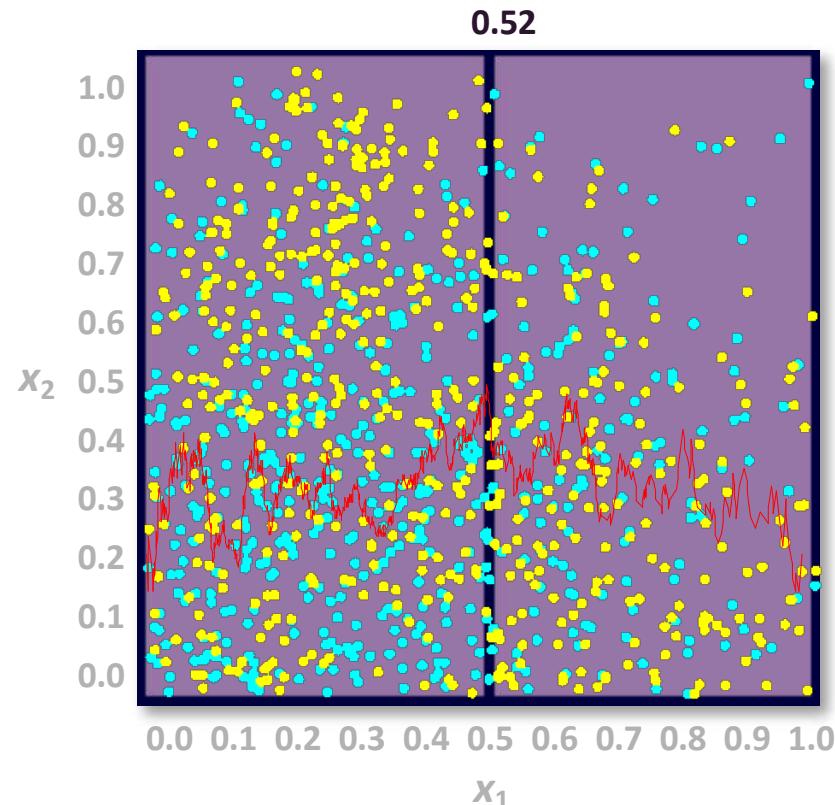
...

# Decision Tree Split Search

	<i>left</i>	<i>right</i>	
●	53%	42%	
●	47%	58%	

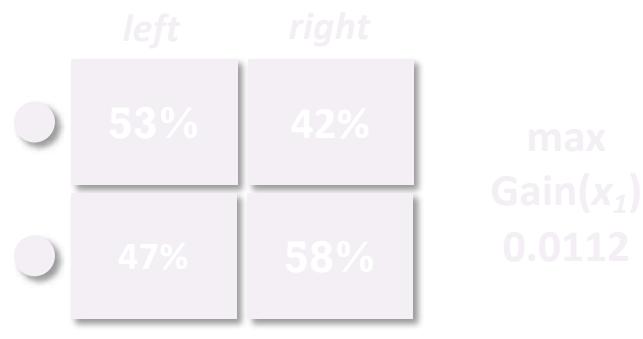
max  
 $\text{gain}(x_1)$   
0.0112

Select the partition with the maximum gain.

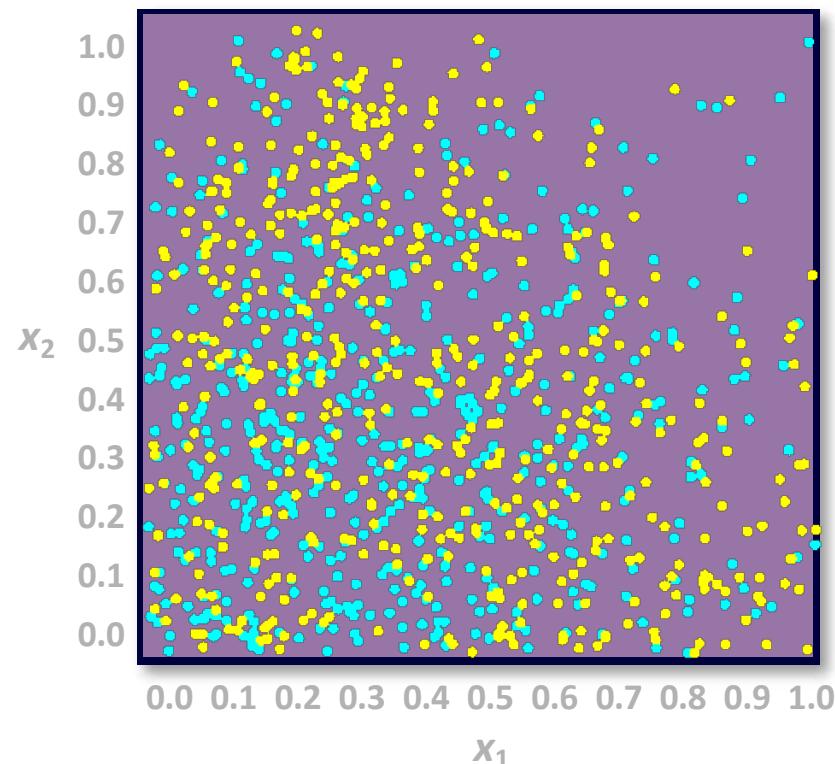


...

# Decision Tree Split Search

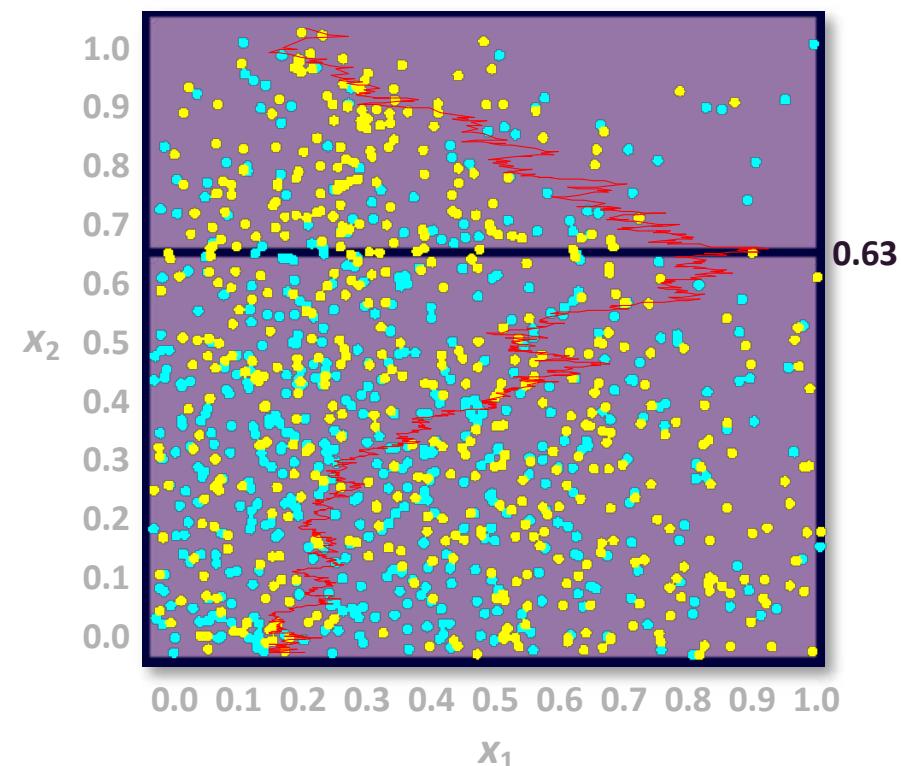
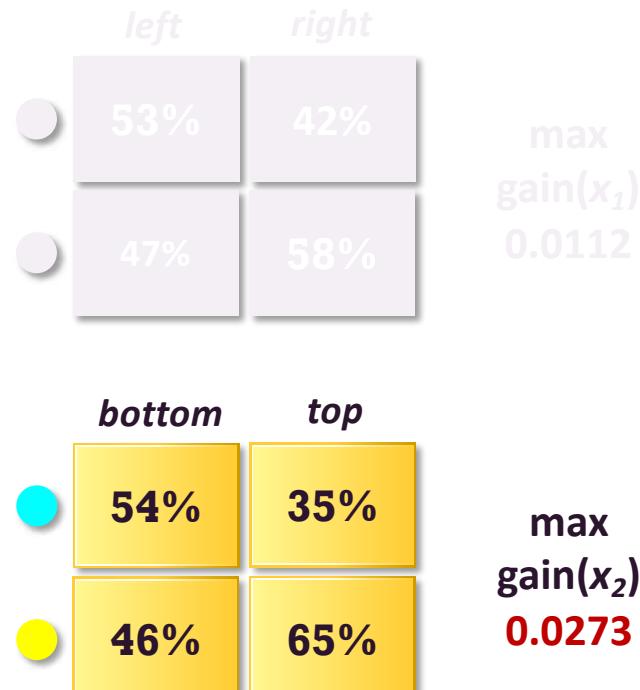


Repeat for input  $x_2$ .



...

# Decision Tree Split Search



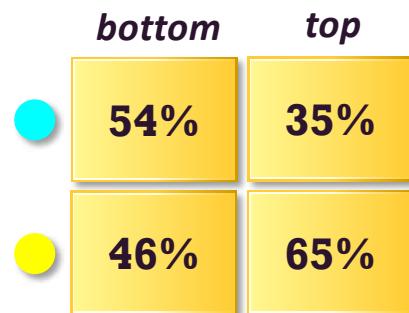
...

# Decision Tree Split Search



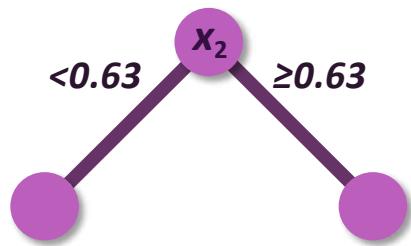
**max  
 $gain(x_1)$**

**max  
 $gain(x_2)$**

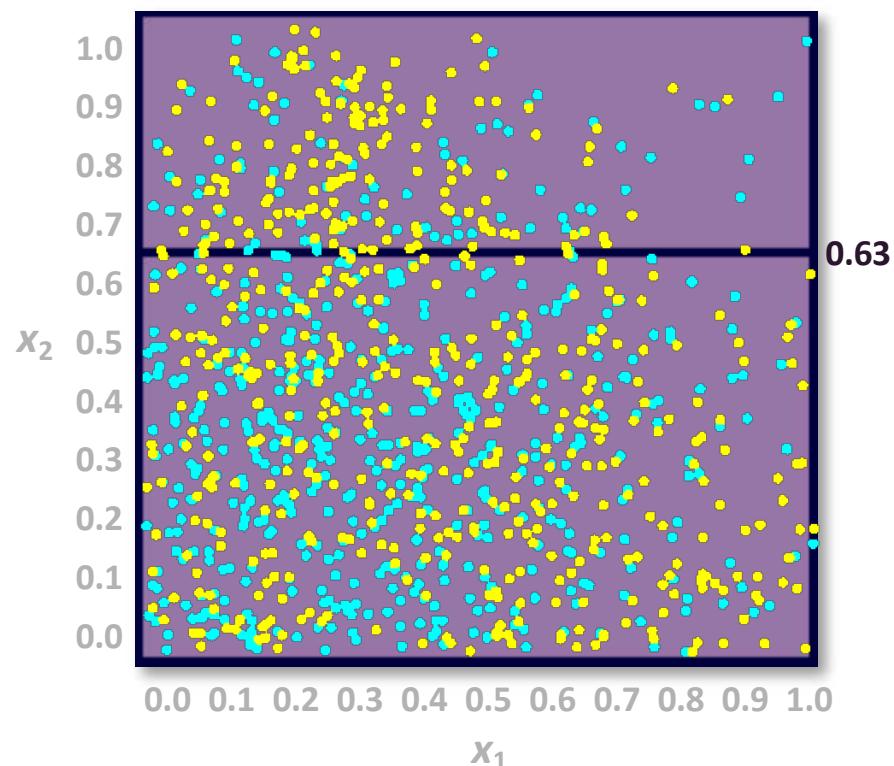


...

# Decision Tree Split Search

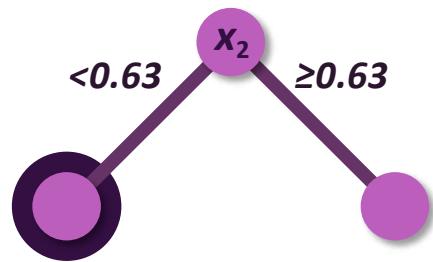


**Create a partition rule  
from the best partition  
across  
all inputs.**

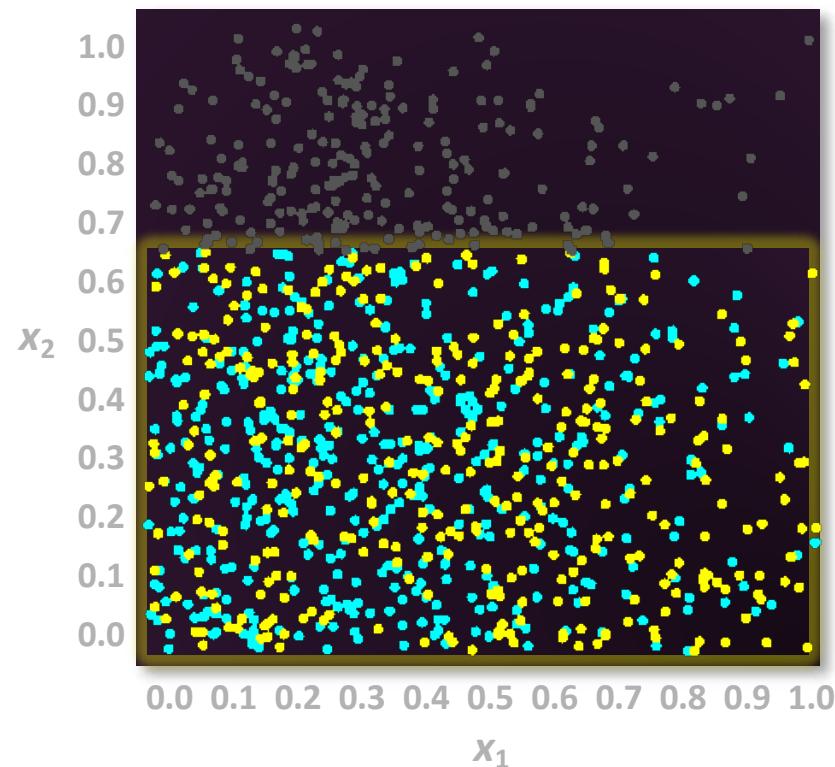


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# Decision Tree Split Search

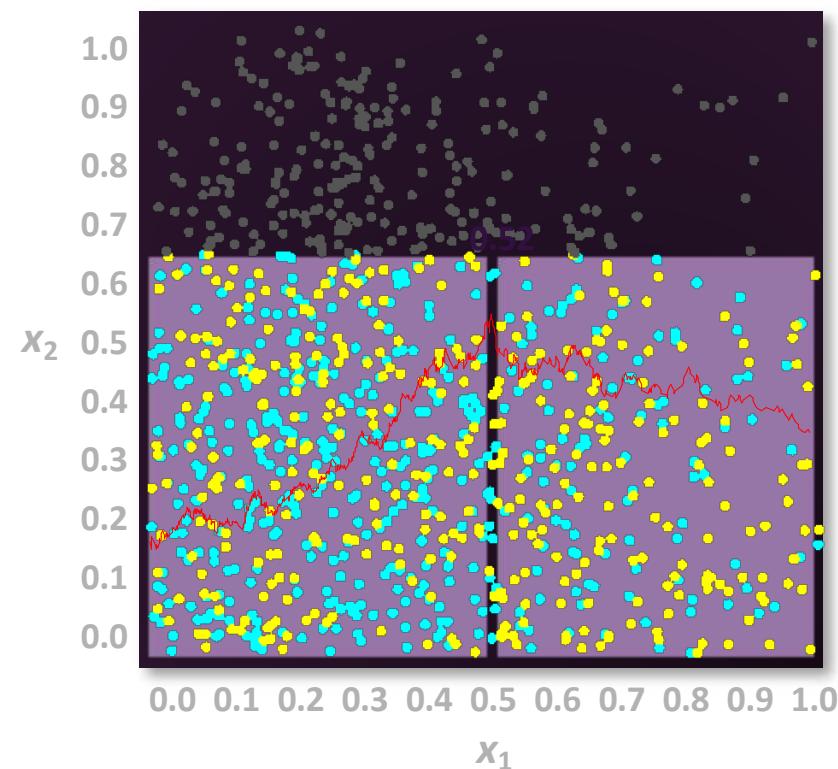


**Repeat the process  
in each subset.**



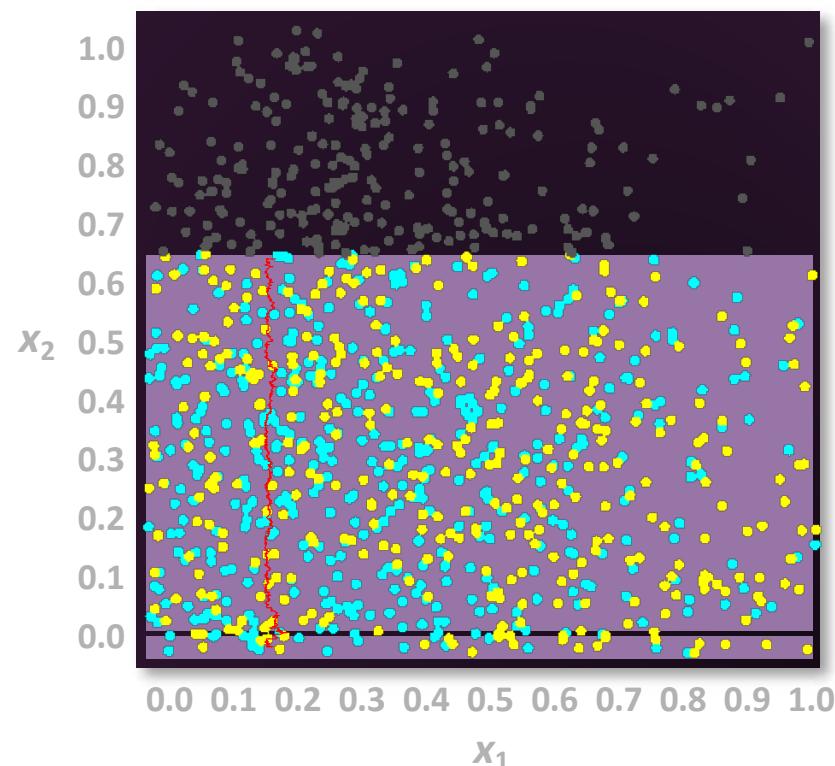
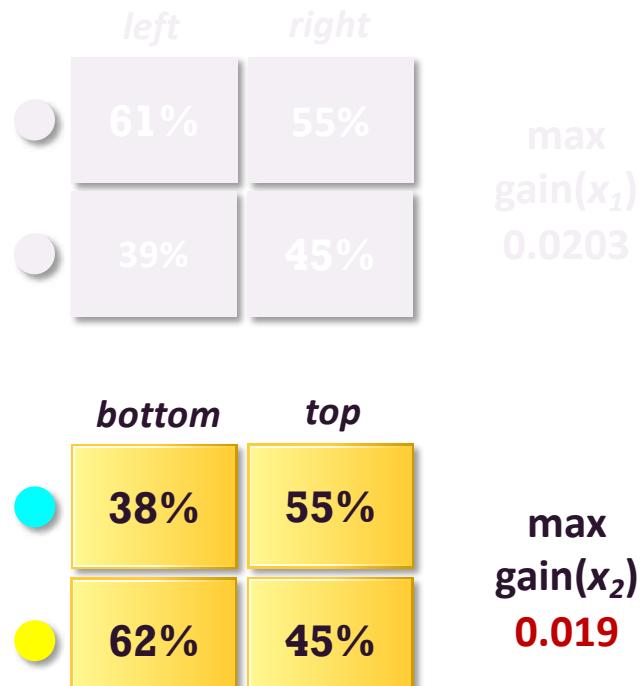
...

# Decision Tree Split Search

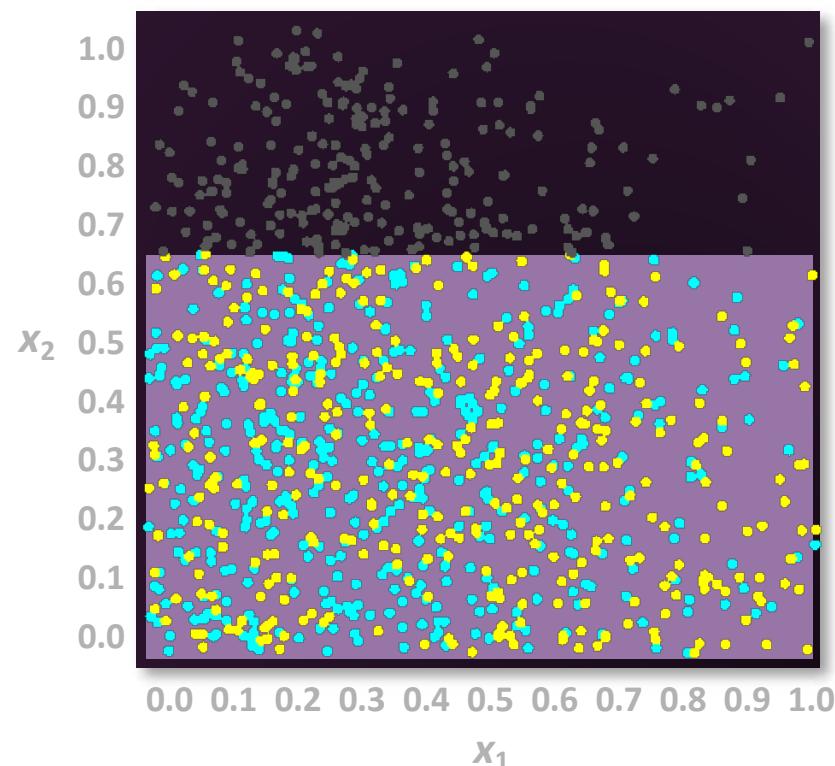
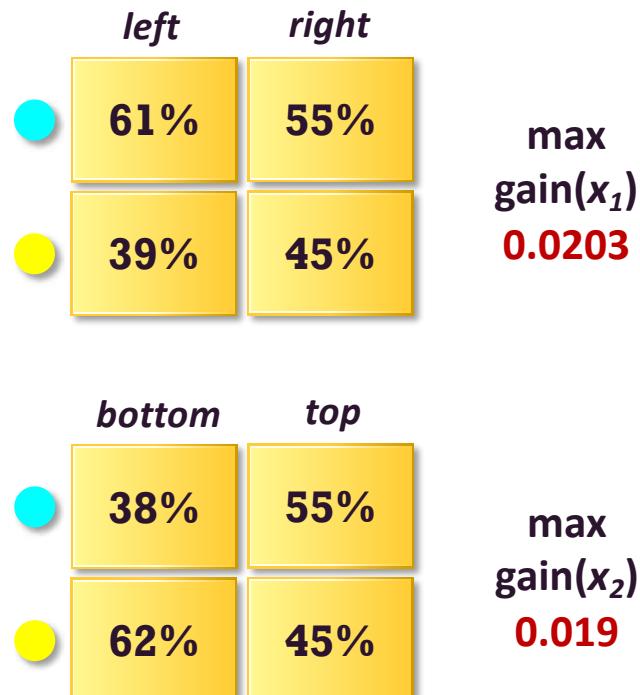


...

# Decision Tree Split Search

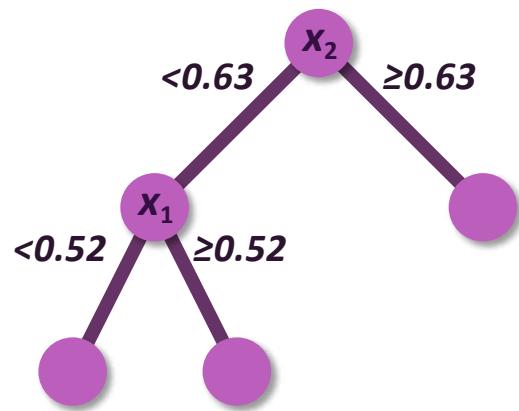


# Decision Tree Split Search

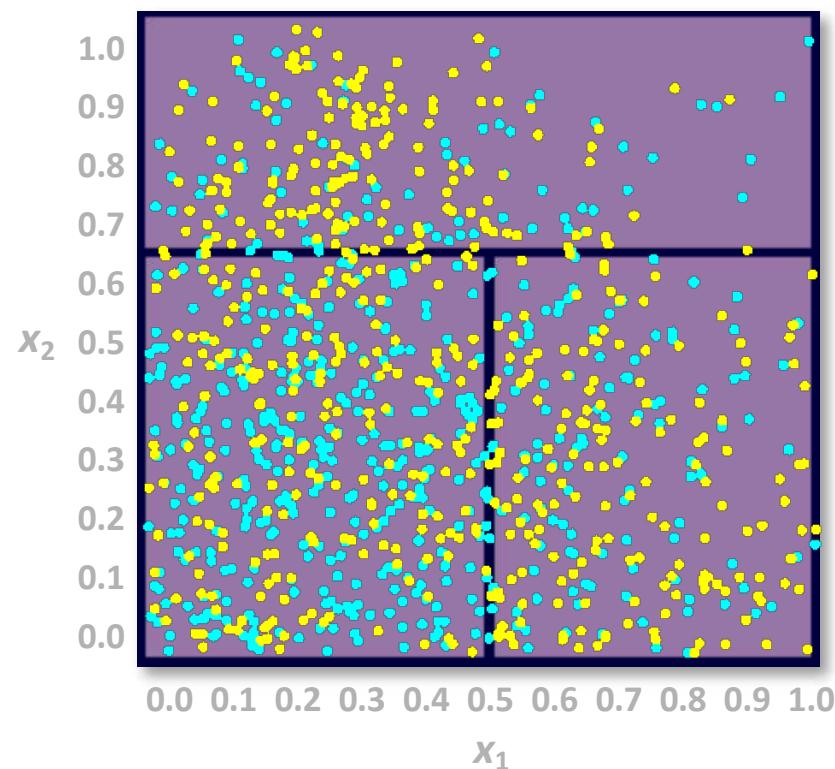


...

# Decision Tree Split Search

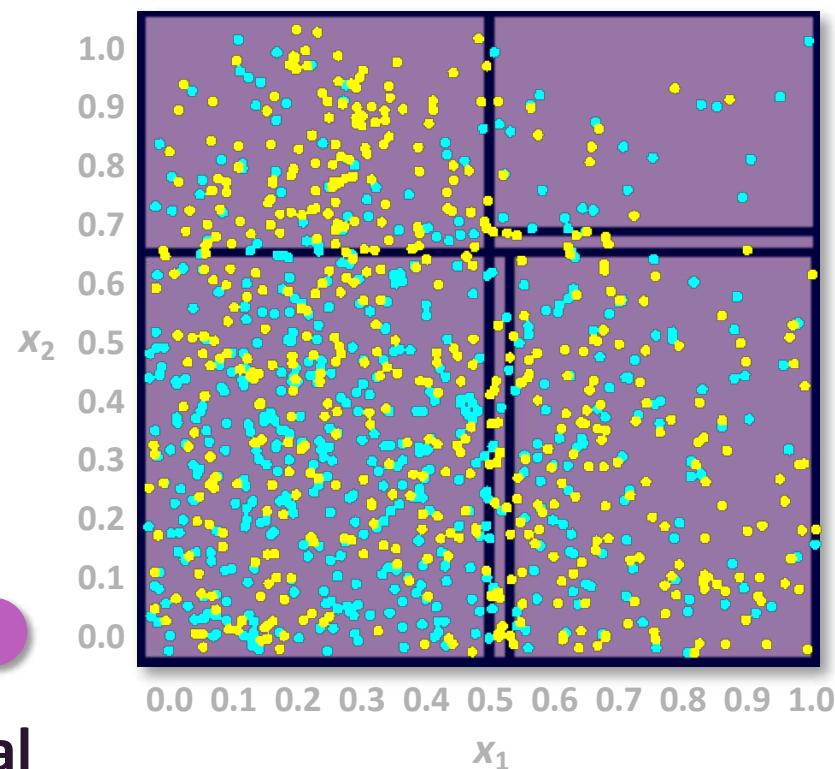
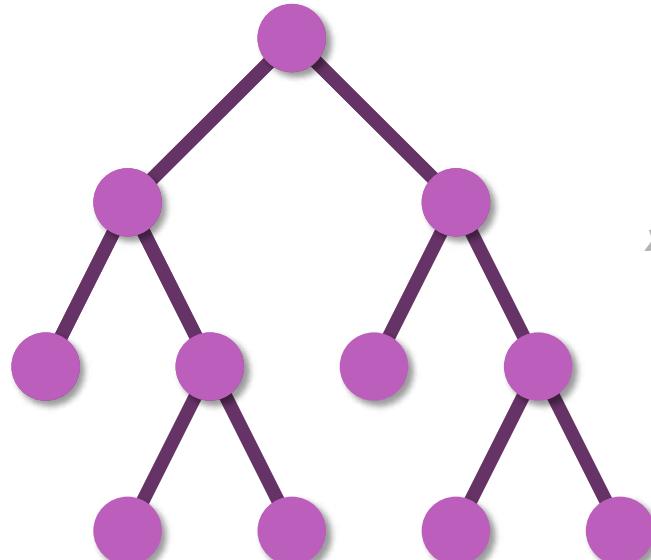


Create a second  
partition rule.



...

# Decision Tree Split Search



**Repeat to form a maximal tree.**



## 1) Entropy (impurity)

- **Entropy** is a measure of disorder or uncertainty and the goal of machine learning models and general is to reduce uncertainty.

$$\text{Entropy} = \sum_{i=1}^n -p_i \log_2 p_i$$

`scipy.stats.entropy`

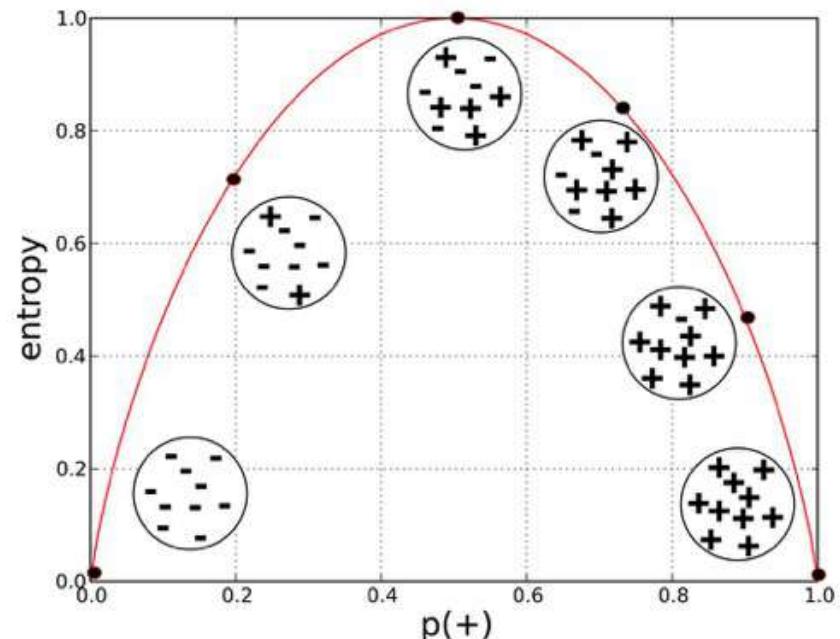
`scipy.stats.entropy(pk, qk=None, base=None, axis=0)`

Calculate the entropy of a distribution for given probability values.

If only probabilities `pk` are given, the entropy is calculated as `S = -sum(pk * log(pk), axis=axis)`.

If `qk` is not `None`, then compute the Kullback-Leibler divergence `S = sum(pk * log(pk / qk), axis=axis)`.

This routine will normalize `pk` and `qk` if they don't sum to 1.



Source: Data Science for Business: What You Need to Know about Data Mining and Data-Analytic Thinking



# Information Gain

## *Before - After*

- Which one is Better ?

Split w/ Age: 70  
 $\sum$  Entropy: 0.350

Split w/ Age: 50  
 $\sum$  Entropy: 0.348

- Information Gain: measure the reduction of this disorder in our target variable/class given additional information

$$\text{InformationGain} = \text{Entropy}(\text{before}) - \sum \text{Entropy}(\text{after})$$

- “Before” = Entropy of Parent Node  
“After” = Entropy of Child Nodes



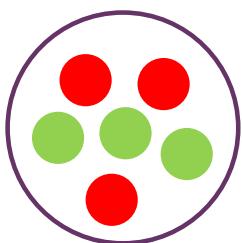
## 2) Gini Impurity

### Gini Reduction = Before - After

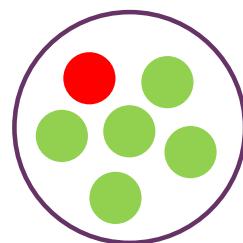
- Another way to measure how well a splitting feature.

$$Gini = 1 - \sum_{i=1}^n (P_i)^2$$

When  $P$  is the probability of class  $i$  in data-set.



$$\begin{aligned} Gini &= 1 - ((3/6)^2 + (3/6)^2) \\ &= 0.5 \end{aligned}$$

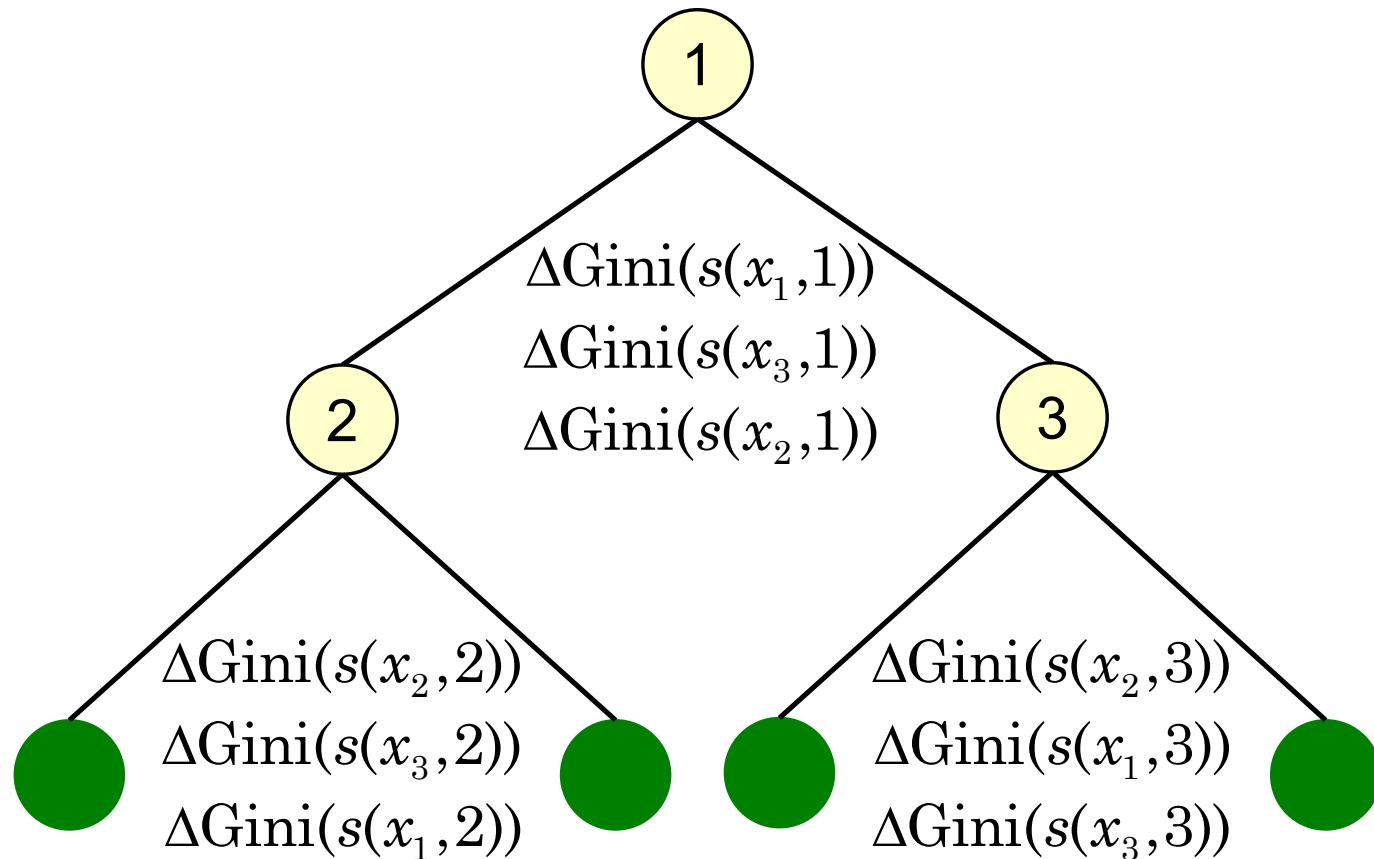
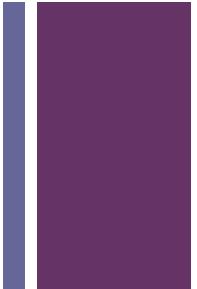


$$\begin{aligned} Gini &= 1 - ((5/6)^2 + (1/6)^2) \\ &= 0.28 \end{aligned}$$

- Easy to calculation, may take less time to build in large dataset.

Source: <https://towardsdatascience.com/understanding-decision-tree-classification-with-scikit-learn-2ddf272731bd>

## + Variable Importance



# Types of Decision Tree

Algorithm	Splitting Measure
ID3	Entropy
C4.5	Gain Ratio
CART	Gini index
CHAID	Chi-squared test



Please [cite us](#) if you use the software.

## sklearn.tree.DecisionTreeClassifier

Examples using

`sklearn.tree.DecisionTreeClassi`

# sklearn.tree.DecisionTreeClassifier

```
class sklearn.tree.DecisionTreeClassifier(criterion='gini', splitter='best', max_depth=None, min_samples_split=2,
min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None, class_weight=None, presort='deprecated', ccp_alpha=0.0)
```

[source]

A decision tree classifier.

Read more in the [User Guide](#).

### Parameters:

#### criterion : {"gini", "entropy"}, default="gini"

The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain.

#### splitter : {"best", "random"}, default="best"

The strategy used to choose the split at each node. Supported strategies are "best" to choose the best split and "random" to choose the best random split.

#### max\_depth : int, default=None

The maximum depth of the tree. If None, then nodes are expanded until all leaves are pure or until all leaves contain less than min\_samples\_split samples.

#### min\_samples\_split : int or float, default=2

The minimum number of samples required to split an internal node:



# Decision Tree with Regression

## `sklearn.tree.DecisionTreeRegressor`

```
class sklearn.tree.DecisionTreeRegressor(criterion='mse', splitter='best', max_depth=None, min_samples_split=2,
min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None, presort='deprecated', ccp_alpha=0.0)
```

[source]

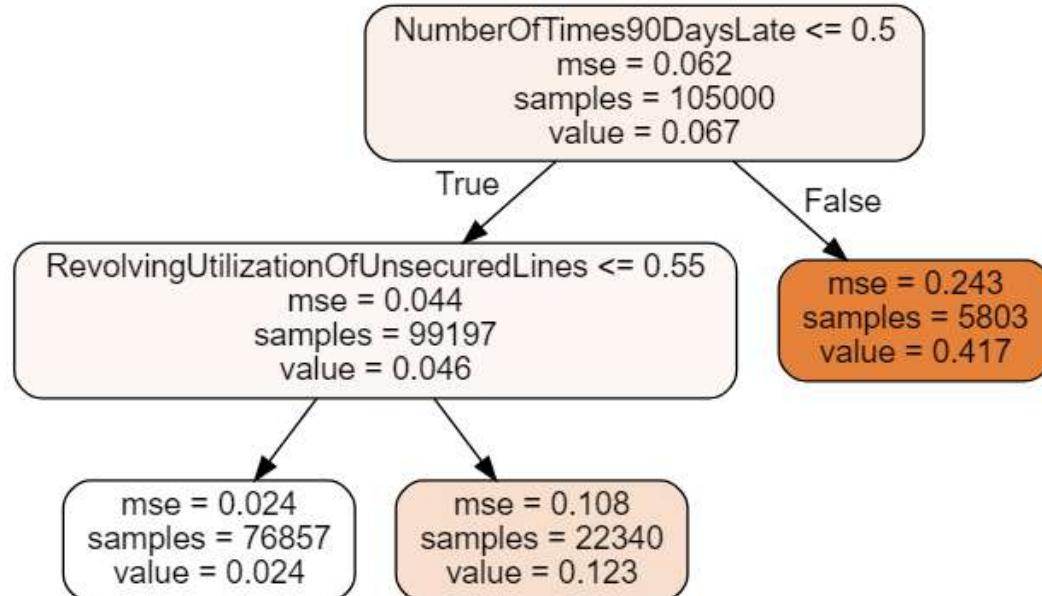
A decision tree regressor.

Read more in the [User Guide](#).

Parameters: `criterion : {"mse", "friedman_mse", "mae"},`

**MSE:** Mean Square Error

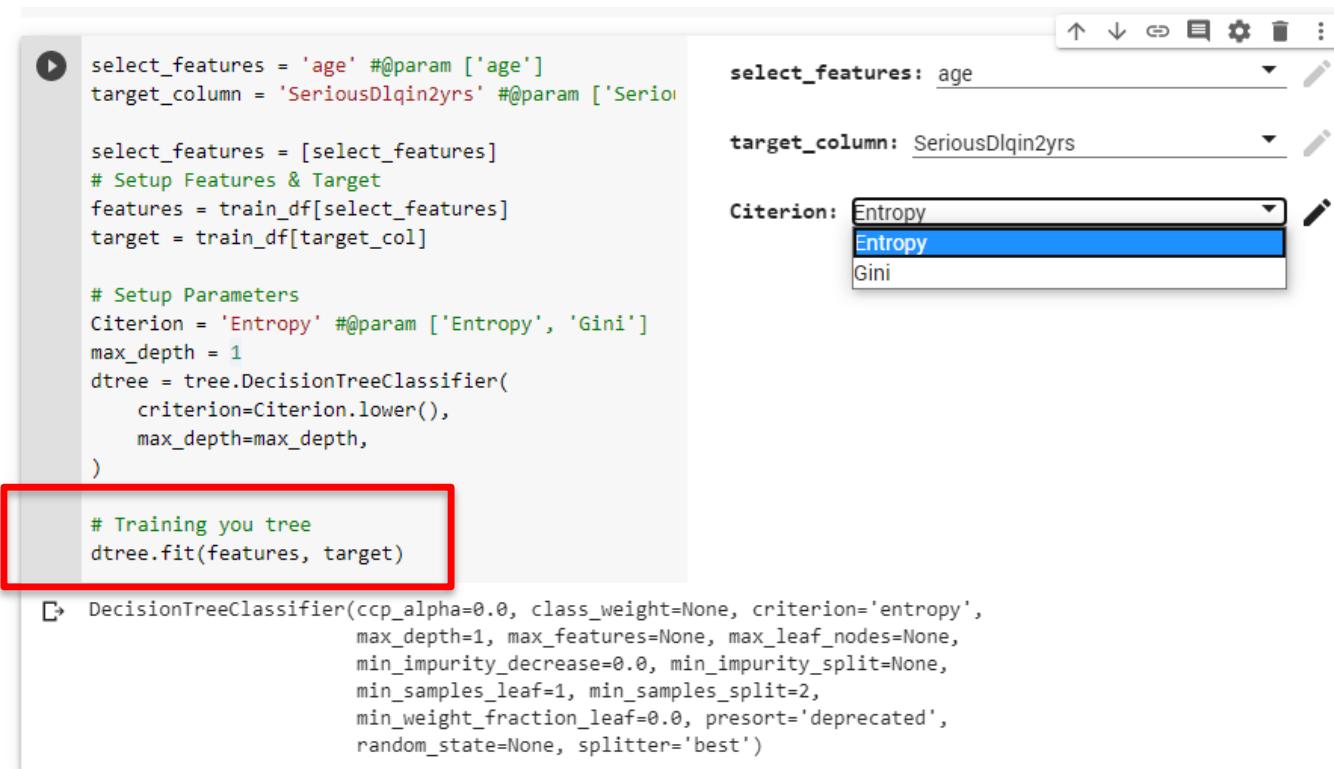
**MAE:** Mean Absolute Error





# Build your Decision Tree (cont.)

## Code Section 2.4



```
select_features = 'age' #@param ['age']
target_column = 'SeriousDlqin2yrs' #@param ['SeriousDlqin2yrs']

select_features = [select_features]
# Setup Features & Target
features = train_df[select_features]
target = train_df[target_col]

# Setup Parameters
Criterion = 'Entropy' #@param ['Entropy', 'Gini']
max_depth = 1
dtree = tree.DecisionTreeClassifier(
    criterion=Criterion.lower(),
    max_depth=max_depth,
)

# Training you tree
dtree.fit(features, target)
```

select\_features: age

target\_column: SeriousDlqin2yrs

Criterion: Entropy

Entropy

Gini



# Model Visualization (read the model)

## Basic Description

1. `get_params` : Get all model parameters
2. `get_depth` : Get depth of trained tree
3. `get_n_leaves` : Get number of nodes
4. `tree_.impurity` : Get Gini/Entropy values

```
1 Parameters: {  
  "ccp_alpha": 0.0,  
  "class_weight": null,  
  "criterion": "entropy",  
  "max_depth": 1,  
  "max_features": null,  
  "max_leaf_nodes": null,  
  "min_impurity_decrease": 0.0,  
  "min_impurity_split": null,  
  "min_samples_leaf": 1,  
  "min_samples_split": 2,  
  "min_weight_fraction_leaf": 0.0,  
  "presort": "deprecated",  
  "random_state": null,  
  "splitter": "best"  
}  
2 Tree Depth: 1  
3 Number of Node: 2  
4 Entropy of Nodes: [0.35401168 0.42690946 0.2175608 ]
```



## Model Visualization (cont.)

### `sklearn.tree.plot_tree`

```
sklearn.tree.plot_tree(decision_tree, *, max_depth=None, feature_names=None, class_names=None, label='all', filled=False, impurity=True, node_ids=False, proportion=False, rounded=False, precision=3, ax=None, fontsize=None) [source]
```

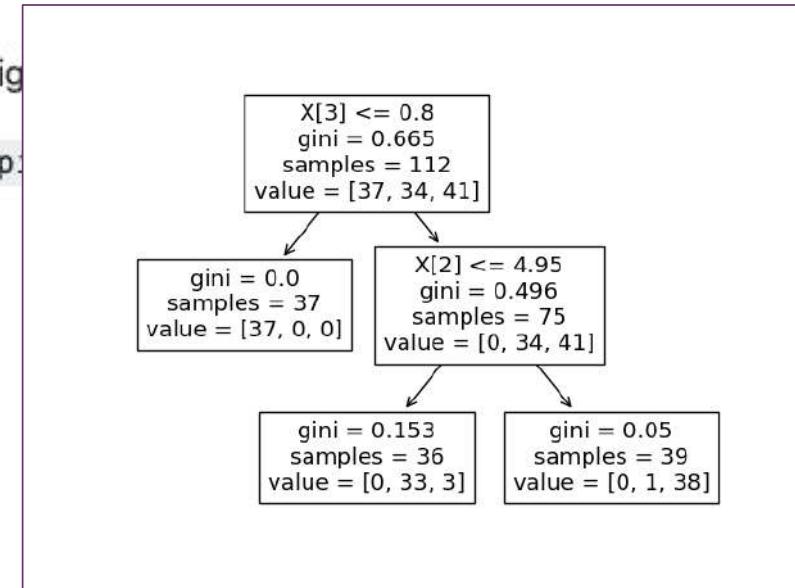
Plot a decision tree.

The sample counts that are shown are weighted with any sample\_weights that might be provided.

The visualization is fit automatically to the size of the axis. Use the `figsize` or `dpi` parameters to control the size of the rendering.

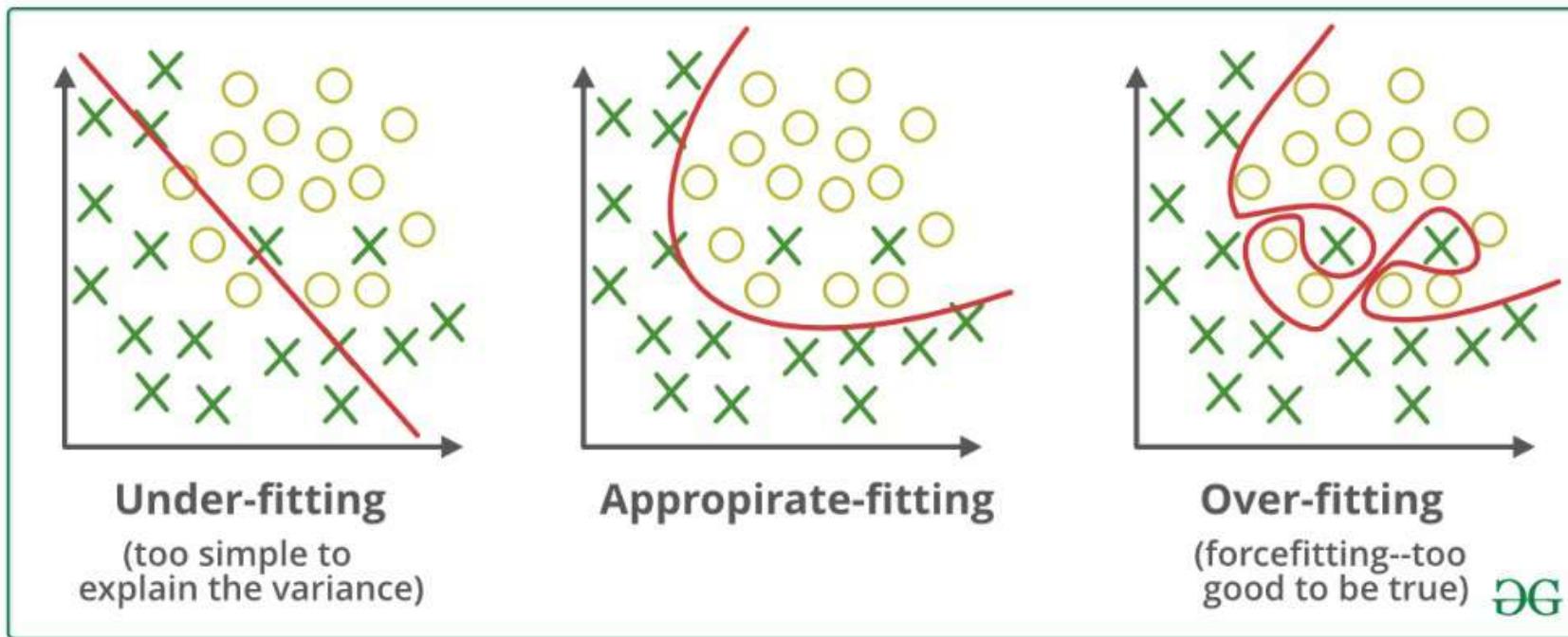
Read more in the [User Guide](#).

*New in version 0.21.*





## Overfitting



Source: <https://towardsdatascience.com/underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6fe4a8a49dbf>

DG

# + Pruning Tree

<https://scikit-learn.org/stable/modules/tree.html#minimal-cost-complexity-pruning/>

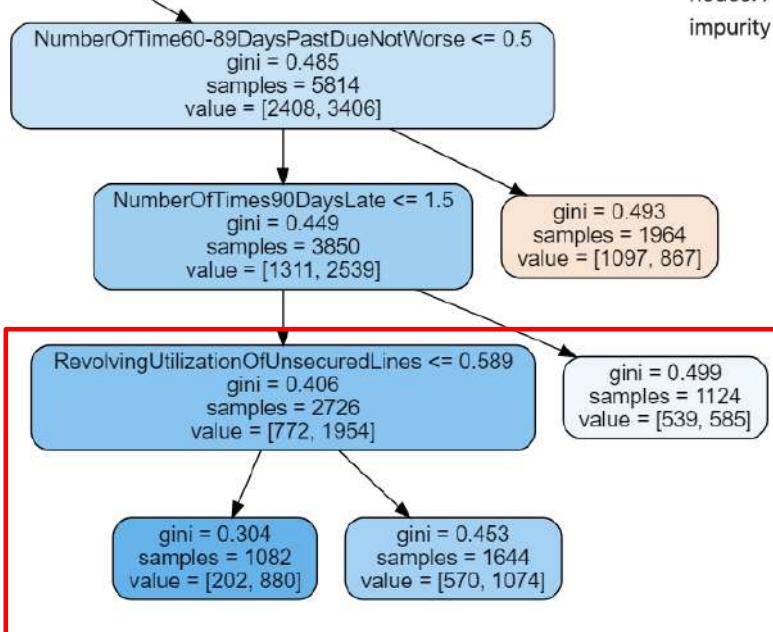
48

`ccp_alpha : non-negative float, default=0.0`

Complexity parameter used for Minimal Cost-Complexity Pruning. The subtree with the largest cost complexity that is smaller than `ccp_alpha` will be chosen. By default, no pruning is performed. See [Minimal Cost-Complexity Pruning](#) for details.

New in version 0.22.

More

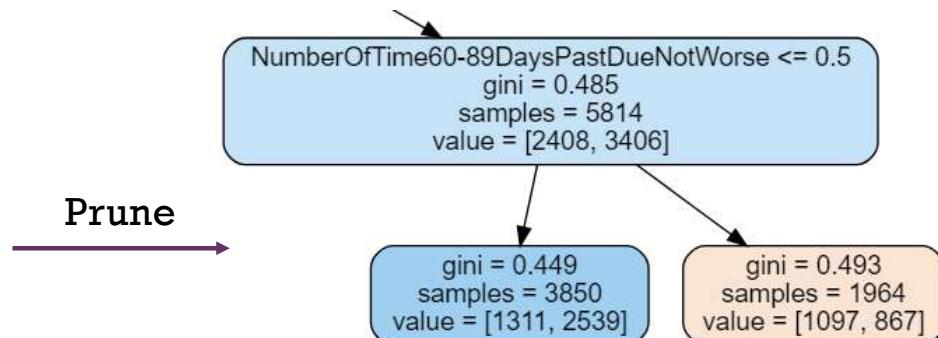


Impurity

Less

When impurity is too low, it cause more overfitting

where  $|T|$  is the number of terminal nodes in  $T$  and  $R(T)$  is traditionally defined as the total misclassification rate of the terminal nodes. Alternatively, scikit-learn uses the total sample weighted impurity of the terminal nodes for  $R(T)$ . As shown above, the impurity of a node depends on the criterion. Minimal cost-complexity pruning finds the subtree of  $T$  that minimizes  $R_\alpha(T)$ .



Prune

Test pruning parameter by `.cost_complexity_pruning_path`

```
dtree.cost_complexity_pruning_path(features, target)
```

```
{
  'ccp_alphas': array([0.0000000e+00, 8.91619910e-05, 1.17039010e-04, 1.29787452e-04,
  1.94525732e-04, 3.18283592e-04, 4.15157131e-04, 5.84363721e-04,
  6.81710606e-04, 1.05951846e-03, 1.17765555e-03, 1.83295138e-03,
  3.24166605e-03, 1.41432990e-02]),
  'impurities': array([0.10075641, 0.10084557, 0.10096261, 0.1010924 , 0.10128692,
  0.10160521, 0.10202036, 0.10260473, 0.10328644, 0.10434596,
  0.10552361, 0.10735656, 0.11059823, 0.12474153])}
}
```

`ccp_alphas`: Values which affect pruning (use lower bound value)

`Impurities`: Impurity after pruning (default=0; no pruning)

# Important Parameters in Decision Tree

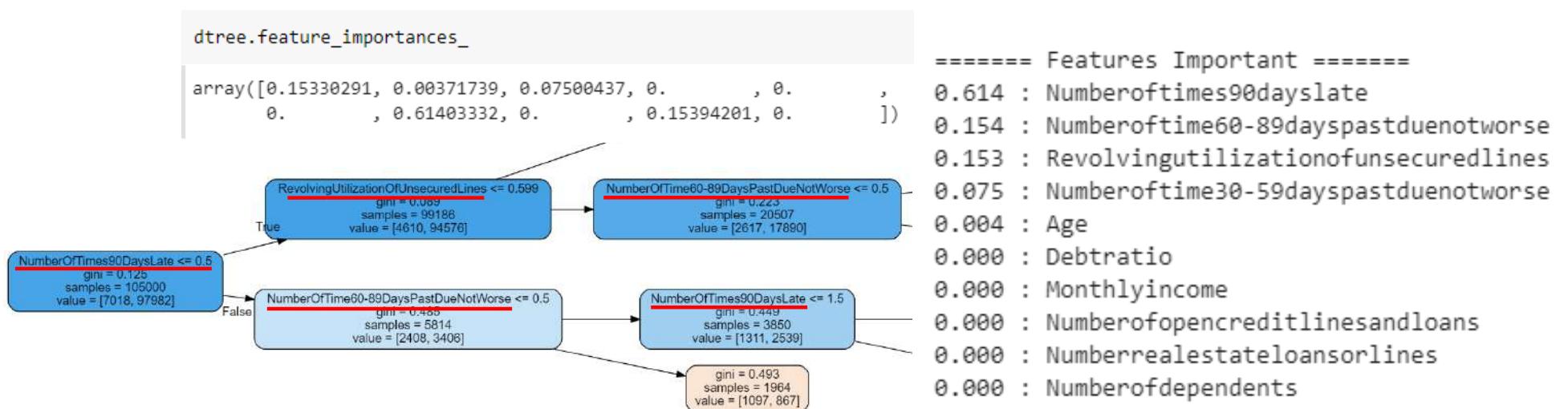


- Splitting measure (criterion) : gini / entropy
- Maximum depth : ~5-10 (depend on number of feature)
- Maximum leaf nodes : depend on number of class (target) and feature
- Minimum sample split : 5 – 20% (depend on number of data)
- Minimum impurity decrease : (default 0)
- Pruning adjustment (ccp\_alpha) : 0.001 - 0.01 (depend on size of tree)



# Which features are important ?

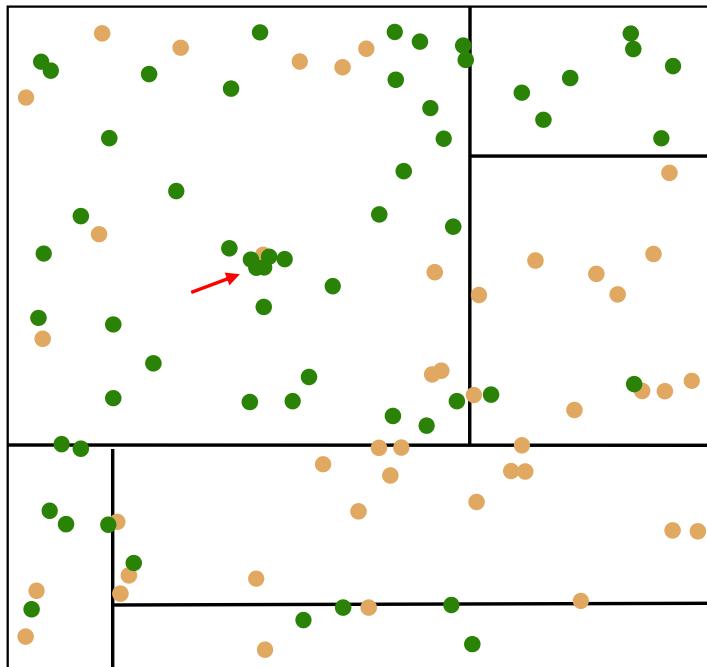
- Check how important by `.feature_importances_`
- The importance of a feature is computed as the (normalized) total reduction of the criterion brought by that feature. It is also known as **the gini importance**.



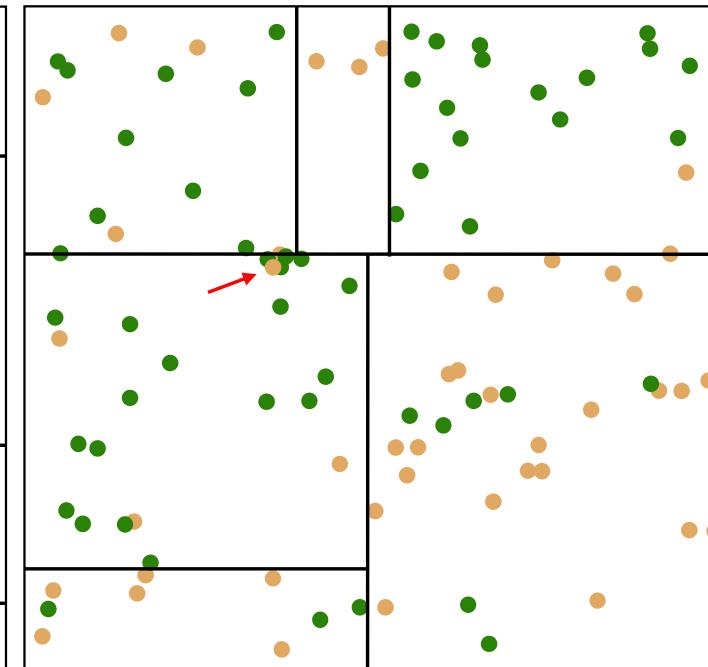
## + Instability

51

One reversal



Accuracy = 81%

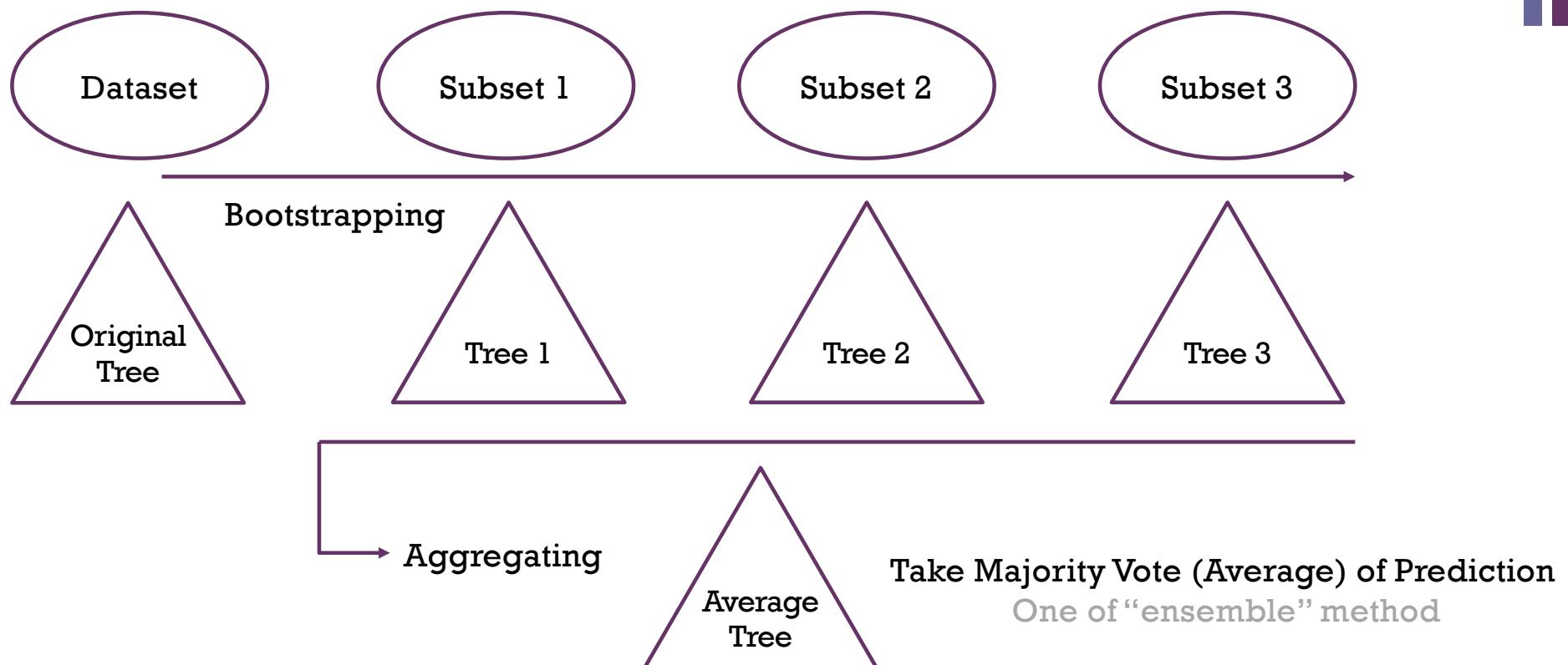


Accuracy = 80%

...



# Bagging (Bootstrap Aggregation)





# Bagging Method in sklearn

## sklearn.ensemble.BaggingClassifier

```
class sklearn.ensemble.BaggingClassifier(base_estimator=None, n_estimators=10, *, max_samples=1.0, max_features=1.0,  
bootstrap=True, bootstrap_features=False, oob_score=False, warm_start=False, n_jobs=None, random_state=None, verbose=0)
```

[\[source\]](#)

## sklearn.ensemble.BaggingRegressor

```
class sklearn.ensemble.BaggingRegressor(base_estimator=None, n_estimators=10, *, max_samples=1.0, max_features=1.0,  
bootstrap=True, bootstrap_features=False, oob_score=False, warm_start=False, n_jobs=None, random_state=None, verbose=0)
```

[\[source\]](#)

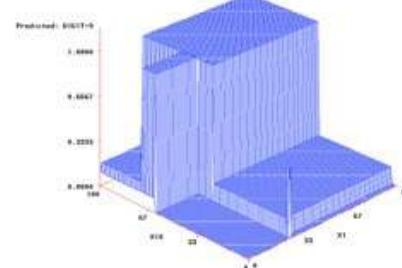
### Example

```
>>> from sklearn.ensemble import BaggingClassifier  
>>> from sklearn.tree import DecisionTreeClassifier  
>>> bagging = BaggingClassifier(DecisionTreeClassifier(),  
...                                max_samples=0.5, max_features=0.5)
```

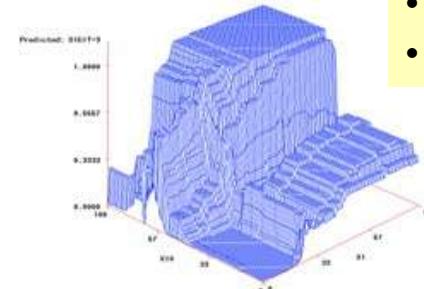
&gt;&gt;&gt;

# Random Forest Algorithm (RF)

- Forest algorithm samples the **rows** and the **columns** at each step.
- Forest takes bootstrap samples of the **rows** in training data (sampling with replacement)
- At each step, a set of variables (**columns**) is sampled.
- This increases variation among trees in the **ensemble** often leads to improved prediction accuracy.



Single Tree

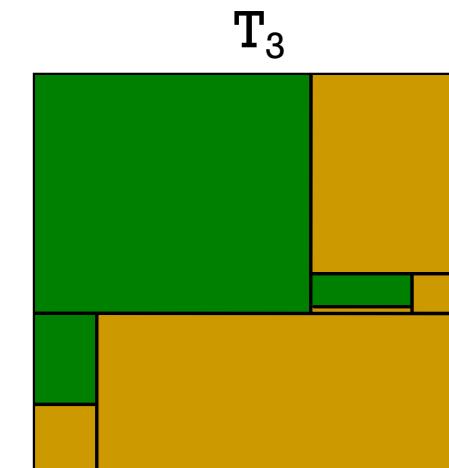
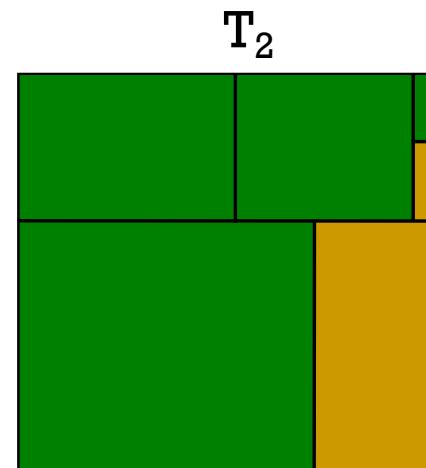
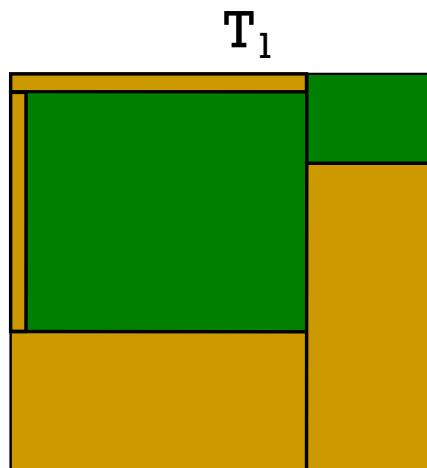


Random Forest

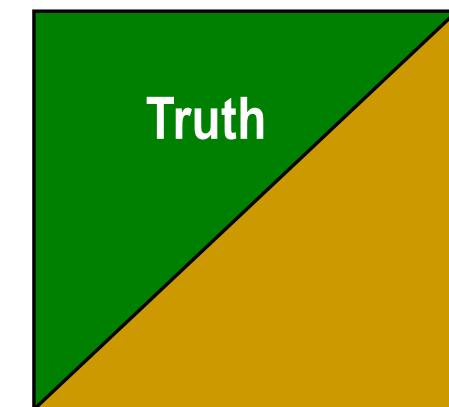
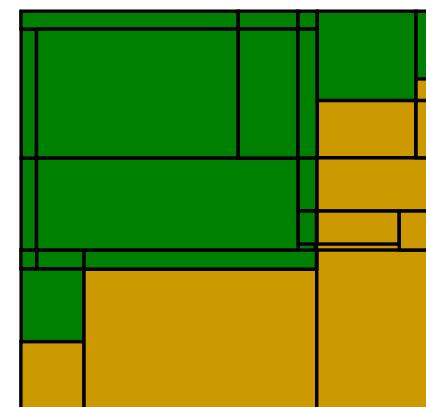
Important Params:

- #Tree
- #Columns (variables)
- #Rows (examples)

# Combine



$$\text{avg}(T_1, T_2, T_3) =$$



...



Prev Up Next

scikit-learn 0.22.2

Other versions

Please [cite us](#) if you use the software.

### 3.2.4.3.1.

#### sklearn.ensemble.RandomFores tClassifier

##### 3.2.4.3.1.1. Examples using

#### sklearn.ensemble.RandomForestC

## 3.2.4.3.1. `sklearn.ensemble.RandomForestClassifier`

```
class sklearn.ensemble.RandomForestClassifier(n_estimators=100, criterion='gini', max_depth=None, min_samples_split=2,
min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, min_impurity_decrease=0.0,
min_impurity_split=None, bootstrap=True, oob_score=False, n_jobs=None, random_state=None, verbose=0, warm_start=False,
class_weight=None, ccp_alpha=0.0, max_samples=None)
```

[\[source\]](#)

A random forest classifier.

A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is always the same as the original input sample size but the samples are drawn with replacement if `bootstrap=True` (default).

Read more in the [User Guide](#).

#### Parameters:

##### `n_estimators : integer, optional (default=100)`

The number of trees in the forest.

*Changed in version 0.22:* The default value of `n_estimators` changed from 10 to 100 in 0.22.

##### `criterion : string, optional (default="gini")`

The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain. Note: this parameter is tree-specific.



Prev Up Next

scikit-learn 0.22.2

Other versions

Please [cite us](#) if you use the software.

### 3.2.4.3.2.

#### sklearn.ensemble.RandomForestRegressor

##### 3.2.4.3.2.1. Examples using `sklearn.ensemble.RandomForestRe`

## 3.2.4.3.2. `sklearn.ensemble.RandomForestRegressor`

```
class sklearn.ensemble.RandomForestRegressor(n_estimators=100, criterion='mse', max_depth=None, min_samples_split=2,
min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, min_impurity_decrease=0.0,
min_impurity_split=None, bootstrap=True, oob_score=False, n_jobs=None, random_state=None, verbose=0, warm_start=False,
ccp_alpha=0.0, max_samples=None) ¶
```

[\[source\]](#)

A random forest regressor.

A random forest is a meta estimator that fits a number of classifying decision trees on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is always the same as the original input sample size but the samples are drawn with replacement if `bootstrap=True` (default).

Read more in the [User Guide](#).

**Parameters:** `n_estimators : integer, optional (default=10)`

The number of trees in the forest.

*Changed in version 0.22:* The default value of `n_estimators` changed from 10 to 100 in 0.22.

**criterion : string, optional (default="mse")**

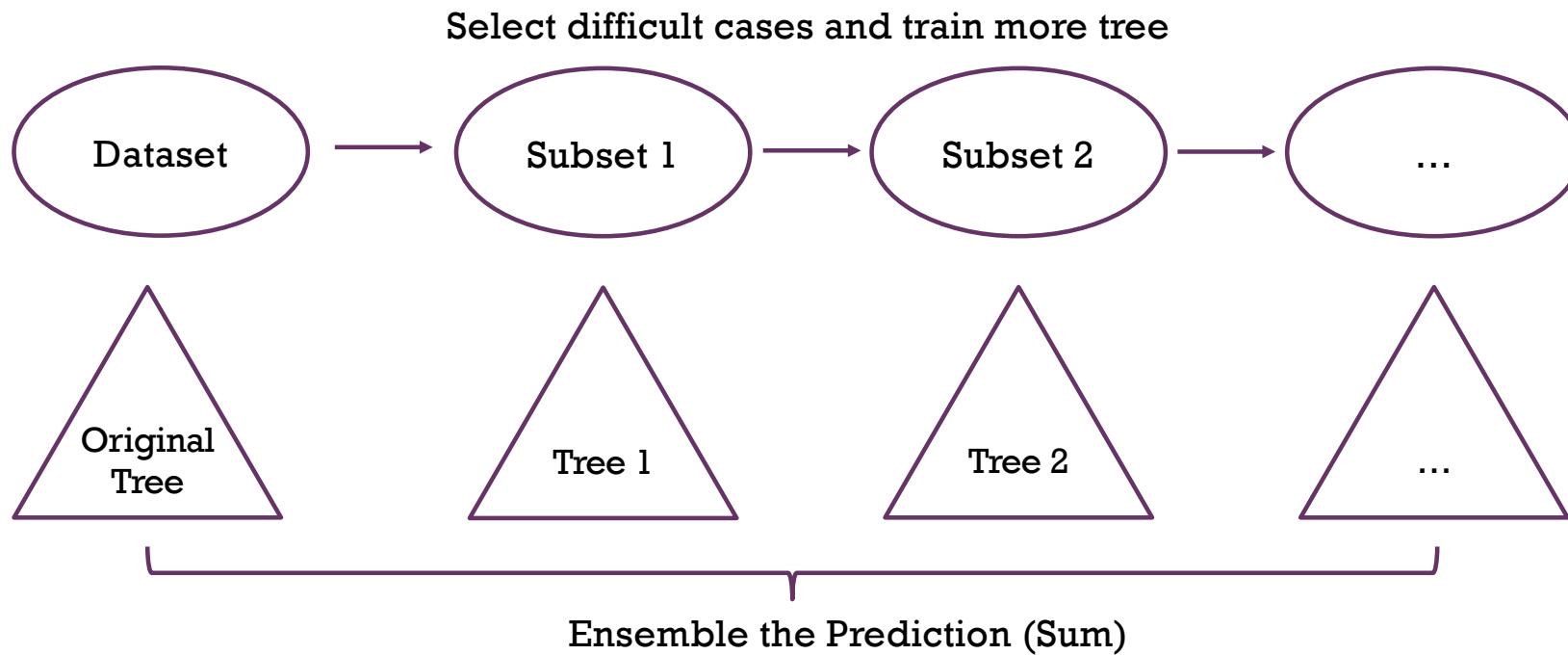
The function to measure the quality of a split. Supported criteria are "mse" for the mean squared error, which is equal to variance reduction as feature selection criterion, and "mae" for the mean absolute error.

*New in version 0.18:* Mean Absolute Error (MAE) criterion.



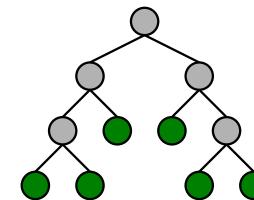
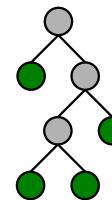
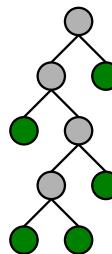
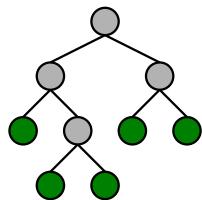
# Boosting

- Boosting is a method of converting **weak learners** into **strong learners**.
- In boosting, each new tree is a fit on a modified version of the original data set.



## Boosting (cont.)

	k=1		k=2		k=3		k=4 ...
<u>case</u>	<u>freq</u>	<u>m</u>	<u>freq</u>	<u>m</u>	<u>freq</u>	<u>m</u>	<u>freq</u>
1	1	1	1.5	1	.5	2	.97
2	1	0	.75	0	.25	0	.06
3	1	1	1.5	2	4.25	3	4.69
4	1	0	.75	1	.5	1	.11
5	1	0	.75	0	.25	0	.06
6	1	0	.75	0	.25	1	.11



\*Shown is Arc-x4, one method of boosting



# Boosting in sklearn

- AdaBoost, short for “Adaptive Boosting”

## sklearn.ensemble.AdaBoostClassifier

```
class sklearn.ensemble.AdaBoostClassifier(base_estimator=None, *, n_estimators=50, learning_rate=1.0, algorithm='SAMME.R', random_state=None)
```

[\[source\]](#)

## sklearn.ensemble.AdaBoostRegressor

```
class sklearn.ensemble.AdaBoostRegressor(base_estimator=None, *, n_estimators=50, learning_rate=1.0, loss='linear', random_state=None)
```

[\[source\]](#)

### Example

```
>>> from sklearn.ensemble import AdaBoostClassifier
>>> from sklearn.tree import DecisionTreeClassifier
>>> boosting = AdaBoostClassifier(DecisionTreeClassifier(),
...                                max_samples=0.5, max_features=0.5)
```

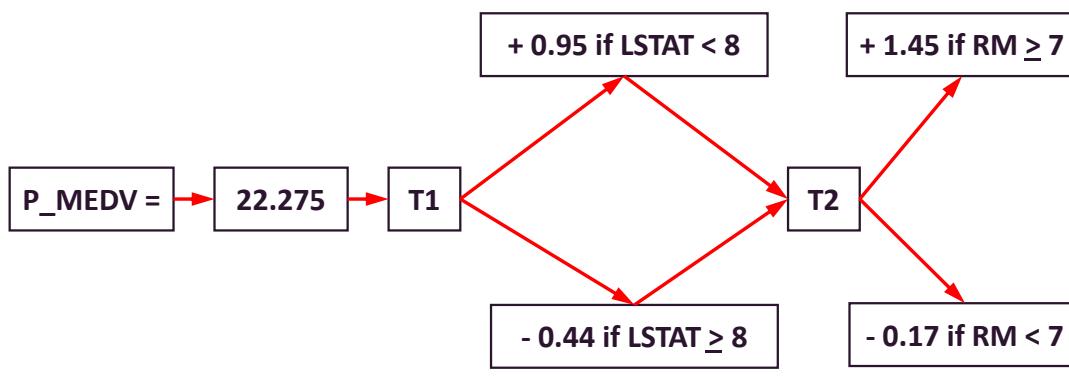
[>>>](#)

<https://towardsdatascience.com/boosting-algorithm-adaboost-b6737a9ee60c#:~:text=AdaBoost,classification%20can%20be%20represented%20as>



# Gradient Boosting Tree

- Boosting the performance by using **ensemble trees**
- Each tree in the next step aims to predict **error**.
- So, the prediction result is **the summation of all trees** (not average any more).
- In the final step, **weights** are assigned to all leaf nodes using **gradient descent** in order to finally reduce errors.



Boston House Price Prediction

- 'RM' is the average number of rooms among homes in the neighborhood.
- 'LSTAT' is the percentage of homeowners in the neighborhood considered "lower class" (working poor).

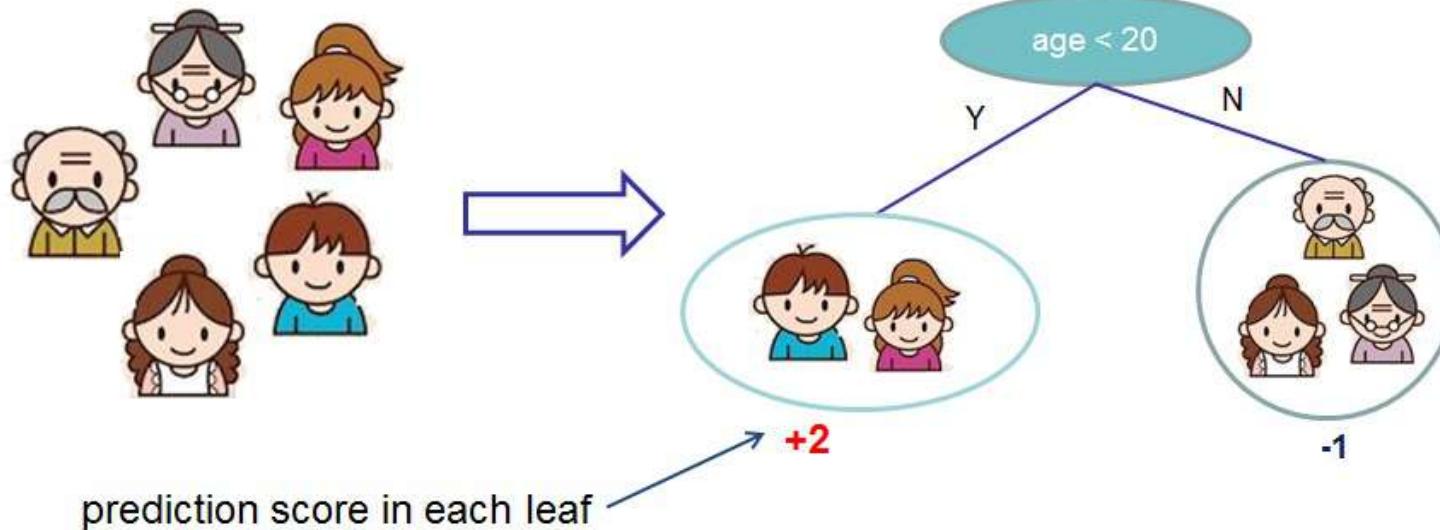


# Intro to Gradient Boosting Tree

## ■ Decision Tree

Input: age, gender, occupation, ...

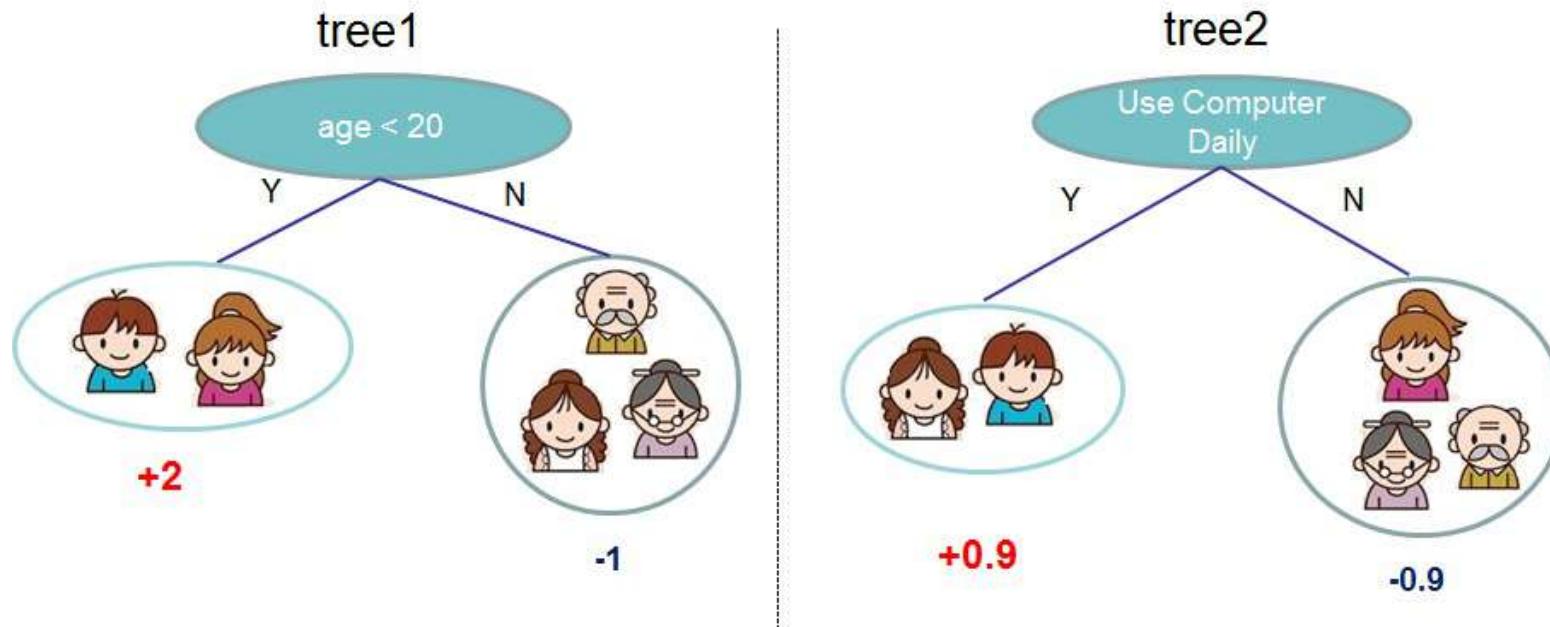
Like the computer game X





# Intro to Gradient Boosting Tree (cont.)

- Ensemble by weight on leaf nodes



$$f(\text{boy}) = 2 + 0.9 = 2.9$$

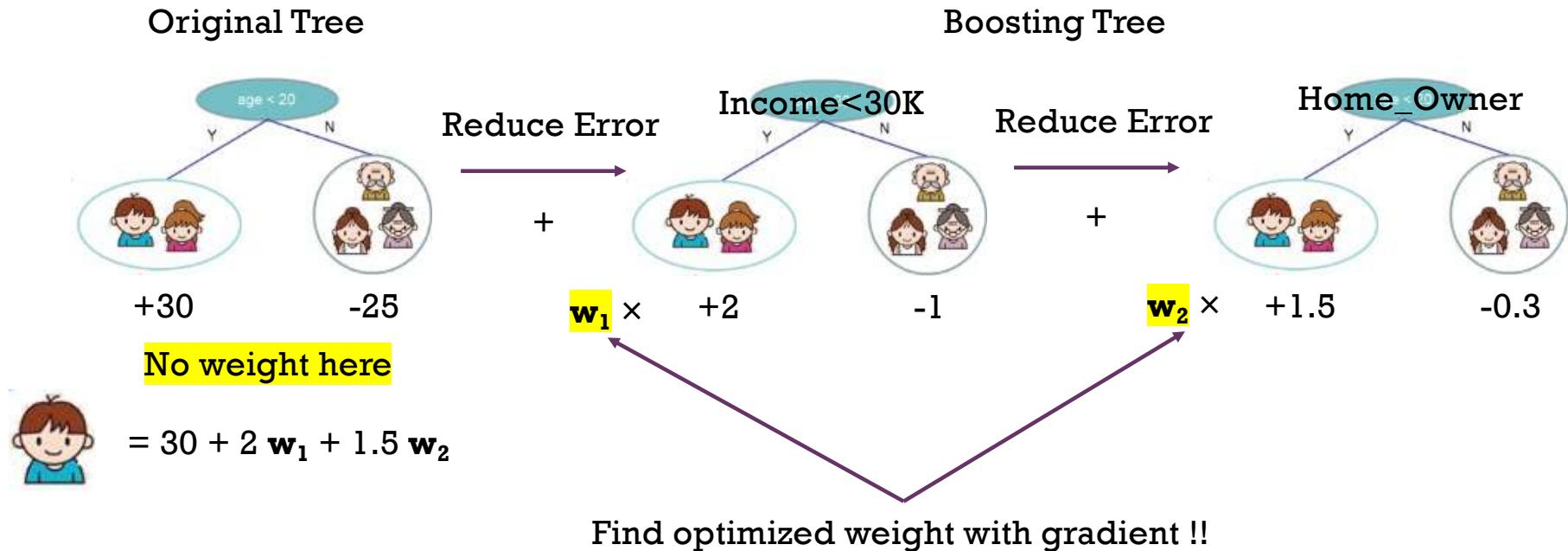


$$f(\text{elderly man}) = -1 - 0.9 = -1.9$$



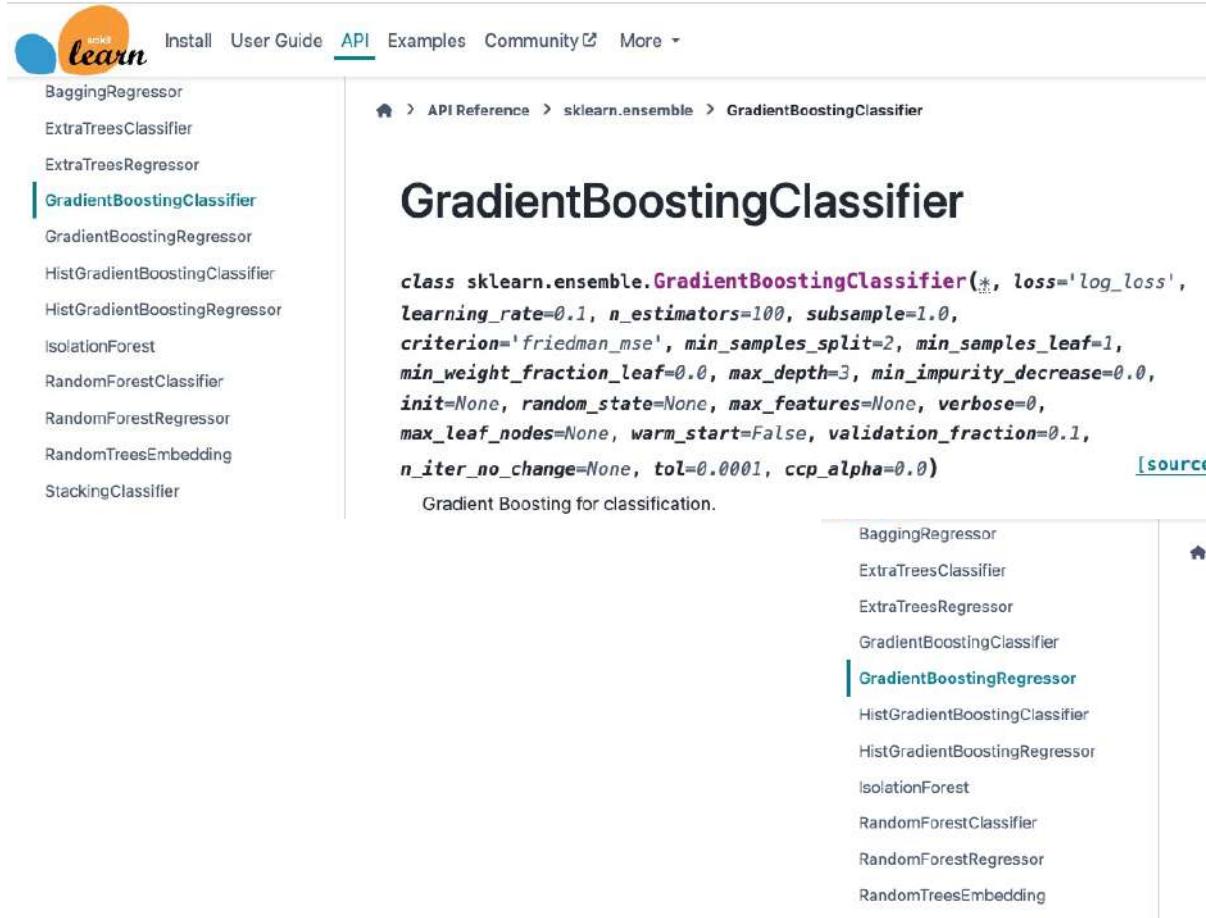
# Intro to Gradient Boosting Tree (cont.)

- Optimize weight of leaf nodes by gradient descent





# Gradient Boosting Tree in sklearn



The screenshot shows the scikit-learn API Reference page for the `GradientBoostingClassifier`. The left sidebar lists various classifiers, with `GradientBoostingClassifier` highlighted. The main content area shows the class definition:

```
class sklearn.ensemble.GradientBoostingClassifier(*, loss='log_loss',
    learning_rate=0.1, n_estimators=100, subsample=1.0,
    criterion='friedman_mse', min_samples_split=2, min_samples_leaf=1,
    min_weight_fraction_leaf=0.0, max_depth=3, min_impurity_decrease=0.0,
    init=None, random_state=None, max_features=None, verbose=0,
    max_leaf_nodes=None, warm_start=False, validation_fraction=0.1,
    n_iter_no_change=None, tol=0.0001, ccp_alpha=0.0)
```

Below the code, it says "Gradient Boosting for classification." To the right, there is a link to the source code and navigation links for examples, community, and more.



The screenshot shows the scikit-learn API Reference page for the `GradientBoostingRegressor`. The left sidebar lists various regressors, with `GradientBoostingRegressor` highlighted. The main content area shows the class definition:

```
class sklearn.ensemble.GradientBoostingRegressor(*,
    loss='squared_error', learning_rate=0.1, n_estimators=100, subsample=1.0,
    criterion='friedman_mse', min_samples_split=2, min_samples_leaf=1,
    min_weight_fraction_leaf=0.0, max_depth=3, min_impurity_decrease=0.0,
    init=None, random_state=None, max_features=None, alpha=0.9, verbose=0,
    max_leaf_nodes=None, warm_start=False, validation_fraction=0.1,
    n_iter_no_change=None, tol=0.0001, ccp_alpha=0.0)
```

Below the code, it says "Gradient Boosting for regression." To the right, there is a link to the source code and navigation links for examples, community, and more.

<https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.GradientBoostingClassifier.html>



# eXtreme Gradient Boosting Tree (XGBoost)

- XGBoost stands for “Extreme Gradient Boosting”, where the term “Gradient Boosting” originates from the paper *Greedy Function Approximation: A Gradient Boosting Machine*, by Friedman.
- XGBoost is exactly a tool motivated by the formal principle introduced in this tutorial! More importantly, it is developed with both deep consideration in terms of **systems optimization** and **principles in machine learning**. The goal of this library is to push the extreme of the computation limits of machines to provide a **scalable, portable and accurate library**

Aspect	Traditional GBDT	XGBoost
Tree building	Sequential	Sequential
In-tree parallelism	Limited	✓ Yes
Split strategy	Exact greedy	Histogram-based

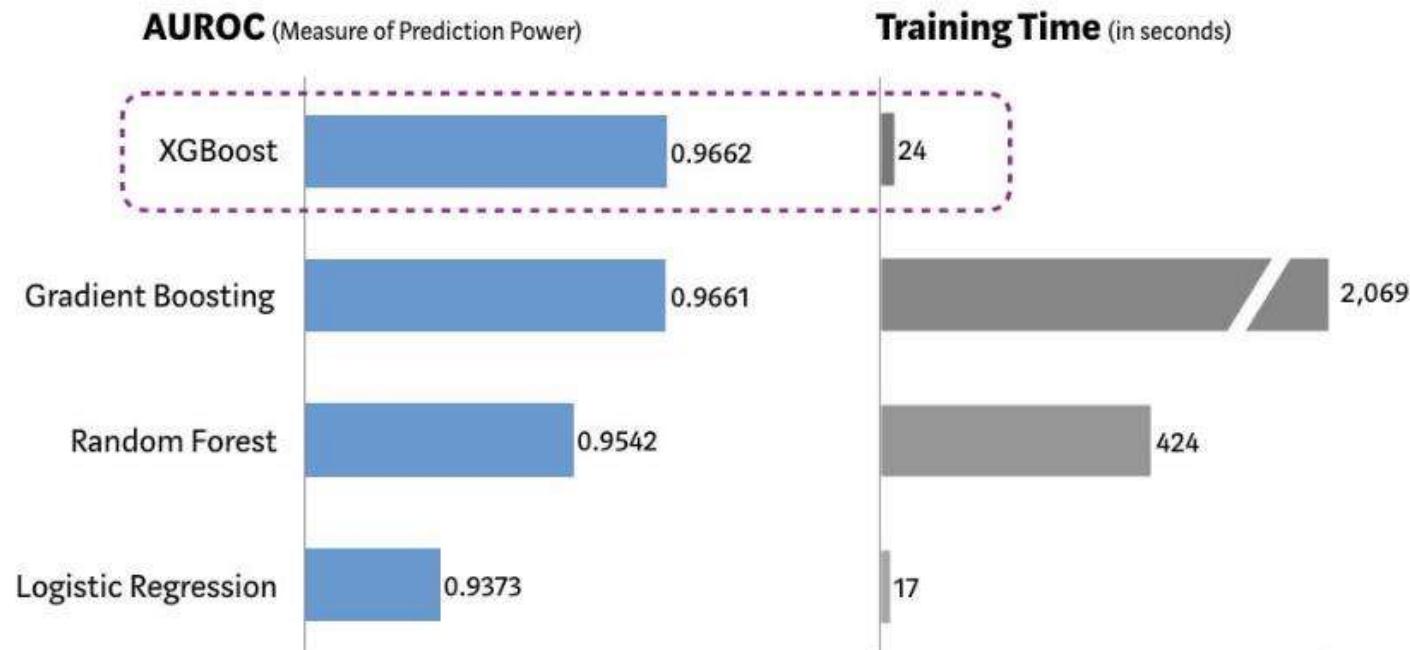
*dmlc*  
**XGBoost**



# Models Performance

## Performance Comparison using SKLearn's 'Make\_Classification' Dataset

(5 Fold Cross Validation, 1MM randomly generated data sample, 20 features)





# XGBoost Package

- Multiple Language Support 
- Distributed Model on Cloud
  - AWS
  - Kubernetes
  - Spark
  - Dask
- Compatible with sklearn interface

Python package

R package

JVM package

Ruby package

Swift package

Julia package

C Package

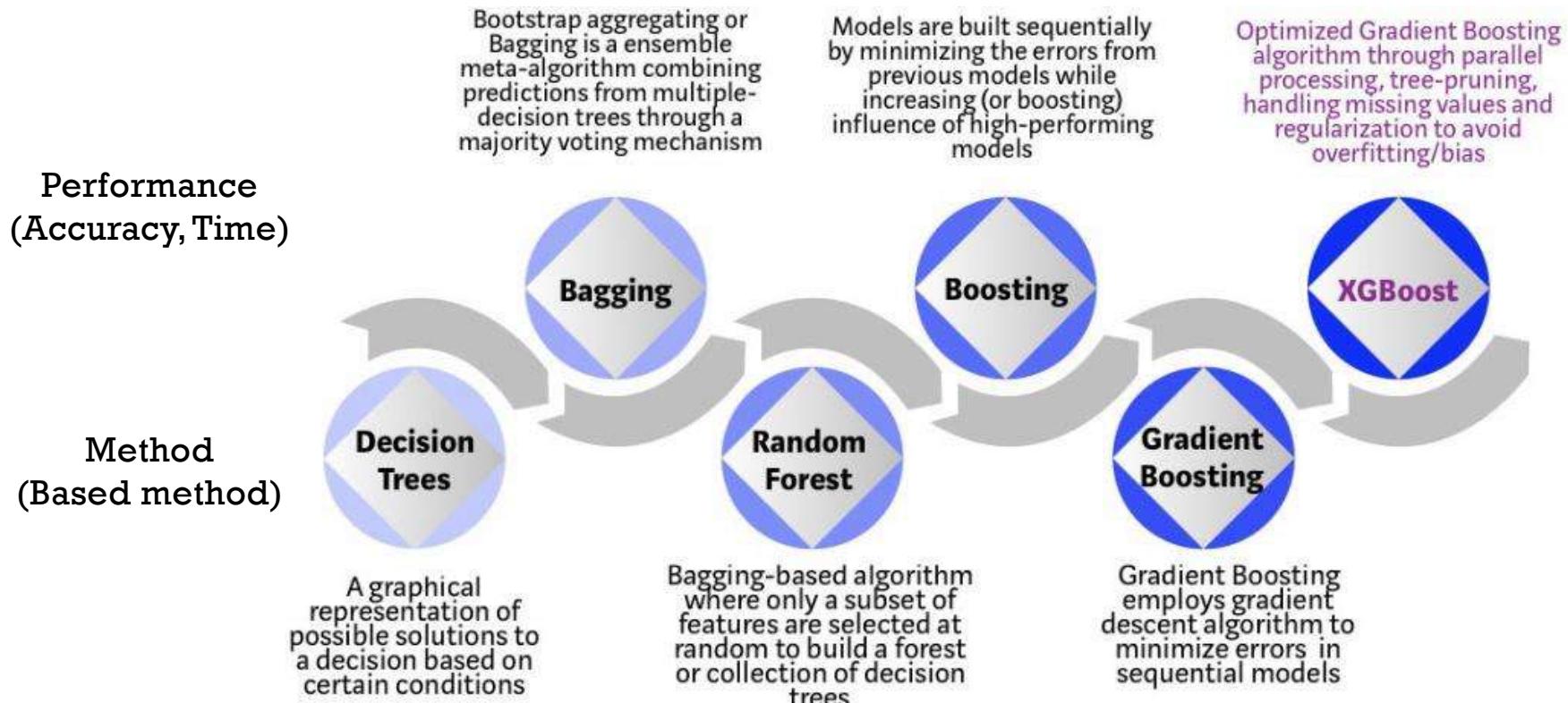


## XGBoost Important Parameter



- `n_jobs` : Number of parallel tasks (`-1 = all cores`)
- `objective` : Type of Prediction
  - for Classification `'binary:hinge'`, `'binary:logistic'` (prob) or `'multi:softmax'` (multi-class)
  - for Regression `'reg:squarederror'`
- `learning_rate` : Step size used in update weights
- `n_estimators` : Number of trees
- `subsample (0, 1]`: Number of training data to growing trees, will prevent overfitting
- `importance_type` : Get feature importance of each feature.
  - `'weight'`: the number of times a feature is used to split the data across all trees.
  - `'gain'`: the average gain across all splits the feature is used in.
  - `'cover'`: the average coverage across all splits the feature is used in.
  - `'total_gain'`: the total gain across all splits the feature is used in.
  - `'total_cover'`: the total coverage across all splits the feature is used in.

# Evolution of Decision Trees



Source: <https://towardsdatascience.com/https-medium-com-vishalmorde-xgboost-algorithm-long-she-may-rein-edd9f99be63d>



## Note: Always set random\_state in tree-based model

- **Randomness in Splitting Criteria:** During training, if multiple splits have the same quality (e.g., information gain, Gini impurity), the algorithm chooses one randomly. This randomness can cause variations in the resulting tree structure.

Without random\_state:

```
python

from sklearn.tree import DecisionTreeClassifier
from sklearn.datasets import load_iris

# Load dataset
data = load_iris()
X, y = data.data, data.target

# Train decision tree multiple times
model1 = DecisionTreeClassifier()
model2 = DecisionTreeClassifier()
model1.fit(X, y)
model2.fit(X, y)

# Check if results are the same
print(model1.feature_importances_)
print(model2.feature_importances_)
```

You might get **different feature importances** or splits each time you run the code.

With random\_state:

```
python

model1 = DecisionTreeClassifier(random_state=42)
model2 = DecisionTreeClassifier(random_state=42)
model1.fit(X, y)
model2.fit(X, y)

# Check if results are the same
print(model1.feature_importances_)
print(model2.feature_importances_)
```

Now, the results are consistent.

[Prev](#) [Up](#) [Next](#)**scikit-learn 1.2.1**[Other versions](#)Please [cite us](#) if you use the software.

[sklearn.feature\\_selection.SelectFromModel](#)  
[SelectFromModel](#)  
Examples using  
[sklearn.feature\\_selection.Select](#)

## sklearn.feature\_selection.SelectFromModel ¶

```
class sklearn.feature_selection.SelectFromModel(estimator, *, threshold=None, prefit=False, norm_order=1,
max_features=None, importance_getter='auto')
```

[\[source\]](#)

Meta-transformer for selecting features based on importance weights.

New in version 0.17.

Read more in the [User Guide](#).

**Parameters:** **estimator : object**

The base estimator from which the transformer is built. This can be both a fitted (if `prefit` is set to True) or a non-fitted estimator. The estimator should have a `feature_importances_` or `coef_` attribute after fitting. Otherwise, the `importance_getter` parameter should be used.

**threshold : str or float, default=None**

The threshold value to use for feature selection. Features whose absolute importance value is greater or equal are kept while the others are discarded. If "median" (resp. "mean"), then the `threshold` value is the median (resp. the mean) of the feature importances. A scaling factor (e.g., "1.25\*mean") may also be used. If None and if the estimator has a parameter penalty set to l1, either explicitly or implicitly (e.g, Lasso), the threshold used is 1e-5. Otherwise, "mean" is used by default.

**prefit : bool, default=False**

Whether a prefit model is expected to be passed into the constructor directly or not. If True, estimator

[https://scikit-learn.org/stable/modules/generated/sklearn.feature\\_selection.SelectFromModel.html](https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.SelectFromModel.html)

[Toggle Menu](#)[https://scikit-learn.org/stable/modules/classes.html#module-sklearn.feature\\_selection](https://scikit-learn.org/stable/modules/classes.html#module-sklearn.feature_selection)



```

from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from sklearn.feature_selection import SelectFromModel
import pandas as pd

# Load dataset
data = load_iris()
X = data.data # Features
y = data.target # Target
feature_names = data.feature_names

# Train a Decision Tree Classifier
tree_model = DecisionTreeClassifier(random_state=42)
tree_model.fit(X, y)

# Use SelectFromModel with threshold=0
selector = SelectFromModel(tree_model, prefit=True, threshold=0)

# Transform the dataset to keep only selected features
X_selected = selector.transform(X)

# Get selected feature names
selected_features = [feature_names[i] for i in selector.get_support(indices=True)]

# Display results
print("Selected Features (Threshold = 0):")
print(selected_features)

# Optionally, display feature importances for reference
feature_importances = pd.DataFrame({
    'Feature': feature_names,
    'Importance': tree_model.feature_importances_
}).sort_values(by='Importance', ascending=False)

print("\nFeature Importances:")
print(feature_importances)

print("\nShape of Original Dataset:", X.shape)
print("Shape of Dataset After Feature Selection:", X_selected.shape)

```

Selected Features (Threshold = 0):  
['sepal length (cm)', 'petal length (cm)', 'petal width (cm)']

	Feature	Importance
2	petal length (cm)	0.734006
3	petal width (cm)	0.239972
0	sepal length (cm)	0.026022
1	sepal width (cm)	0.000000

Shape of Original Dataset: (150, 4)  
Shape of Dataset After Feature Selection: (150, 3)



```
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from sklearn.feature_selection import SelectFromModel
import pandas as pd

# Load the Iris dataset (replace this with your own dataset if needed)
data = load_iris()
X = data.data # Features
y = data.target # Target
feature_names = data.feature_names

# Train a Decision Tree Classifier
tree_model = DecisionTreeClassifier(random_state=42)
tree_model.fit(X, y)

# Extract feature importances
feature_importances = tree_model.feature_importances_

# Display feature importances for better understanding
importance_df = pd.DataFrame({
    'Feature': feature_names,
    'Importance': feature_importances
}).sort_values(by='Importance', ascending=False)

print("Feature Importances:")
print(importance_df)

# Use SelectFromModel for feature selection
selector = SelectFromModel(tree_model, prefit=True, threshold="mean")

# Transform the dataset to keep only selected features
X_selected = selector.transform(X)

# Get selected feature names
selected_features = [feature_names[i] for i in selector.get_support(indices=True)]

# Output results
print("\nSelected Features:")
print(selected_features)

print("\nShape of Original Dataset:", X.shape)
print("Shape of Dataset After Feature Selection:", X_selected.shape)
```

## Default threshold=mean

### Feature Importances:

	Feature	Importance
2	petal length (cm)	0.734006
3	petal width (cm)	0.239972
0	sepal length (cm)	0.026022
1	sepal width (cm)	0.000000

### Selected Features:

```
['petal length (cm)', 'petal width (cm)']
```

Shape of Original Dataset: (150, 4)

Shape of Dataset After Feature Selection: (150, 2)



```

from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from sklearn.feature_selection import SelectFromModel
import numpy as np
import pandas as pd

# Load the Iris dataset
data = load_iris()
X = data.data # Features
y = data.target # Target
feature_names = data.feature_names

# Train a Decision Tree Classifier
tree_model = DecisionTreeClassifier(random_state=42)
tree_model.fit(X, y)

# Use SelectFromModel with threshold=-np.inf to consider all features and limit to top 2 features
selector = SelectFromModel(estimator=tree_model, prefit=True, threshold=-np.inf, max_features=2)
X_selected = selector.transform(X)

# Get the names of the selected features
selected_features = [feature_names[i] for i in selector.get_support(indices=True)]

# Display the results
print("Selected Features (Top 2):")
print(selected_features)

# Optionally, show the feature importances
feature_importances = pd.DataFrame({
    'Feature': feature_names,
    'Importance': tree_model.feature_importances_
}).sort_values(by='Importance', ascending=False)

print("\nFeature Importances:")
print(feature_importances)

print("\nShape of Original Dataset:", X.shape)
print("Shape of Dataset After Feature Selection:", X_selected.shape)

```

**max\_features=2****threshold=-inf**

Ensures that all features are considered for selection

Selected Features (Top 2):  
['petal length (cm)', 'petal width (cm)']

Feature Importances:

	Feature	Importance
2	petal length (cm)	0.734006
3	petal width (cm)	0.239972
0	sepal length (cm)	0.026022
1	sepal width (cm)	0.000000

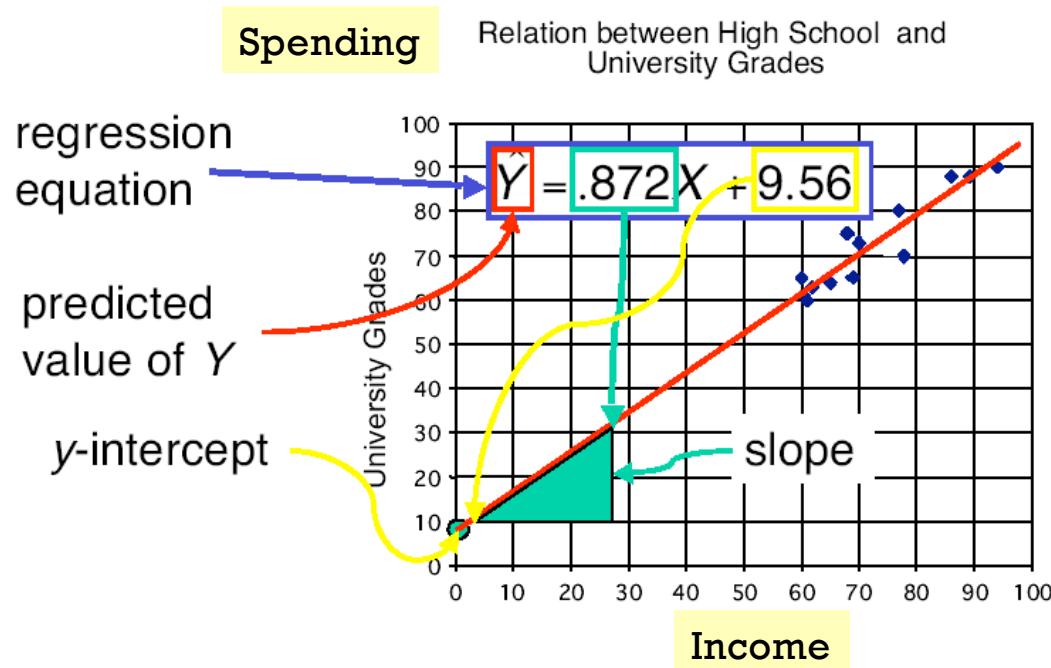
Shape of Original Dataset: (150, 4)  
Shape of Dataset After Feature Selection: (150, 2)

+

## 2) Regression



## 2) Regression



weight, coefficient

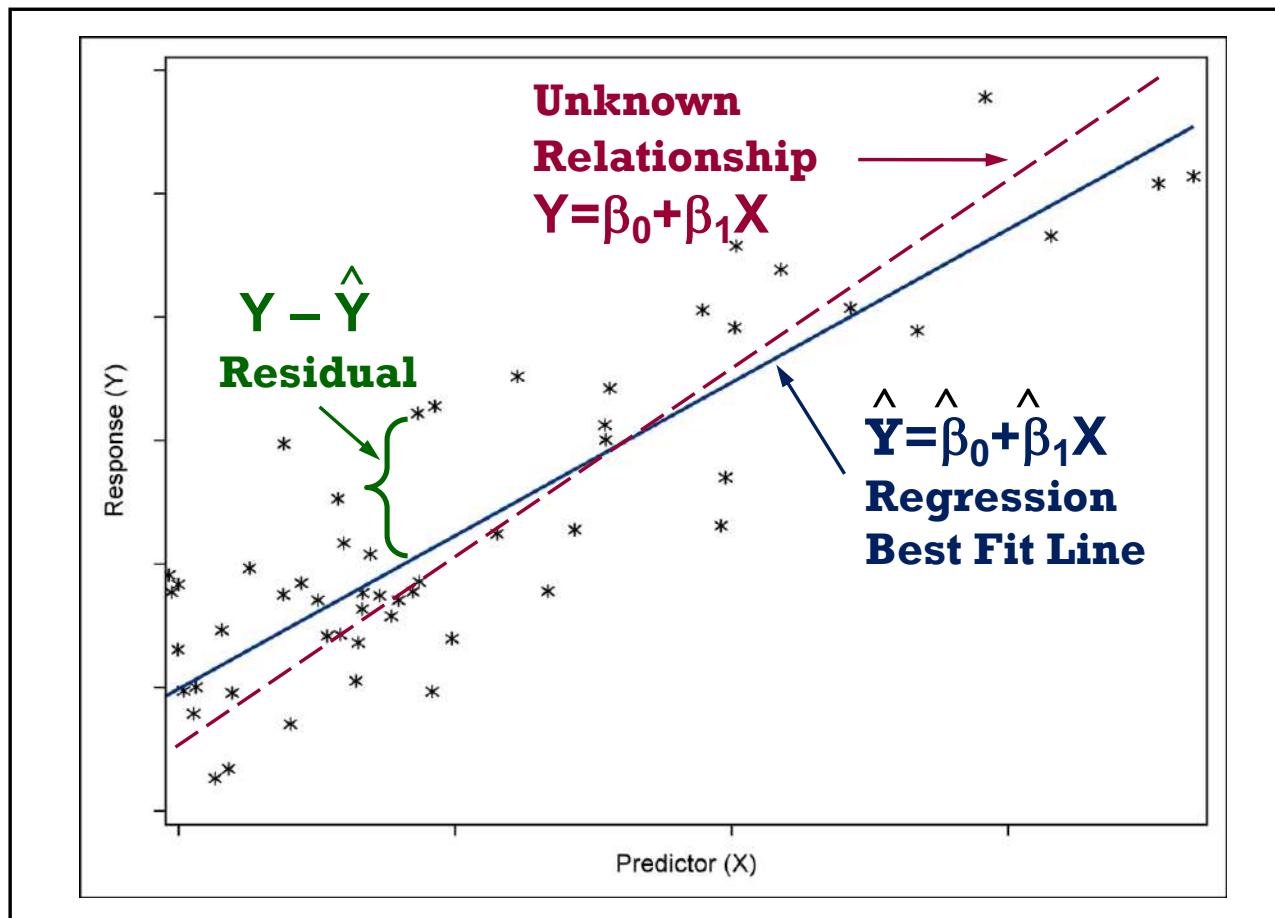
$\hat{y} = \widehat{w}_0 + \widehat{w}_1 x_1 + \widehat{w}_2 x_2$

target      intercept      input

- The least square method aims to minimize the following term

$$\sum_{\text{training data}} (y_i - \hat{y}_i)^2$$

# Ordinary Least Squares (OLS) Regression



# Multiple Linear Regression Model Matrix Multiplication Approach

	inputs	target
Age	Income in k\$	Spending
25	25	400
35	50	500
32	35	550

$$Y = \beta_0(1) + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$

$$[Y] = [X][\beta]$$

$$[\beta] = [X]^{-1}[Y]$$

General least-squares solution:

$$\beta = (X^T X)^{-1} X^T Y$$

$$y = \begin{bmatrix} 400 \\ 500 \\ 550 \end{bmatrix} \quad X = \begin{bmatrix} 1 & 25 & 25 \\ 1 & 35 & 50 \\ 1 & 32 & 35 \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

In this toy example,  $X$  is  $3 \times 3$  and invertible, so it fits exactly and you can also use:  
 $\beta = X^{-1}y$

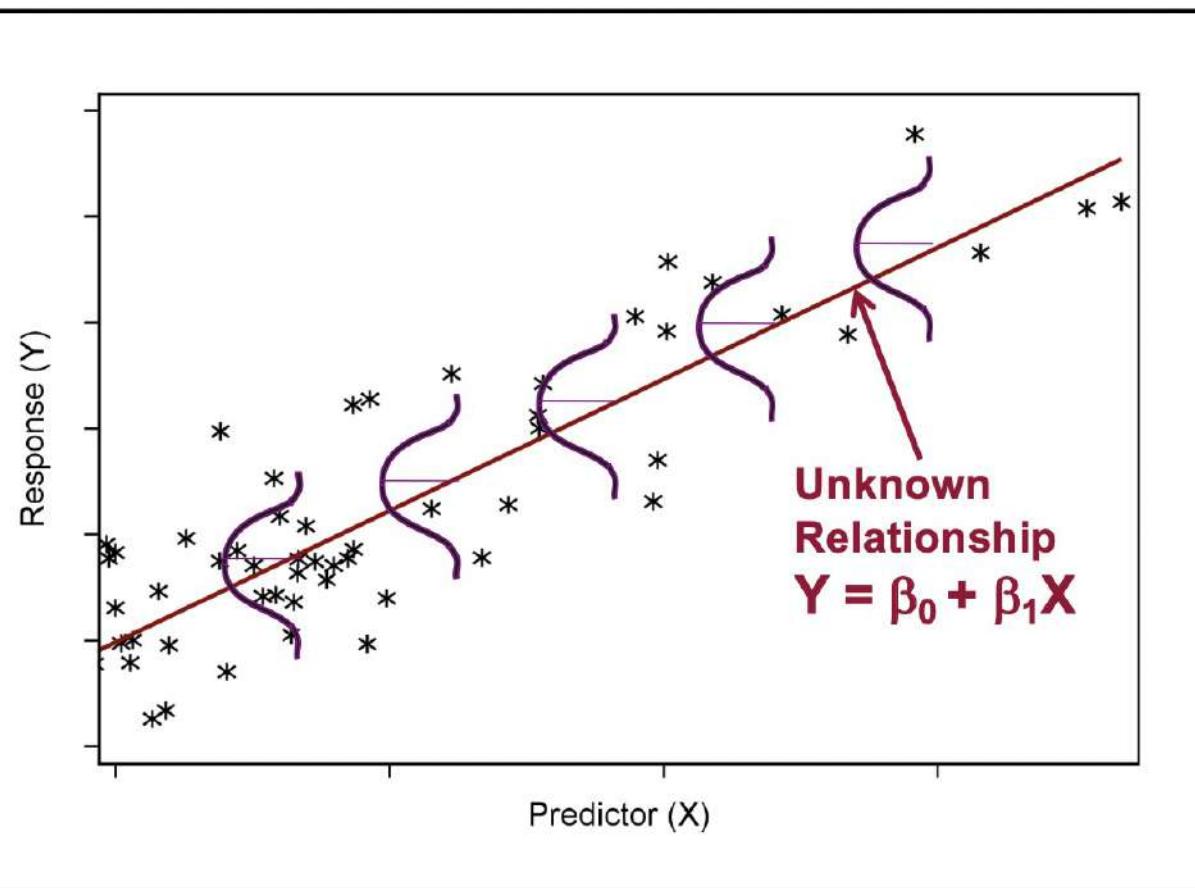
$$\beta = \begin{bmatrix} -250 \\ \frac{110}{3} \\ -\frac{32}{3} \end{bmatrix} \approx \begin{bmatrix} -250 \\ 36.6667 \\ -10.6667 \end{bmatrix}$$

$$\widehat{\text{Spending}} = -250 + 36.6667(\text{Age}) - 10.6667(\text{Income in k\$})$$



# Linear Regression Assumption

$$\text{Spending} = 500 + 10 \times \text{Income10K} + 2 \times \text{Age}$$



- Linear relationship between  $(y, x_i)$ . [Pearson correlation]
- Error is normal distributed. [remove outliers, log-transformation]
- Error has equal variance (homoscedasticity) [remove outliers, log-transformation]
- Errors are independent from each other. [design new data correction]



## sklearn.linear\_model.LinearRegression

```
class sklearn.linear_model.LinearRegression(fit_intercept=True, normalize=False, copy_X=True, n_jobs=None)
```

[source]

Ordinary least squares Linear Regression.

LinearRegression fits a linear model with coefficients  $w = (w_1, \dots, w_p)$  to minimize the residual sum of squares between the observed targets in the dataset, and the targets predicted by the linear approximation.

**Parameters:** `fit_intercept : bool, optional, default True`

Whether to calculate the intercept for this model. If set to False, no intercept will be used in calculations (i.e. data is expected to be centered).

`normalize : bool, optional, default False`

This parameter is ignored when `fit_intercept` is set to True. It is there for consistency with other estimators that perform regression by subtracting the mean and dividing by the L2-norm. If you wish to standardize, please use `StandardScaler` before calling `fit` on an estimator with `normalize=False`.

`normalize : bool, default=False`

This parameter is ignored when `fit_intercept` is set to False. If True, the regressors  $X$  will be normalized before regression by subtracting the mean and dividing by the L2-norm. If you wish to standardize, please use `StandardScaler` before calling `fit` on an estimator with `normalize=False`.

*Deprecated since version 1.0: `normalize` was deprecated in version 1.0 and will be removed in 1.2.*

**Attributes::** `coef_ : array of shape (n_features, ) or (n_targets, n_features)`

Estimated coefficients for the linear regression problem. If multiple targets are passed during the fit (y 2D),

`intercept_ : float or array of shape (n_targets, )`

Independent term in the linear model. Set to 0.0 if `fit_intercept = False`.

`n_features_in_ : int`

Number of features seen during `fit`.

New in version 0.24.

for  $n_{targets} > 1$  and sufficient

`one` means 1 unless in a `joblib.parallel_backend` context. `-1` means using all processors.

more details.

`feature_names_in_ : ndarray of shape (n_features_in_, )`

Names of features seen during `fit`. Defined only when  $X$  has feature names that are all strings.

New in version 1.0.



# Regression with Regularization

## ■ Lasso Regression (L1 Regularization)

**Lasso Regression** (Least Absolute Shrinkage and Selection Operator) adds “absolute value of magnitude” of coefficient as penalty term to the loss function.

$$\sum_{i=1}^n (Y_i - \sum_{j=1}^p X_{ij}\beta_j)^2 + \lambda \sum_{j=1}^p |\beta_j|$$

Cost function

## ■ Ridge Regression (L2 Regularization)

**Ridge regression** adds “squared magnitude” of coefficient as penalty term to the loss function. Here the *highlighted* part represents L2 regularization element.

$$\sum_{i=1}^n (y_i - \sum_{j=1}^p x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^p \beta_j^2$$

Cost function

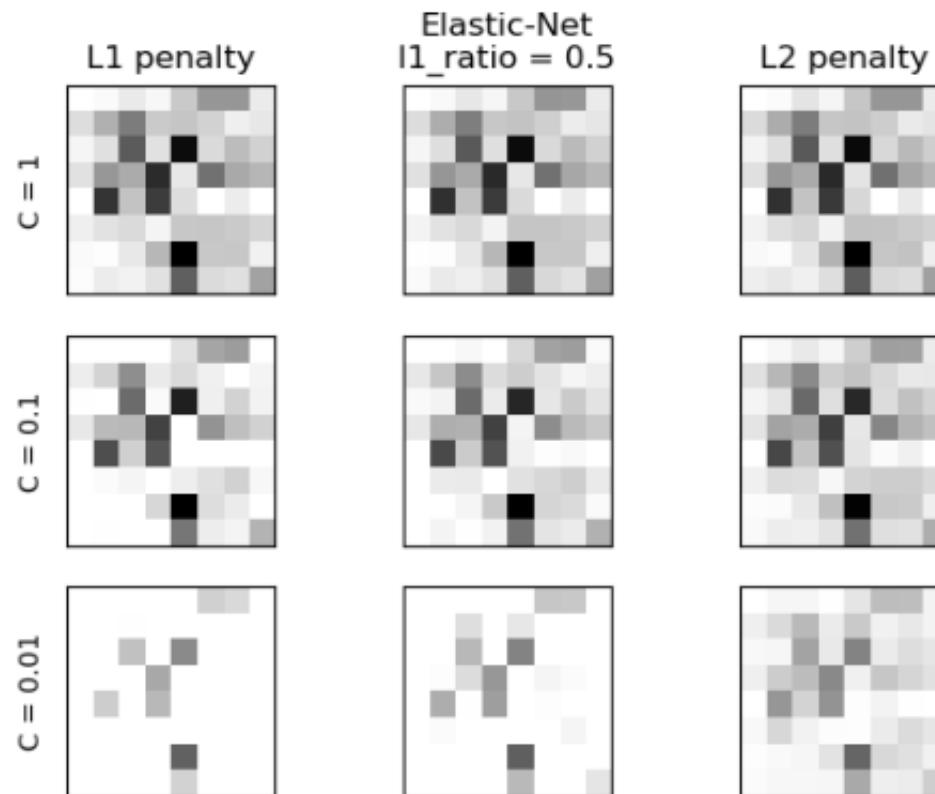
The function of both the regularization methods are almost the same. The **key difference** between these techniques is that Lasso shrinks the less important feature's coefficient to zero thus, removing some feature altogether. So, this works well for **feature selection** in case we have a huge number of features.

<https://towardsdatascience.com/l1-and-l2-regularization-methods-ce25e7fc831c>

# ElasticNet

`l1_ratio : float, default=0.5`

The ElasticNet mixing parameter, with  $0 \leq l1\_ratio \leq 1$ . For  $l1\_ratio = 0$  the penalty is an L2 penalty. For  $l1\_ratio = 1$  it is an L1 penalty. For  $0 < l1\_ratio < 1$ , the penalty is a combination of L1 and L2.



[https://scikit-learn.org/stable/auto\\_examples/linear\\_model/plot\\_logistic\\_l1\\_l2\\_sparsity.html#:~:text=Comparison%20of%20the%20sparsity%20\(percentage,C%20constrain%20the%20model%20more](https://scikit-learn.org/stable/auto_examples/linear_model/plot_logistic_l1_l2_sparsity.html#:~:text=Comparison%20of%20the%20sparsity%20(percentage,C%20constrain%20the%20model%20more)

**See also:****Ridge**

Ridge regression addresses some of the problems of Ordinary Least Squares by imposing a penalty on the size of the coefficients with L2 regularization.

**Lasso**

The Lasso is a linear model that estimates sparse coefficients with L1 regularization.

**ElasticNet**

Elastic-Net is a linear regression model trained with both L1 and L2 -norm regularization of the coefficients.

## sklearn.linear\_model.Ridge

```
class sklearn.linear_model.Ridge(alpha=1.0, *, fit_intercept=True,
max_iter=None, tol=0.001, solver='auto', positive=False, random_
state=None)
```

Linear least squares with L2 regularization.

Minimizes the objective function:

$$\|y - Xw\|_2^2 + \alpha * \|w\|_2^2$$

This model solves a regression model where the loss function is the L2-norm. Also known as Ridge Regression or Tikhonov regularization (i.e., when y is a 2d-array of shape (n\_samples, n\_targets)).

Read more in the [User Guide](#).

**Parameters:** `alpha : {float, ndarray of shape (n_targets, n_features)}`  
Constant that multiplies the L2 term, controlling regularization strength. `alpha` must be a float i.e. in [0, inf).

When `alpha = 0`, the objective is equivalent to ordinary least squares, solved by the `LinearRegression` object. For numerical reasons, using `alpha = 0` with the `Lasso` object is not advised.

If an array is passed, penalties are assumed to be column vectors.

**fit\_intercept : bool, default=True**  
Whether to fit the intercept for this model. If set to False, no intercept will be used (i.e. data is expected to be centered).

**normalize : bool, default=False**  
This parameter is ignored when `fit_intercept` is set to False. If True, the regressor is fit by subtracting the mean from the input features before fitting the regression by dividing the sum of the squares of the differences of all values by the number of samples.

## sklearn.linear\_model.Lasso

```
class sklearn.linear_model.Lasso(alpha=1.0, *, fit_intercept=True, normalize='deprecated',
precompute=False, max_iter=1000, tol=0.001, warm_start=False, positive=False, random_state=None,
selection='cyclic')
```

Linear Model trained with L1 prior as regularizer (aka the Lasso).

The optimization objective for Lasso is:

$$(1 / (2 * n\_samples)) * \|y - Xw\|_2^2 + \alpha * \|w\|_1$$

Technically the Lasso model is optimizing the same objective function as the Elastic Net with `l1_ratio=1`.

Read more in the [User Guide](#).

**Parameters:** `alpha : float, default=1.0`

Constant that multiplies the L1 term, controlling regularization strength. `alpha` must be a float i.e. in [0, inf).

When `alpha = 0`, the objective is equivalent to ordinary least squares, solved by the `LinearRegression` object. For numerical reasons, using `alpha = 0` with the `Lasso` object is not advised.

**fit\_intercept : bool, default=True**

Whether to calculate the intercept for this model. If set to False, no intercept will be used (i.e. data is expected to be centered).

**normalize : bool, default=False**

This parameter is ignored when `fit_intercept` is set to False. If True, the regressor is fit by subtracting the mean from the input features before fitting the regression by dividing the sum of the squares of the differences of all values by the number of samples.

*Deprecated since version 1.0: normalize was deprecated in version 1.0 and will be removed in 2.0.*

## sklearn.linear\_model.ElasticNet

```
class sklearn.linear_model.ElasticNet(alpha=1.0, *, l1_ratio=0.5, fit_intercept=True, normalize='deprecated',
precompute=False, max_iter=1000, copy_X=True, tol=0.0001, warm_start=False, positive=False, random_state=None,
selection='cyclic')
```

[\[source\]](#)

Linear regression with combined L1 and L2 priors as regularizer.

Minimizes the objective function:

$$1 / (2 * n\_samples) * \|y - Xw\|_2^2 + \alpha * l1\_ratio * \|w\|_1 + 0.5 * \alpha * (1 - l1\_ratio) * \|w\|_2^2$$

If you are interested in controlling the L1 and L2 penalty separately, keep in mind that this is equivalent to:

$$a * \|w\|_1 + 0.5 * b * \|w\|_2^2$$

where:

$$\alpha = a + b \text{ and } l1\_ratio = a / (a + b)$$

The parameter `l1_ratio` corresponds to `alpha` in the `glmnet` R package while `alpha` corresponds to the `lambda` parameter in `glmnet`. Specifically, `l1_ratio = 1` is the Lasso penalty. Currently, `l1_ratio <= 0.01` is not reliable, unless you supply your own sequence of `alpha`.

Read more in the [User Guide](#).

**Parameters:** `alpha : float, default=1.0`

Constant that multiplies the penalty terms. Defaults to 1.0. See the notes for the exact mathematical meaning of this parameter. `alpha = 0` is equivalent to an ordinary least square, solved by the `LinearRegression` object. For numerical reasons, using `alpha = 0` with the `Lasso` object is not advised. Given this, you should use the `LinearRegression` object.

**l1\_ratio : float, default=0.5**

The ElasticNet mixing parameter, with  $0 \leq l1\_ratio \leq 1$ . For `l1_ratio = 0` the penalty is an L2 penalty. For `l1_ratio = 1` it is an L1 penalty. For  $0 < l1\_ratio < 1$ , the penalty is a combination of L1 and L2.

**fit\_intercept : bool, default=True**

Whether the intercept should be estimated or not. If `False`, the data is assumed to be already centered.

**normalize : bool, default=False**

# Adjust input ranges

## StandardScaler

```
class sklearn.preprocessing.StandardScaler(*, copy=True, with_mean=True,  
with_std=True) [source]
```

Standardize features by removing the mean and scaling to unit variance.

The standard score of a sample  $x$  is calculated as:

$$z = (x - u) / s$$

where  $u$  is the mean of the training samples or zero if `with_mean=False`, and  $s$  is the standard deviation of the training samples or one if `with_std=False`.

Centering and scaling happen independently on each feature by computing the relevant statistics on the samples in the

using `transform`

```
>>> from sklearn.preprocessing import StandardScaler
```

```
>>> data = [[0, 0], [0, 0], [1, 1], [1, 1]]
```

Standardization of

```
>>> scaler = StandardScaler()
```

might behave bad

```
>>> print(scaler.fit(data))
```

distributed data (

```
StandardScaler()
```

For instance man

```
>>> print(scaler.mean_)
```

kernel of Support

```
[0.5 0.5]
```

```
>>> print(scaler.transform(data))
```

```
[[ -1. -1.]
```

```
[-1. -1.]
```

```
[ 1.  1.]
```

```
[ 1.  1.]
```

```
>>> print(scaler.transform([[2, 2]]))
```

```
[[ 3.  3.]]
```

<https://scikit-learn.org/1.6/modules/generated/sklearn.preprocessing.StandardScaler.html>

## MinMaxScaler

```
class sklearn.preprocessing.MinMaxScaler(feature_range=(0, 1), *, copy=True,  
clip=False) [source]
```

Transform features by scaling each feature to a given range.

This estimator scales and translates each feature individually such that it is in the given range on the training set, e.g. between zero and one.

The transformation is given by:

$$\begin{aligned} X_{\text{std}} &= (X - X.\min(\text{axis}=0)) / (X.\max(\text{axis}=0) - X.\min(\text{axis}=0)) \\ X_{\text{scaled}} &= X_{\text{std}} * (\text{max} - \text{min}) + \text{min} \end{aligned}$$

where  $\text{min}$ ,  $\text{max} = \text{f}$

This transformation

`MinMaxScaler` does

range, where the la

one corresponds to

[other scalers](#).

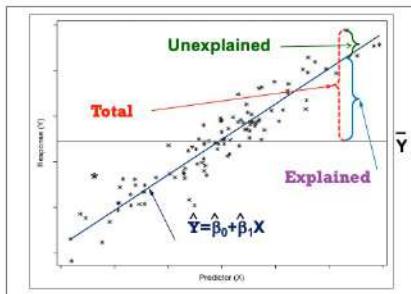
Read more in the [U](#)

```
>>> from sklearn.preprocessing import MinMaxScaler  
>>> data = [[-1, 2], [-0.5, 6], [0, 10], [1, 18]]  
>>> scaler = MinMaxScaler()  
>>> print(scaler.fit(data))  
MinMaxScaler()  
>>> print(scaler.data_max_)  
[ 1. 18.]  
>>> print(scaler.transform(data))  
[[0. 0.]  
[0.25 0.25]  
[0.5 0.5 ]  
[1. 1. ]]  
>>> print(scaler.transform([[2, 2]]))  
[[1.5 0. ]]
```

<https://scikit-learn.org/1.6/modules/generated/sklearn.preprocessing.MinMaxScaler.html>

## Evaluation: RMSE, (MAE), R<sup>2</sup>

$$\widehat{bp} = 57.8355 + 0.3116 \times chol$$



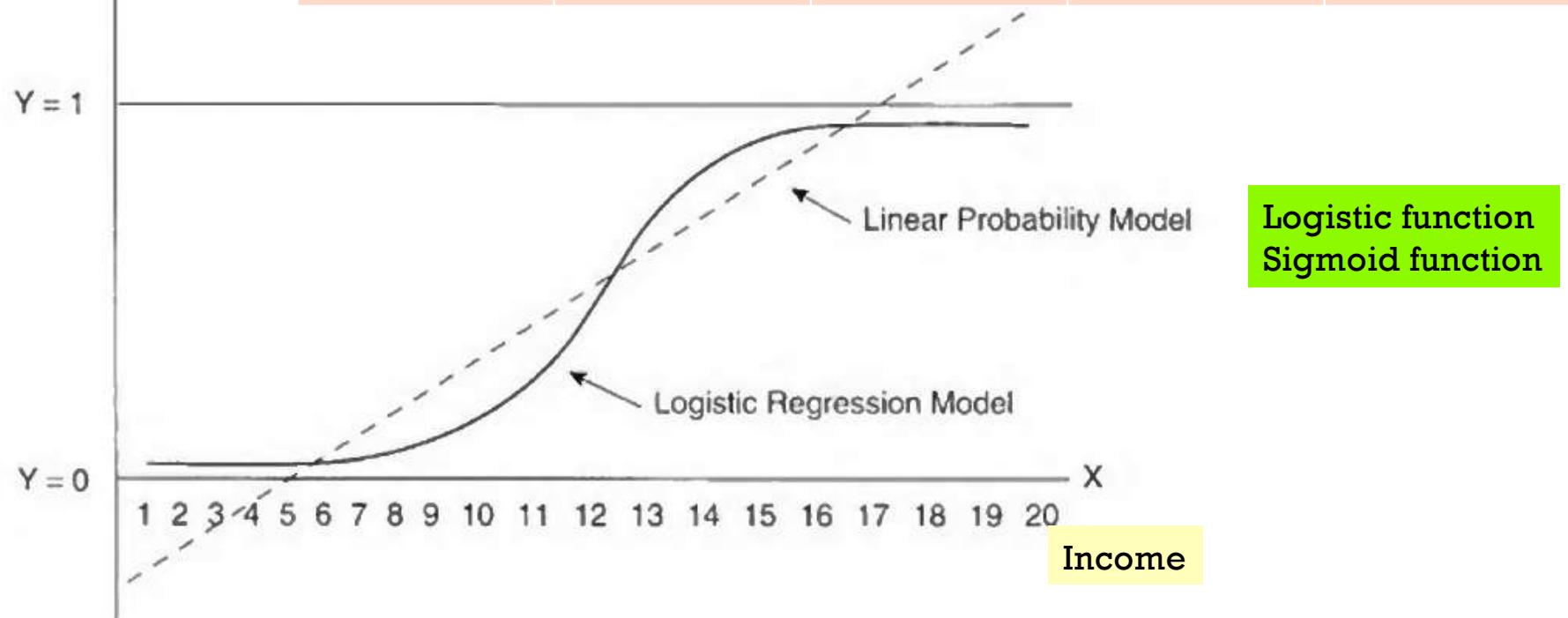
$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSE}{SST}$$

id	chol (x)	bp (y)	predict	error	squared error (SE)	guess	(y - y_bar )	squared total (ST)
1	437	194	196.1897	(2.1897)	4.7948	143.4286	50.5714	2,557.4694
2	264	121	141.4179	(20.4179)	416.8906	143.4286	(22.4286)	503.0408
3	249	131	136.6689	(5.6689)	32.1364	143.4286	(12.4286)	154.4694
4	297	159	151.8657	7.1343	50.8982	143.4286	15.5714	242.4694
5	243	123	134.7693	(11.7693)	138.5164	143.4286	(20.4286)	417.3265
6	272	161	143.9507	17.0493	290.6786	143.4286	17.5714	308.7551
7	161	115	108.8081	6.1919	38.3396	143.4286	(28.4286)	808.1837
average	274.7143	143.4286		SSE	972.2548		SST	4,991.7143
)				MSE	138.8935			
				RMSE	11.7853			
	R <sup>2</sup>	1 - (SSE/SST)	0.8052					



## Classification Problem

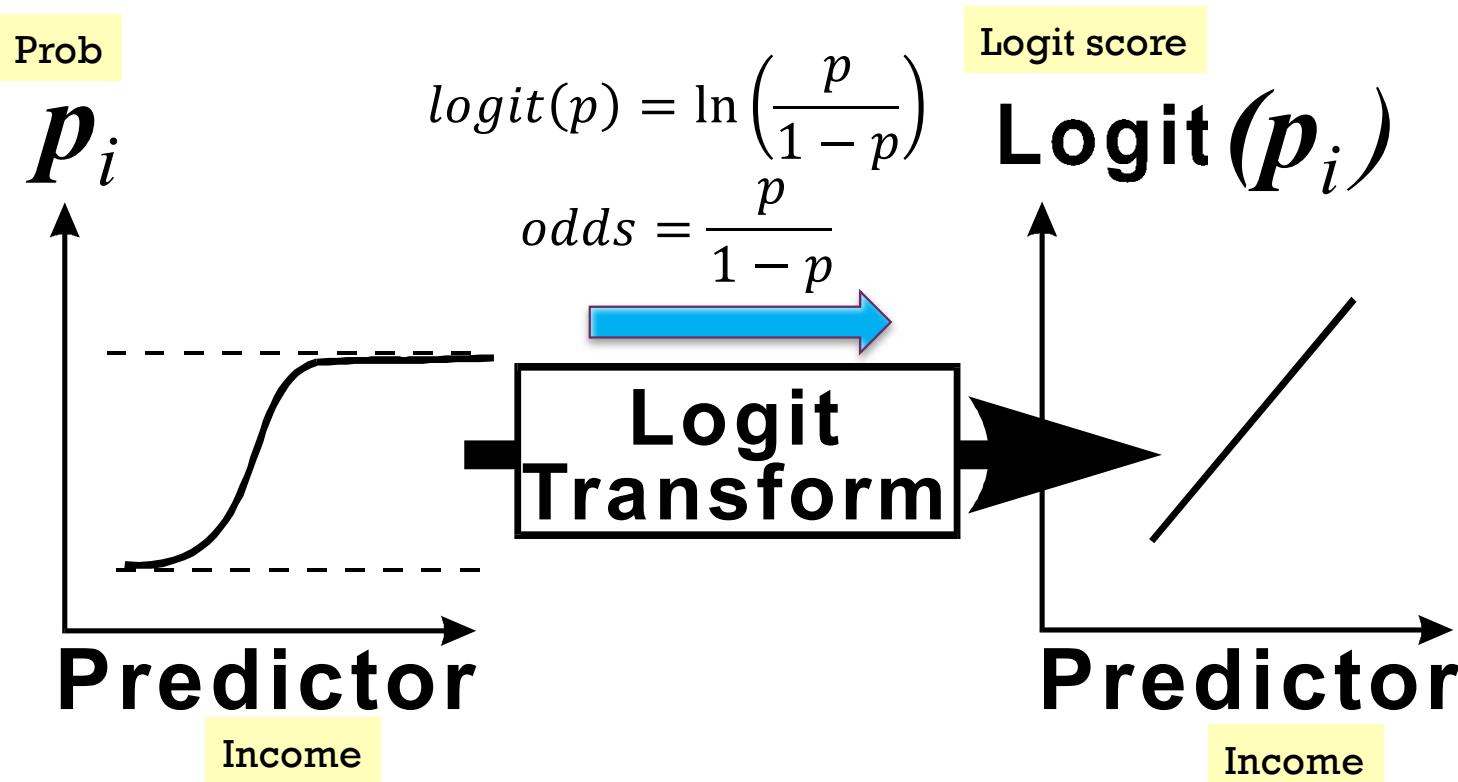
Prob. of purchase	Age	Income	Gender	Province	Purchase
	25	25,000	Female	Bangkok	Yes (1)
	35	50,000	Female	Nontaburi	Yes (1)
	32	35,000	Male	Bangkok	No (0)





## Logistic Regression (forward pass)

Logit link function: Non-linear to Linear



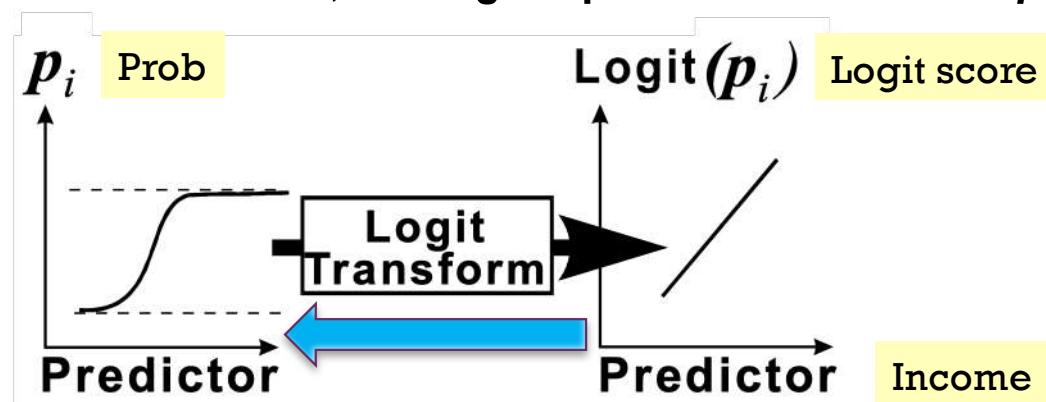
## + Logit Link Function (backward pass)

$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2 = \text{logit}(\hat{p})$$

■ Maximum likelihood estimates

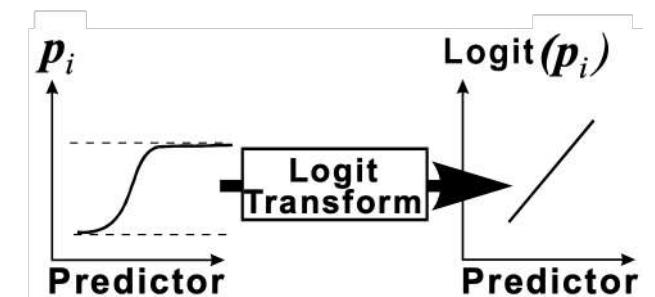
$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$

To obtain prediction estimates, the logit equation is solved for  $\hat{p}$ .



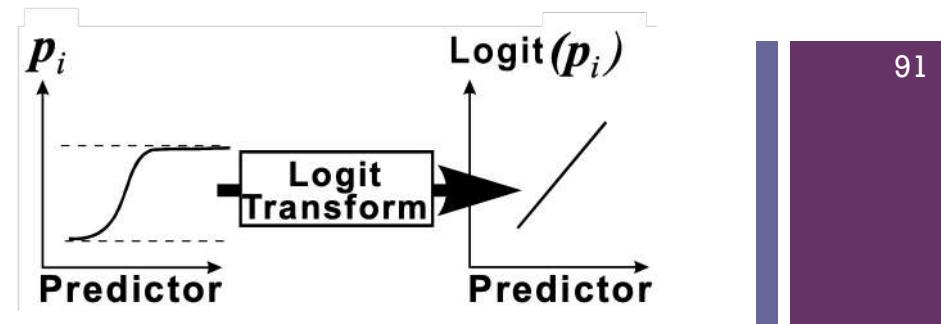
# Assumptions for Logistic Regression

- The mean of the logit is accurately modeled by a linear function of the  $X_i$ .
  - (logit,  $x_i$ ) = linear relationship
- The random error term,  $\epsilon$ , is assumed to have a normal distribution with a mean of zero.
- The random error term,  $\epsilon$ , is assumed to have a constant variance,  $\sigma^2$ .
  - Not skew
- The errors are independent.





## Quiz



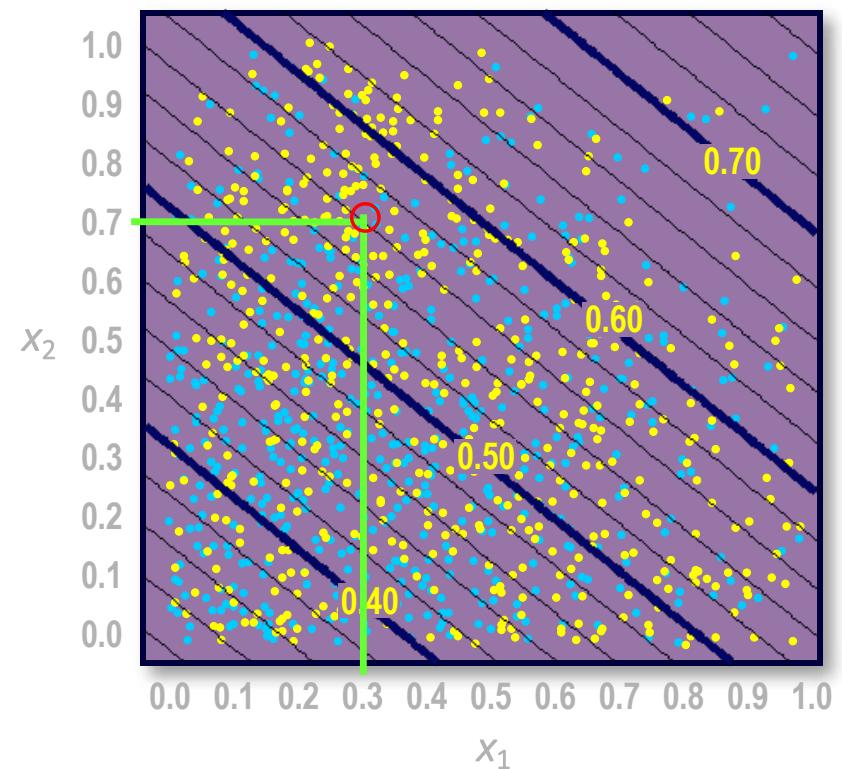
91

- What is the logistic regression prediction for the indicated point?

- a. 0.243
- b. 0.56
- c. yellow
- d. It depends.

$$\text{logit}(\hat{p}) = -0.81 + 0.92x_1 + 1.11x_2$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$





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scikit-learn 0.22.1

[Other versions](#)

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## sklearn.linear\_model.LogisticRegression

```
class sklearn.linear_model.LogisticRegression(penalty='l2', dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None) ¶
```

[\[source\]](#)

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi\_class' option is set to 'ovr', and uses the cross-entropy loss if the 'multi\_class' option is set to 'multinomial'. (Using the 'multinomial' setting with newton-cg, sag or liblinear solvers will yield results that differ from version 0.17 to 0.18 due to a change in the solver's default behavior.)

This class implements regularized logistic regression using 'liblinear' solver by default. It can handle both dense and sparse input formats. By default, it uses L2 regularization and dual coordinate descent. It is also possible to use L1 regularization and dual coordinate descent, which is more appropriate for sparse datasets. The 'newton-cg', 'sag' and 'lbfgs' solvers support only L2 regularization. The 'liblinear' solver supports both L1 and L2 regularization, with a dual formulation only for the former. The 'saga' solver only supports L1 regularization with a dual formulation.

The 'newton-cg', 'sag', and 'lbfgs' solvers support only L2 regularization. The 'liblinear' solver supports both L1 and L2 regularization, with a dual formulation only for the former. The 'saga' solver only supports L1 regularization with a dual formulation.

Read more in the [User Guide](#).

### Parameters:

`penalty : {'l1', 'l2', 'elasticnet', 'none'}, default='l2'`

Used to specify the norm used in the penalization. The 'newton-cg', 'sag' and 'lbfgs' solvers support only L2 regularization. The 'liblinear' solver supports both L1 and L2 regularization, with a dual formulation only for the former. The 'saga' solver only supports L1 regularization with a dual formulation.

*New in version 0.19: l1 penalty with SAGA solver (allowing 'multinomial' + L1)*

***l1\_ratio : float, default=None***

The Elastic-Net mixing parameter, with  $0 \leq l1\_ratio \leq 1$ . Only used if `penalty='elasticnet'`. Setting `l1_ratio=0` is equivalent to using `penalty='l2'`, while setting `l1_ratio=1` is equivalent to using `penalty='l1'`. For  $0 < l1\_ratio < 1$ , the penalty is a combination of L1 and L2.

***C : float, default=1.0***

Inverse of regularization strength; must be a positive float. Like in support vector machines, smaller values specify stronger regularization.

Here, we are going to check how sparsity increases as we increase lambda (or decrease C, as  $C = 1/\lambda$ ) when L1 Regularizer is used.

```
from sklearn.linear_model import LogisticRegression
clf = LogisticRegression(C= 1000, penalty= 'l1')
clf.fit(x_train,y_train)
pred = clf.predict(x_test)
print("Non Zero weights:",np.count_nonzero(clf.coef_))

clf = LogisticRegression(C= 1, penalty= 'l1')
clf.fit(x_train,y_train)
pred = clf.predict(x_test)
print("Non Zero weights:",np.count_nonzero(clf.coef_))

clf = LogisticRegression(C= 0.01, penalty= 'l1')
clf.fit(x_train,y_train)
pred = clf.predict(x_test)
print("Non Zero weights:",np.count_nonzero(clf.coef_))
```

Non Zero weights: 50470

Non Zero weights: 8228

Non Zero weights:396

<https://medium.com/@aditya97p/l1-and-l2-regularization-237438a9caa6>

**class\_weight : dict or 'balanced', default=None**

Weights associated with classes in the form {class\_label: weight}. If not given, all classes are supposed to have weight one.

The "balanced" mode uses the values of y to automatically adjust weights inversely proportional to class frequencies in the input data as n\_samples / (n\_classes \* np.bincount(y)).

Note that these weights will be multiplied with sample\_weight (passed through the fit method) if sample\_weight is specified.

*New in version 0.17: class\_weight='balanced'*

**random\_state : int, RandomState instance, default=None**

Used when solver == 'sag', 'saga' or 'liblinear' to shuffle the data. See [Glossary](#) for details.

**Examples**

```
>>> np.bincount(np.arange(5))
array([1, 1, 1, 1, 1])
>>> np.bincount(np.array([0, 1, 1, 3, 2, 1, 7]))
array([1, 3, 1, 1, 0, 0, 0, 1])
```

- 100 (20:80)
- $W_{c1} = 100 / (2 * 20) = 2.5$
- $W_{c2} = 100 / (2 * 80) = 0.625$



# Linear Regression Limitation

- Manage missing value
- Handle outliers (skewness)
- Handle categorical variables (dummy codes)
- Variable selection:
  - Forward, Backward, Stepwise (**not exist in scikit-learn**)
- Accounted for nonlinearities

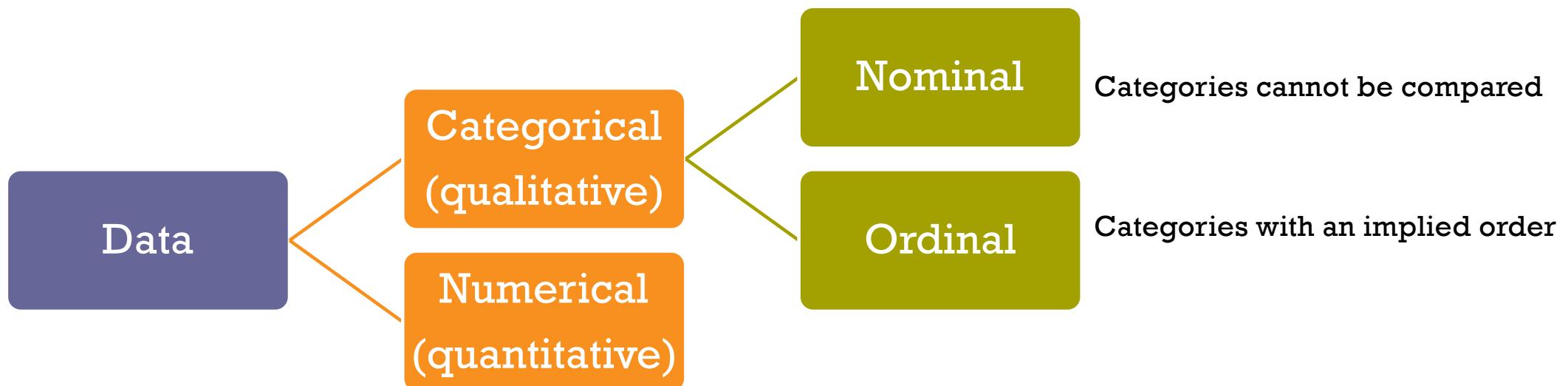


Important Params:

- Require good data preparation
- Variable selection



## Terminology: Kinds of data (recap)





# Ordinal: Recode

Grade	GradeNum
A	4.00
B+	3.50
B	3.00
C+	2.50
C	2.00
D+	1.50
D	1.00
F	0.00

Size	SizeNum
XL	5
L	4
M	3
S	2
XS	1



# Categorical

- Dummy coding =  $(n-1)$  dummy codes

Branch	BranchNum	D_BKK	B_Patum	D_Non	D_BKK	B_Patum
BKK	1	1	0	0	1	0
Patumtani	2	0	1	0	0	1
Nontaburi	3	0	0	1	0	0 reference

Search the docs ...

Input/output

**General functions**

Series

DataFrame

Pandas arrays

Panel

Index objects

Date offsets

Window

GroupBy

Resampling

Style

# pandas.get\_dummies

`pandas.get_dummies(data, prefix=None, prefix_sep='_', dummy_na=False, columns=None, sparse=False, drop_first=False, dtype=None) → 'DataFrame'` [\[source\]](#)

Convert categorical variable into dummy/indicator variables.

**Parameters:** `data : array-like, Series, or DataFrame`

Data of which to get dummy indicators.

`prefix : str, list of str, or dict of str, default None`

String to append DataFrame column names. Pass a list with length equal to the number of columns when calling `get_dummies` on a DataFrame. Alternatively, `prefix` can be a dictionary mapping column names to prefixes.

`prefix_sep : str, default '_'`

If appending prefix, separator/delimiter to use. Or pass a list or dictionary as with `prefix`.

`dummy_na : bool, default False`

Add a column to indicate NaNs, if False NaNs are ignored.

```
>>> pd.get_dummies(pd.Series(list('abcaa')), drop_first=True)
      b   c
0    0   0
1    1   0
2    0   1
3    0   0
4    0   0
```

`drop_first : bool, default None`

Drop the first column in the DataFrame to be encoded. If `columns` is None then all the columns with `object` or `category` dtypes are converted.

`sparse : bool, default False`

Dummy-encoded columns should be backed by a `SparseArray` (True) or a regular NumPy array (False).



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Other versions

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sklearn.preprocessing.OneHotEncoder  
OneHotEncoder  
Examples using  
sklearn.preprocessing.OneHotEncoder

## sklearn.preprocessing.OneHotEncoder

```
class sklearn.preprocessing.OneHotEncoder(*, categories='auto', drop=None, sparse='deprecated',
                                         sparse_output=True, dtype=<class 'numpy.float64'>, handle_unknown='error', min_frequency=None, max_categories=None)
[source]
```

Encode categorical features as a one-hot numeric array.

The input to this transformer should be an array-like of integers or strings, denoting the values taken on by categorical (discrete) features. The features are encoded using a one-hot (aka 'one-of-K' or 'dummy') encoding scheme. This creates a binary column for each category and returns a sparse matrix or dense array (depending on the `sparse_output` parameter).

By default, the encoder derives the categories based on the unique values in each feature. Alternatively, one can specify the categories manually.

This encoding is needed for feeding categorical data to many scikit-learn estimators, notably linear models with standard kernels.

Note: a one-hot encoding of y labels should use a LabelBinarizer instead.

### drop : {'first', 'if\_binary'} or an array-like of shape (n\_features,), default=None

Specifies a methodology to use to drop one of the categories per feature. This is useful in situations where perfectly collinear features cause problems, such as when feeding the resulting data into an unregularized linear regression model.

However, dropping one category breaks the symmetry of the original representation and can therefore induce a bias in downstream models, for instance for penalized linear classification or regression models.

- None : retain all features (the default).
- 'first' : drop the first category in each feature. If only one category is present, the feature will be dropped entirely.
- 'if\_binary' : drop the first category in each feature with two categories. Features with 1 or more than 2 categories are left intact.
- array : `drop[i]` is the category in feature `X[:, i]` that should be dropped.

New in version 0.21: The parameter `drop` was added in 0.21.

Changed in version 0.23: The option `drop='if_binary'` was added in 0.23.

Changed in version 1.1: Support for dropping infrequent categories.

```
>>> X = [['Male', 1], ['Female', 3], ['Female', 2]]
```

One can always drop the first column for each feature:

```
>>> drop_enc = OneHotEncoder(drop='first').fit(X)
>>> drop_enc.categories_
[array(['Female', 'Male'], dtype=object), array([1, 2, 3], dtype=object)]
>>> drop_enc.transform([[['Female', 1], ['Male', 2]]]).toarray()
array([[0., 0., 0.],
       [1., 1., 0.]])
```

Or drop a column for feature only having 2 categories:

```
>>> drop_binary_enc = OneHotEncoder(drop='if_binary').fit(X)
>>> drop_binary_enc.transform([[['Female', 1], ['Male', 2]]]).toarray()
array([[0., 1., 0., 0.],
       [1., 0., 1., 0.]])
```



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Other versions

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sklearn.feature\_selection.SelectFromModel  
SelectFromModel  
Examples using  
sklearn.feature\_selection.Select

## sklearn.feature\_selection.SelectFromModel Recap

```
class sklearn.feature_selection.SelectFromModel(estimator, *, threshold=None, prefit=False, norm_order=1,  
max_features=None, importance_getter='auto')
```

[source]

Meta-transformer for selecting features based on importance weights.

New in version 0.17.

Read more in the [User Guide](#).

**Parameters:** *estimator : object*

The base estimator from which the transformer is built. This can be both a fitted (if `prefit` is set to True) or a non-fitted estimator. The estimator should have a `feature_importances_` or `coef_` attribute after fitting. Otherwise, the `importance_getter` parameter should be used.

**threshold : str or float, default=None**

The threshold value to use for feature selection. Features whose absolute importance value is greater or equal are kept while the others are discarded. If "median" (resp. "mean"), then the `threshold` value is the median (resp. the mean) of the feature importances. A scaling factor (e.g., "1.25\*mean") may also be used. If None and if the estimator has a parameter penalty set to l1, either explicitly or implicitly (e.g, Lasso), the threshold used is 1e-5. Otherwise, "mean" is used by default.

**prefit : bool, default=False**

Whether a prefit model is expected to be passed into the constructor directly or not. If True, estimator

[https://scikit-learn.org/stable/modules/generated/sklearn.feature\\_selection.SelectFromModel.html](https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.SelectFromModel.html)

Toggle Menu

[https://scikit-learn.org/stable/modules/classes.html#module-sklearn.feature\\_selection](https://scikit-learn.org/stable/modules/classes.html#module-sklearn.feature_selection)

# Negative coefficients are handled by their absolute values

```
from sklearn.datasets import load_diabetes
from sklearn.linear_model import Lasso
from sklearn.feature_selection import SelectFromModel
import pandas as pd
import numpy as np

# Load dataset
data = load_diabetes()
X = data.data # Features
y = data.target # Target
feature_names = data.feature_names

# Train a Lasso Regression Model
lasso = Lasso(alpha=0.1, random_state=42)
lasso.fit(X, y)

# Use SelectFromModel with threshold=0 to select all non-zero absolute coefficient features
selector = SelectFromModel(estimator=lasso, prefit=True, threshold=0)
X_selected = selector.transform(X)

# Get the names of the selected features
selected_features = [feature_names[i] for i in selector.get_support(indices=True)]

# Display results
print("Selected Features (Non-zero Coefficients):")
print(selected_features)

# Display feature coefficients for reference
feature_coefficients = pd.DataFrame({
    'Feature': feature_names,
    'Coefficient': lasso.coef_
}).sort_values(by='Coefficient', ascending=False)

print("\nFeature Coefficients:")
print(feature_coefficients)
```

Selected Features (Non-zero Coefficients):  
['bmi', 's5']

Feature Coefficients:

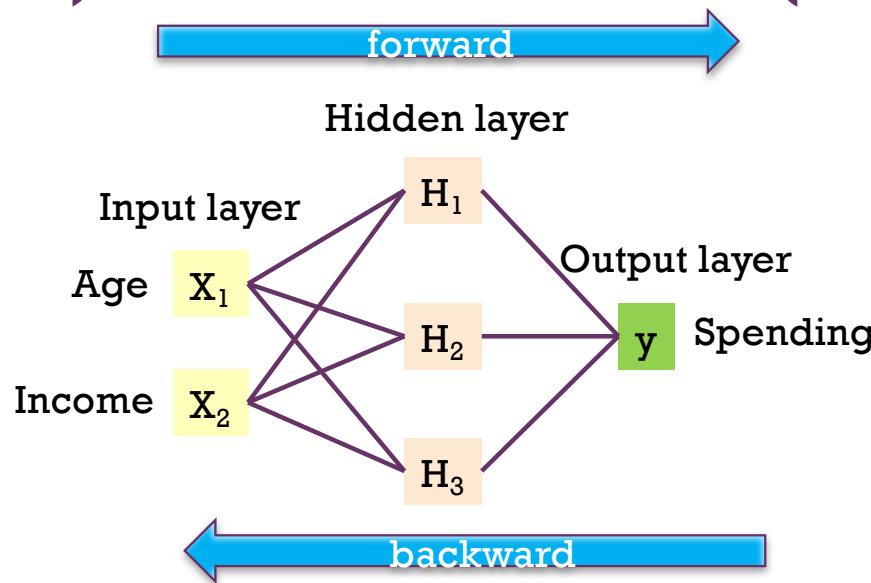
	Feature	Coefficient
2	bmi	502.679024
8	s5	293.543915
3	bp	0.000000
...		
1	sex	0.000000
4	tc	-0.000000
0	age	-0.000000

+

### 3) Neural Networks



### 3) Neural Networks (universal approximator)

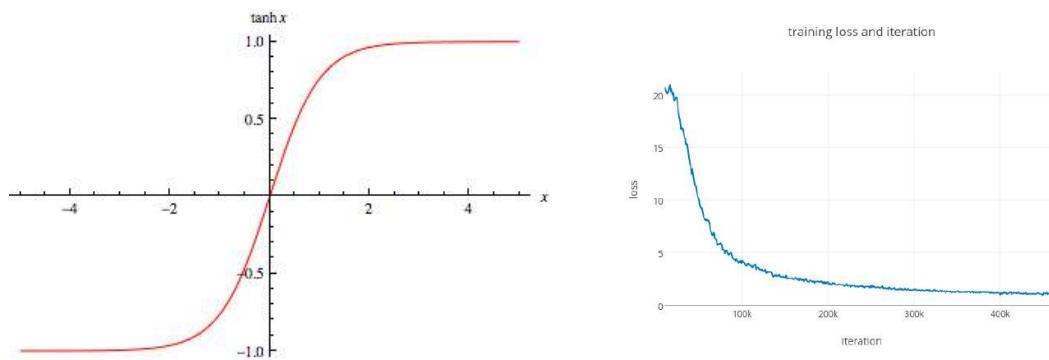


$$\text{Spending} = \hat{w}_0 + \hat{w}_1 H_1 + \hat{w}_2 H_2 + \hat{w}_3 H_3$$

$$H_1 = \tanh(\hat{w}_{10} + \hat{w}_{11}x_1 + \hat{w}_{12}x_2)$$

$$H_2 = \tanh(\hat{w}_{20} + \hat{w}_{21}x_1 + \hat{w}_{22}x_2)$$

$$H_3 = \tanh(\hat{w}_{30} + \hat{w}_{31}x_1 + \hat{w}_{32}x_2)$$



How to update weight

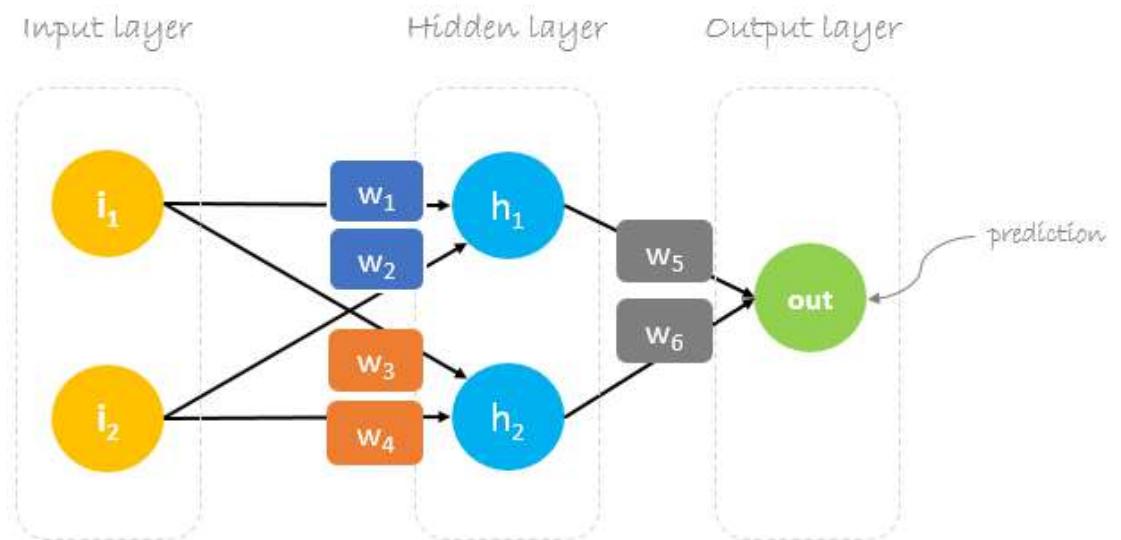
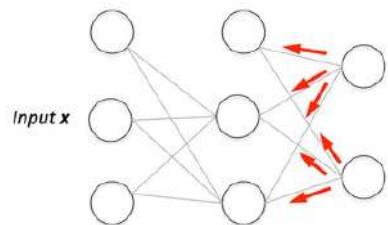
<https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/>

# + NN Example: Forward & backwork passes

HMKCODE

## Backpropagation Step by Step

03 NOV 2019

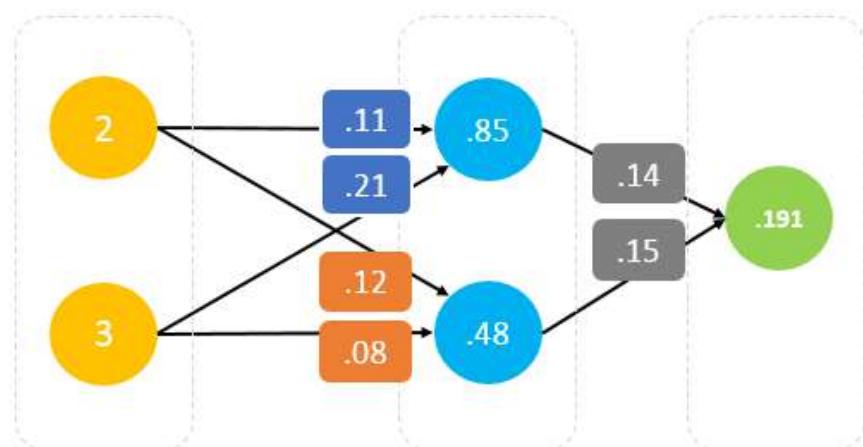


<https://hmkcode.com/ai/backpropagation-step-by-step/>

Our single sample is as following `inputs=[2, 3]` and `output=[1]`.

## + 1) Forward pass (prediction)

Input layer      Hidden layer      Output layer



Forward Pass

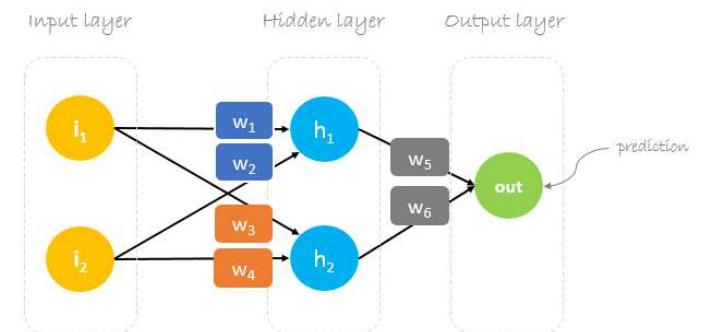
$$[2 \ 3] \cdot \begin{bmatrix} 0.11 & 0.12 \\ 0.21 & 0.08 \end{bmatrix} = [0.85 \ 0.48] \cdot \begin{bmatrix} 0.14 \\ 0.15 \end{bmatrix} = [0.191]$$

$$2 \times 0.11 + 3 \times 0.21 = 0.85$$

$$0.85 \times 0.14 + 0.48 \times 0.15 = 0.191$$

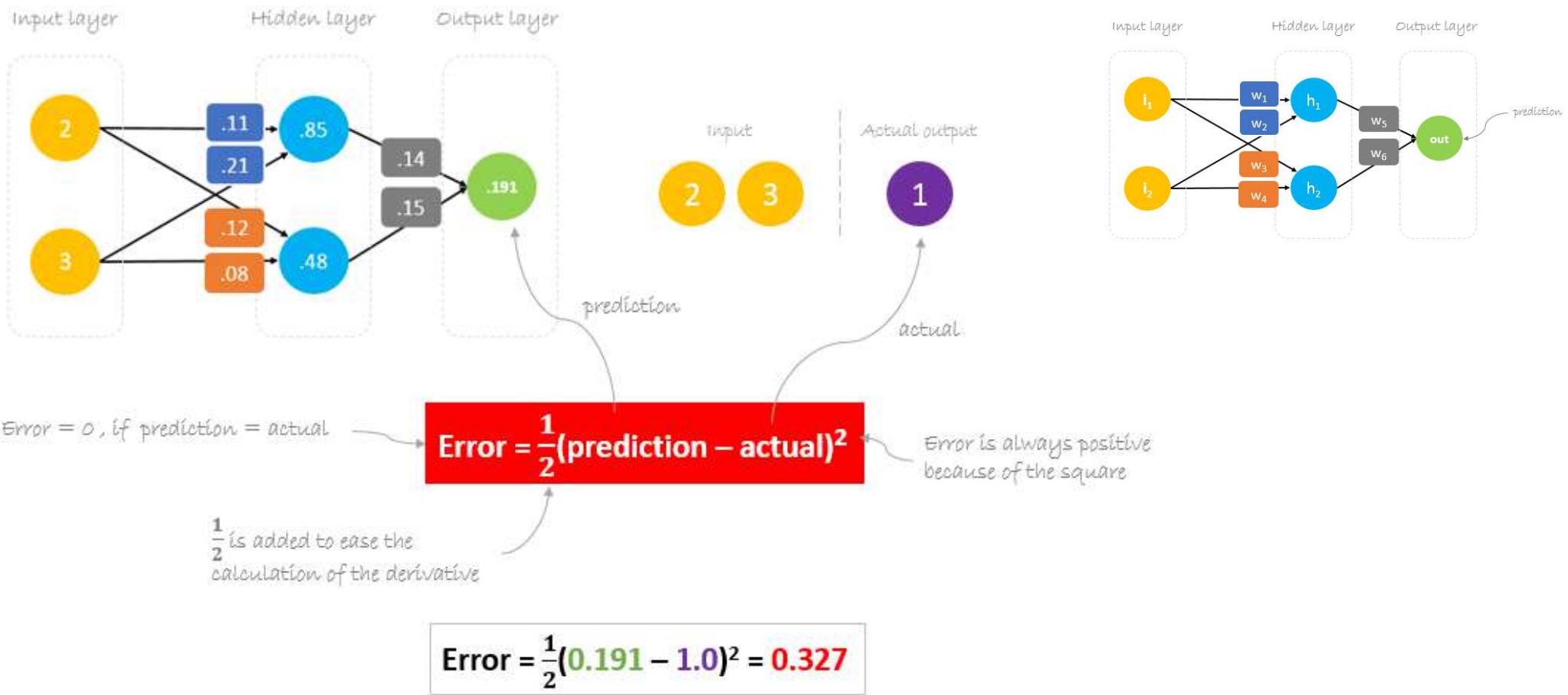
$$2 \times 0.12 + 3 \times 0.08 = 0.48$$

Matrix multiplication  
Details



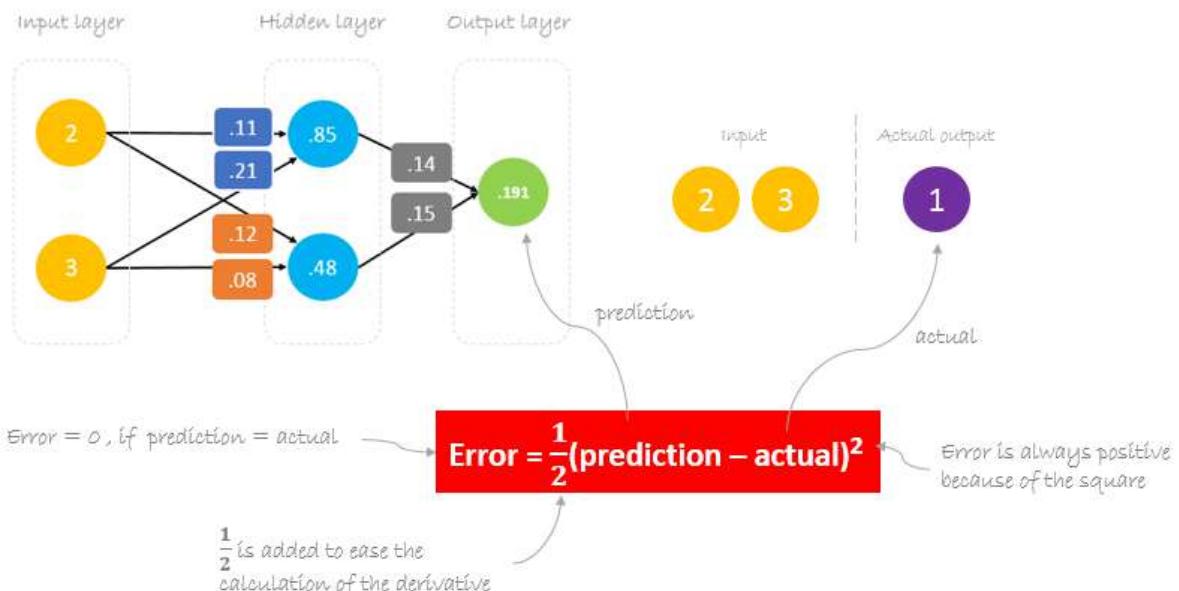


## 2) Backward pass (aka. backpropagation) Calculation error

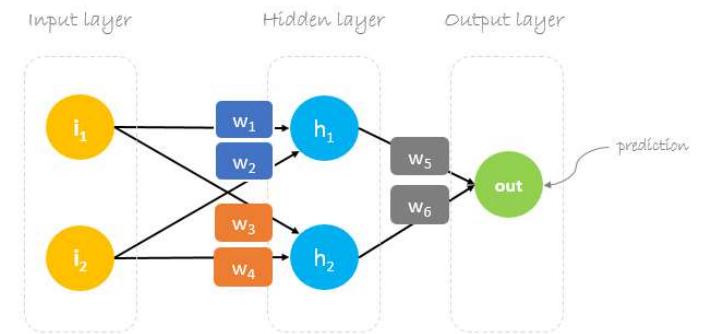




# Reducing error



$$\text{Error} = \frac{1}{2}(0.191 - 1.0)^2 = 0.327$$



**prediction** = **out**

$$\text{prediction} = (h_1) w_5 + (h_2) w_6$$

$$h_1 = i_1 w_1 + i_2 w_2$$

$$h_2 = i_1 w_3 + i_2 w_4$$

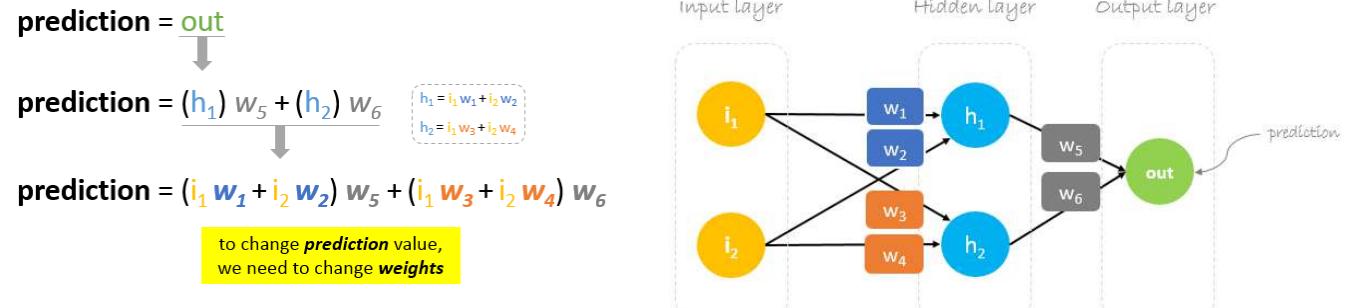
$$\text{prediction} = (i_1 w_1 + i_2 w_2) w_5 + (i_1 w_3 + i_2 w_4) w_6$$

to change **prediction** value, we need to change **weights**

+

# Backpropagation

## w5,w6



$$\frac{\partial \text{Error}}{\partial W_6} = \frac{\partial \text{Error}}{\partial \text{prediction}} * \frac{\partial \text{prediction}}{\partial W_6}$$

chain rule

$$\frac{\partial \text{Error}}{\partial W_6} = \frac{1}{2}(\text{predictoin} - \text{actula})^2 * \frac{\partial ((i_1 w_1 + i_2 w_2) w_5 + (i_1 w_3 + i_2 w_4) w_6)}{\partial W_6}$$

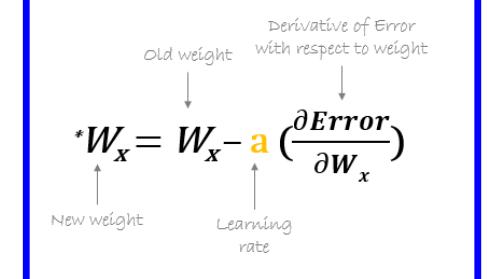
$$\frac{\partial \text{Error}}{\partial W_6} = 2 * \frac{1}{2}(\text{predictoin} - \text{actula}) \frac{\partial (\text{predictoin} - \text{actula})}{\partial \text{prediciton}} * (i_1 w_3 + i_2 w_4)$$

$$\frac{\partial \text{Error}}{\partial W_6} = (\text{predictoin} - \text{actula}) * (h_2)$$

$$\frac{\partial \text{Error}}{\partial W_6} = \Delta h_2$$

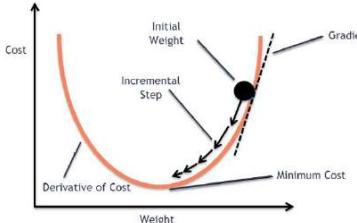
$$\text{Error} = \frac{1}{2}(\text{prediction} - \text{actual})^2$$

$$\text{prediction} = (i_1 w_1 + i_2 w_2) w_5 + (i_1 w_3 + i_2 w_4) w_6$$



$$\Delta = \text{prediction} - \text{actual}$$

delta



$$*W_6 = W_6 - a \Delta h_2$$

$$*W_5 = W_5 - a \Delta h_1$$

+

# Backpropagation

## w1,w2,w3,w4

$$\frac{\partial \text{Error}}{\partial W_1} = \frac{\partial \text{Error}}{\partial \text{prediction}} * \frac{\partial \text{prediction}}{\partial h_1} * \frac{\partial h_1}{\partial W_1}$$

chain rule

$$\frac{\partial \text{Error}}{\partial W_1} = \frac{\partial \frac{1}{2}(\text{predictoin} - \text{actula})^2}{\partial \text{prediciton}} * \frac{\partial (h_1) w_5 + (h_2) w_6}{\partial h_1} * \frac{\partial i_1 w_1 + i_2 w_2}{\partial w_1}$$

$$\frac{\partial \text{Error}}{\partial W_1} = 2 * \frac{1}{2}(\text{predictoin} - \text{actula}) \frac{\partial (\text{predictoin} - \text{actula})}{\partial \text{prediciton}} * (w_5) * (i_1)$$

$$\frac{\partial \text{Error}}{\partial W_1} = (\text{predictoin} - \text{actula}) * (w_5 i_1)$$

$$\frac{\partial \text{Error}}{\partial W_1} = \Delta w_5 i_1$$

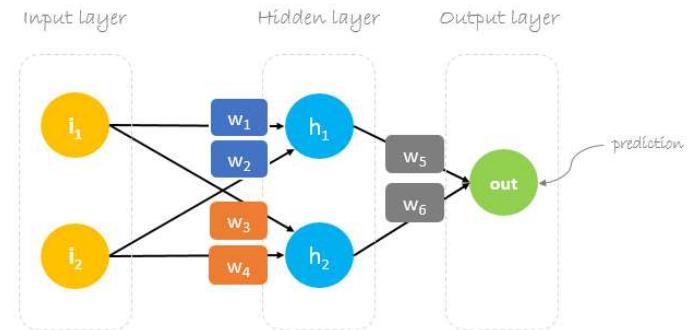
**prediction = out**

$$\text{prediction} = (h_1) w_5 + (h_2) w_6$$

$h_1 = i_1 w_1 + i_2 w_2$   
 $h_2 = i_1 w_3 + i_2 w_4$

**prediction =  $(i_1 w_1 + i_2 w_2) w_5 + (i_1 w_3 + i_2 w_4) w_6$**

to change **prediction** value,  
we need to change **weights**



$$\text{Error} = \frac{1}{2}(\text{prediction} - \text{actual})^2$$

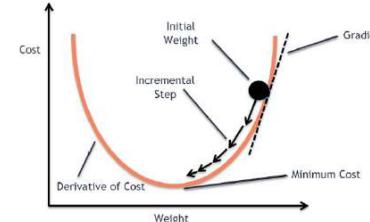
$$\text{prediction} = (h_1) w_5 + (h_2) w_6$$

$$h_1 = i_1 w_1 + i_2 w_2$$

Old weight  
 $\downarrow$   
 $\cdot W_x = W_x - a \left( \frac{\partial \text{Error}}{\partial W_x} \right)$   
 New weight  
 Learning rate

**$\Delta = \text{prediction} - \text{actual}$**

delta

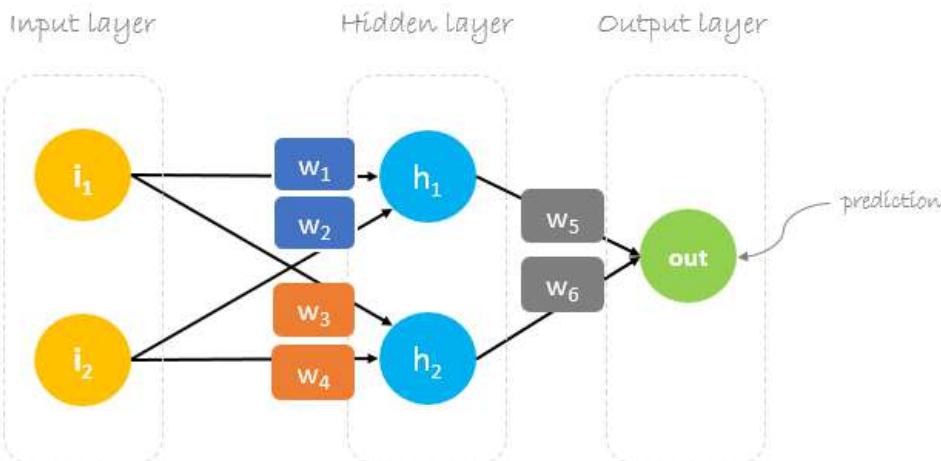


Updated weights  
 $\rightarrow$   
 $*W_6 = W_6 - a (h_2 . \Delta)$   
 $*W_5 = W_5 - a (h_1 . \Delta)$   
 $*W_4 = W_4 - a (i_2 . \Delta w_6)$   
 $*W_3 = W_3 - a (i_1 . \Delta w_5)$   
 $*W_2 = W_2 - a (i_2 . \Delta w_5)$   
 $*W_1 = W_1 - a (i_1 . \Delta w_5)$



# Backpropagation: Matrix Operations

$$\text{New weight} \quad \downarrow \quad \text{Old weight} \quad \downarrow \quad \text{Derivative of Error with respect to weight} \\ *W_x = W_x - a \left( \frac{\partial \text{Error}}{\partial W_x} \right) \quad \uparrow \quad \uparrow \quad \uparrow \\ \text{Learning rate}$$



Updated weights

$$\begin{aligned} *w_6 &= w_6 - a (h_2 \cdot \Delta) \\ *w_5 &= w_5 - a (h_1 \cdot \Delta) \\ *w_4 &= w_4 - a (i_2 \cdot \Delta w_6) \\ *w_3 &= w_3 - a (i_1 \cdot \Delta w_6) \\ *w_2 &= w_2 - a (i_2 \cdot \Delta w_5) \\ *w_1 &= w_1 - a (i_1 \cdot \Delta w_5) \end{aligned}$$

$$\begin{bmatrix} w_5 \\ w_6 \end{bmatrix} = \begin{bmatrix} w_5 \\ w_6 \end{bmatrix} - a \Delta \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} w_5 \\ w_6 \end{bmatrix} - \begin{bmatrix} ah_1 \Delta \\ ah_2 \Delta \end{bmatrix}$$

$$\begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} = \begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} - a \Delta \begin{bmatrix} i_1 \\ i_2 \end{bmatrix} \cdot \begin{bmatrix} w_5 & w_6 \end{bmatrix} = \begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} - \begin{bmatrix} a i_1 \Delta w_5 & a i_1 \Delta w_6 \\ a i_2 \Delta w_5 & a i_2 \Delta w_6 \end{bmatrix}$$

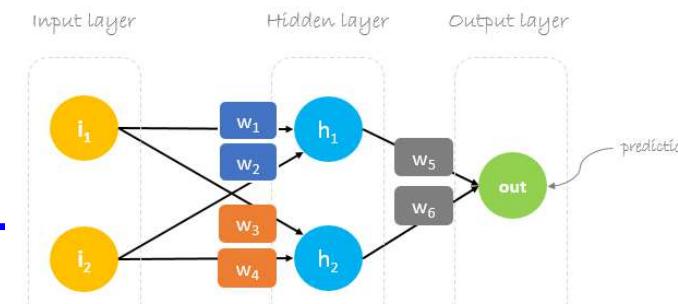
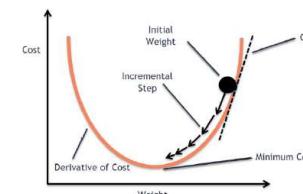
# + Backpropagation: Matrix Operations (cont.)

$$\Delta = 0.191 - 1 = -0.809 \quad \text{← Delta = prediction - actual}$$

$$a = 0.05 \quad \text{← Learning rate, we smartly guess this number}$$

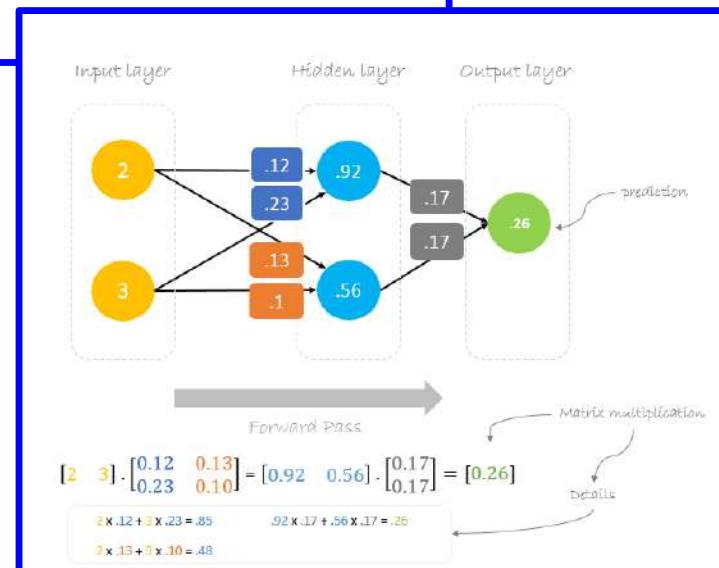
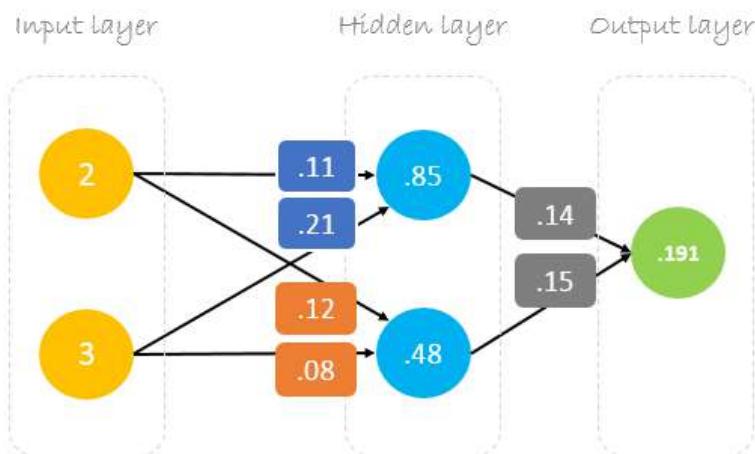
$$\begin{bmatrix} w_5 \\ w_6 \end{bmatrix} = \begin{bmatrix} 0.14 \\ 0.15 \end{bmatrix} - 0.05(-0.809) \begin{bmatrix} 0.85 \\ 0.48 \end{bmatrix} = \begin{bmatrix} 0.14 \\ 0.15 \end{bmatrix} - \begin{bmatrix} -0.034 \\ -0.019 \end{bmatrix} = \begin{bmatrix} 0.17 \\ 0.17 \end{bmatrix}$$

$$\begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} = \begin{bmatrix} .11 & .12 \\ .21 & .08 \end{bmatrix} - 0.05(-0.809) \begin{bmatrix} 2 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} 0.14 & 0.15 \end{bmatrix} = \begin{bmatrix} .11 & .12 \\ .21 & .08 \end{bmatrix} - \begin{bmatrix} -0.011 & -0.012 \\ -0.017 & -0.018 \end{bmatrix} = \begin{bmatrix} .12 & .13 \\ .23 & .10 \end{bmatrix}$$



$$\begin{bmatrix} w_5 \\ w_6 \end{bmatrix} = \begin{bmatrix} w_5 \\ w_6 \end{bmatrix} - a \Delta \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} w_5 \\ w_6 \end{bmatrix} - \begin{bmatrix} ah_1 \Delta \\ ah_2 \Delta \end{bmatrix}$$

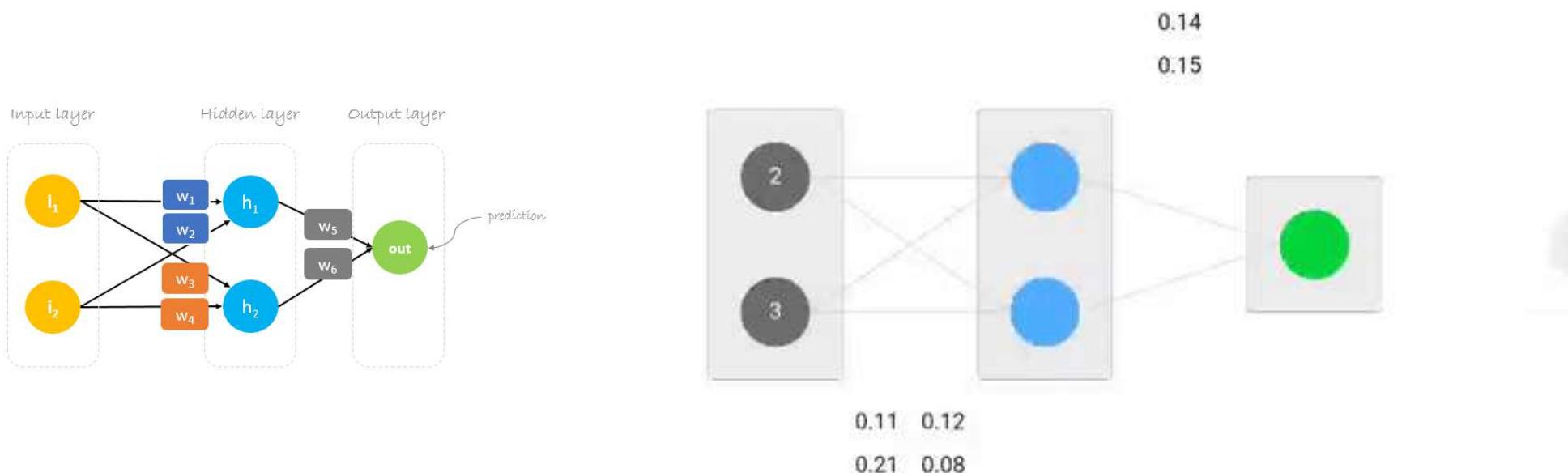
$$\begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} = \begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} - a \Delta \begin{bmatrix} i_1 \\ i_2 \end{bmatrix} \cdot \begin{bmatrix} w_5 & w_6 \end{bmatrix} = \begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix} - \begin{bmatrix} a i_1 \Delta w_5 & a i_1 \Delta w_6 \\ a i_2 \Delta w_5 & a i_2 \Delta w_6 \end{bmatrix}$$



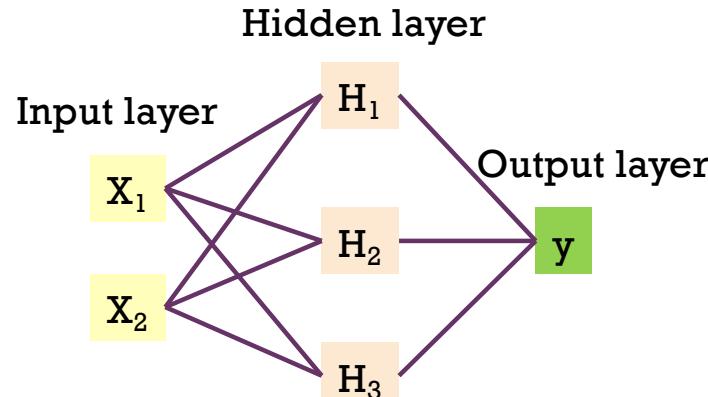
# +

## Backpropagation visualization

<https://hmkcode.com/ai/backpropagation-step-by-step/>

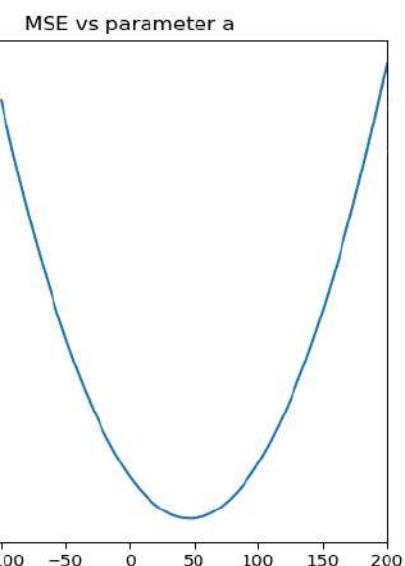
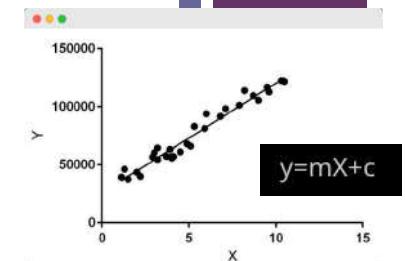
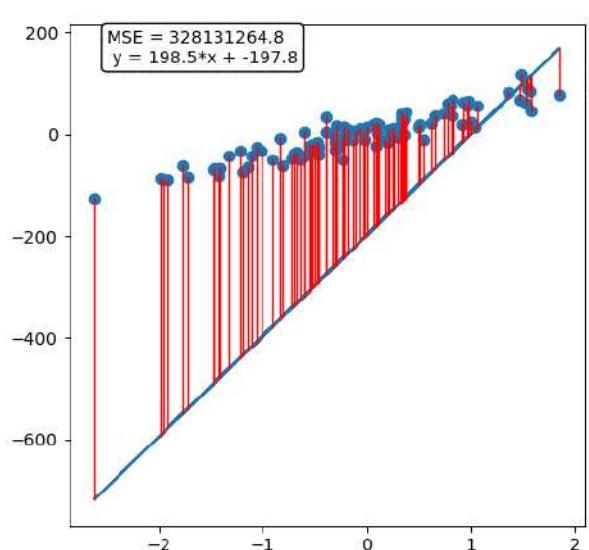
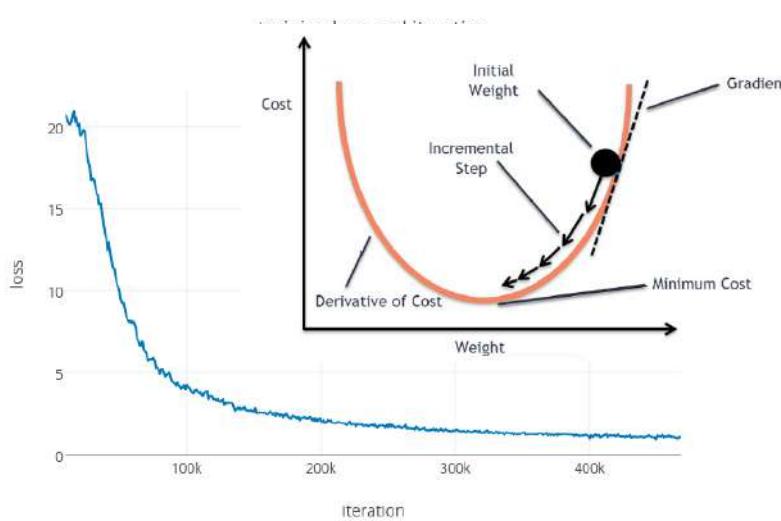


# Gradient descent (solver to find weights)

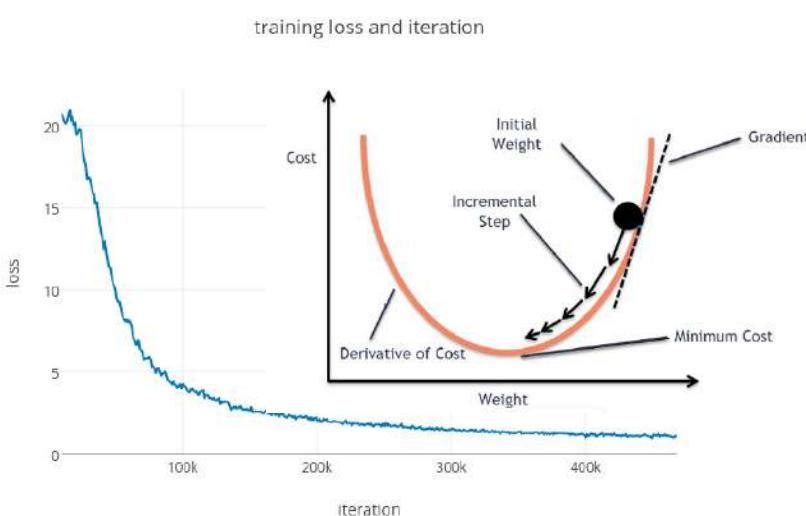
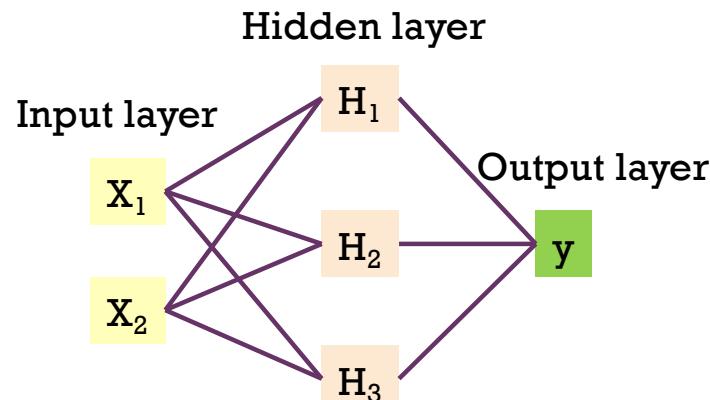


*New weight = weight - Learning rate \* Gradient*

$$\text{New weight} = \text{Old weight} - \text{Learning rate} \left( \frac{\partial \text{Error}}{\partial \text{Weight}} \right)$$



# Batch, Iteration, Epoch



**Stop when?**

- Converge (no change in loss)
- Max epochs

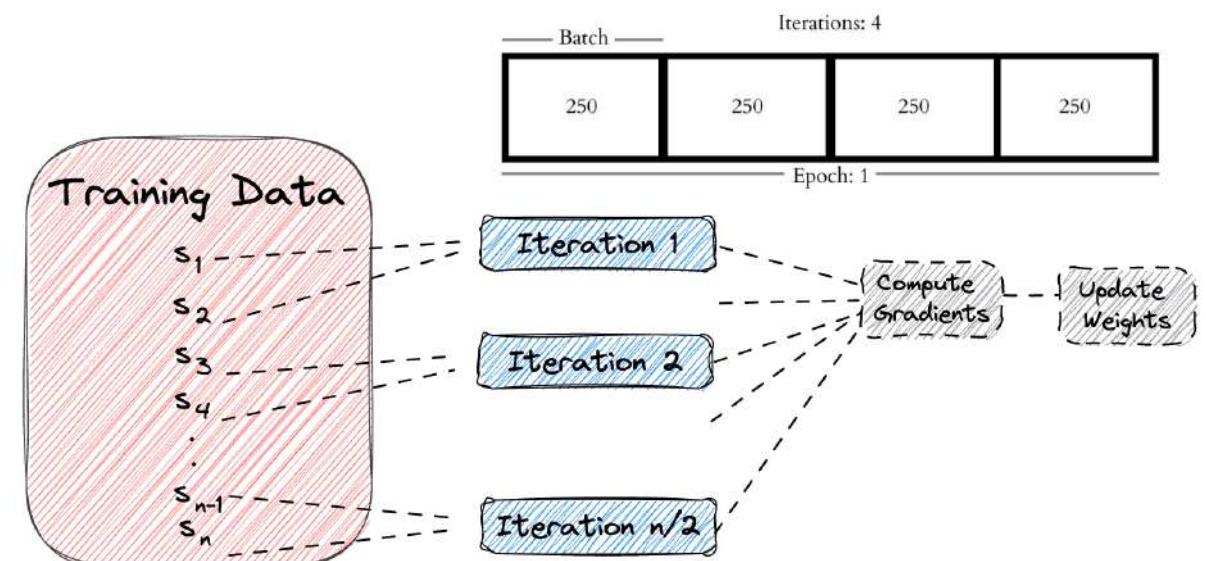
115

**Important Params:**

- Activation functions
- #hidden units, #hidden layers
- Learning rate, momentum, decay
- Seed number, etc.

**Epoch vs Iterations vs Batch**

Example Dataset: 1000

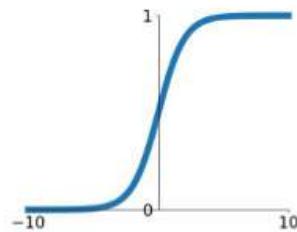




# Activation functions

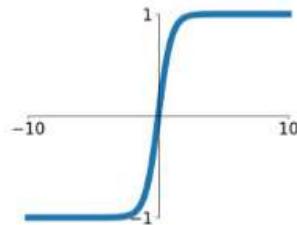
## Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



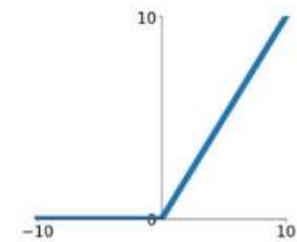
## tanh

$$\tanh(x)$$



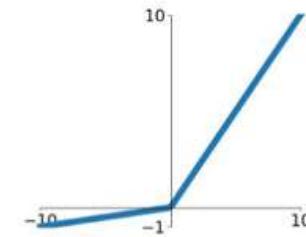
## ReLU

$$\max(0, x)$$



## Leaky ReLU

$$\max(0.1x, x)$$

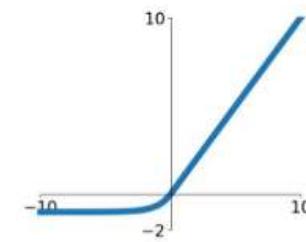


## Maxout

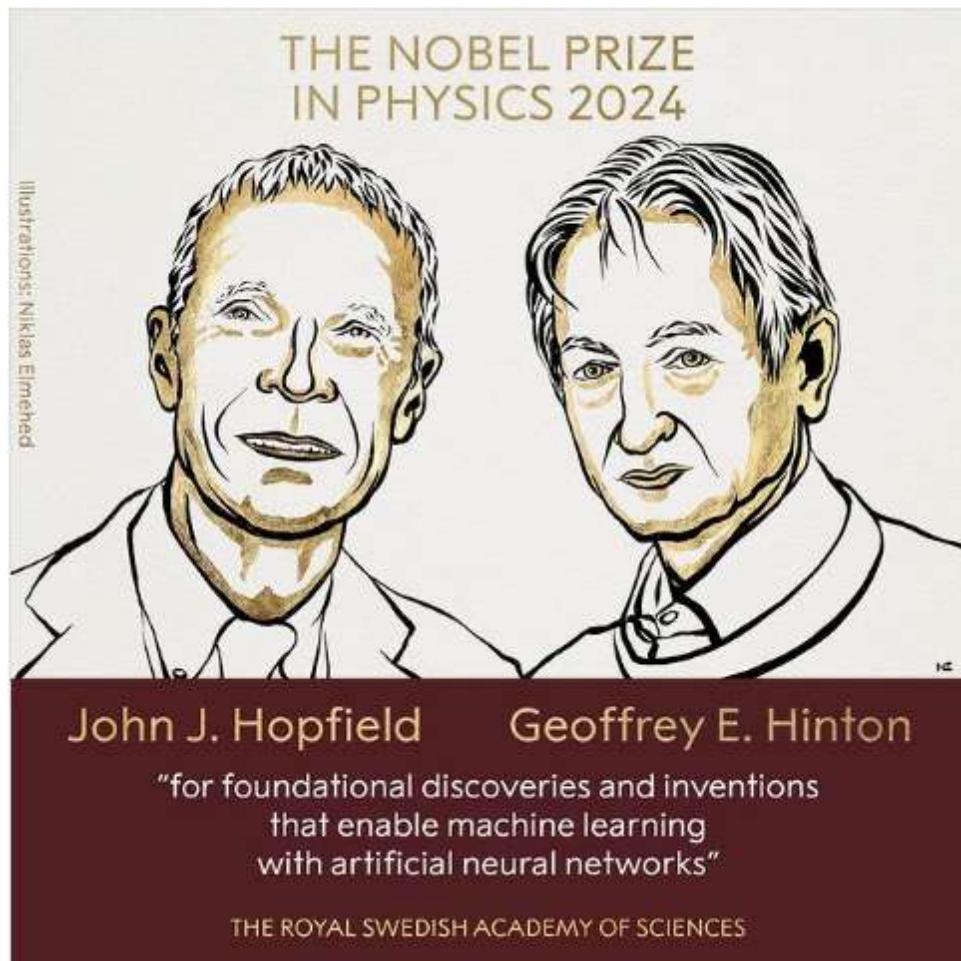
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

## ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Basic research (foundation research)



8 October 2024

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Physics 2024 to

**John J. Hopfield**  
Princeton University, NJ, USA

**Geoffrey E. Hinton**  
University of Toronto, Canada

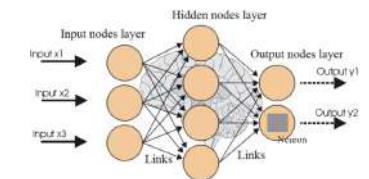
*"for foundational discoveries and inventions that enable machine learning with artificial neural networks"*

They trained artificial neural networks using physics

**John Hopfield** invented a network that uses a method for saving and recreating patterns. We can imagine the nodes as pixels.

The *Hopfield network* utilises physics that describes a material's characteristics due to its atomic spin – a property that makes each atom a tiny magnet.

**Geoffrey Hinton** used the Hopfield network as the foundation for a new network that uses a different method: *the Boltzmann machine*. This can learn to recognise characteristic elements in a given type of data.



# Tinker With a Neural Network Right Here in Your Browser.

## Don't Worry, You Can't Break It. We Promise.

Epoch 000,000      Learning rate 0.03      Activation Tanh      Regularization None      Regularization rate 0      Problem type Classification

DATA      FEATURES      + - 2 HIDDEN LAYERS      OUTPUT

Which dataset do you want to use?  
Which properties do you want to feed in?

Ratio of training to test data: 50%  
Noise: 0  
Batch size: 10

Link

sin(X<sub>1</sub>)

4 neurons

2 neurons

The outputs are mixed with varying weights, shown by the thickness of the lines.

This is the output from one neuron. Hover to see it larger.

Test loss 0.500  
Training loss 0.551

A neural network diagram illustrating a two-hidden-layer model. The input layer consists of five features:  $X_1$ ,  $X_2$ ,  $X_1^2$ ,  $X_2^2$ , and  $X_1X_2$ . These feed into a first hidden layer with 4 neurons and a second hidden layer with 2 neurons. The final output is a classification result. The diagram includes a scatter plot showing the distribution of data points (blue and orange) and their corresponding predictions. Various controls at the top allow for adjusting the epoch, learning rate, activation function, regularization, and problem type. The current state shows an epoch of 000,000, a learning rate of 0.03, Tanh activation, no regularization, and a classification problem. The test loss is 0.500 and the training loss is 0.551.



Please [cite us](#) if you use the software.

[sklearn.neural\\_network.MLPClassifier](#)  
[Examples using sklearn.neural\\_network.MLPClassifi...](#)

## sklearn.neural\_network.MLPClassifier

```
class sklearn.neural_network.MLPClassifier(hidden_layer_sizes=(100,), activation='relu', solver='adam', alpha=0.0001, batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True, random_state=None, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000) ¶ [source]
```

Multi-layer Perceptron classifier.

This model optimizes the log-loss function using LBFGS or stochastic gradient descent.

*New in version 0.18.*

**Parameters:** `hidden_layer_sizes : tuple, length = n_layers - 2, default=(100,)`

The ith element represents the number of neurons in the ith hidden layer.

`activation : {'identity', 'logistic', 'tanh', 'relu'}, default='relu'`

Activation function for the hidden layer.

- 'identity', no-op activation, useful to implement linear bottleneck, returns  $f(x) = x$
- 'logistic', the logistic sigmoid function, returns  $f(x) = 1 / (1 + \exp(-x))$ .
- 'tanh', the hyperbolic tan function, returns  $f(x) = \tanh(x)$ .
- 'relu', the rectified linear unit function, returns  $f(x) = \max(0, x)$

`solver : {'lbfgs', 'sgd', 'adam'}, default='adam'`

The solver for weight optimization.



Prev Up Next

scikit-learn 0.22.2

Other versions

Please [cite us](#) if you use the software.[sklearn.neural\\_network.MLPRegressor](#)

Examples using

[sklearn.neural\\_network.MLPRegressor](#)

## sklearn.neural\_network.MLPRegressor

```
class sklearn.neural_network.MLPRegressor(hidden_layer_sizes=(100,), activation='relu', solver='adam', alpha=0.0001,
batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True, random_state=None,
tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False,
validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000) ¶ [source]
```

Multi-layer Perceptron regressor.

This model optimizes the squared-loss using LBFGS or stochastic gradient descent.

New in version 0.18.

**Parameters:**

**hidden\_layer\_sizes : tuple, length = n\_layers - 2, default=(100,)**

The ith element represents the number of neurons in the ith hidden layer.

**activation : {'identity', 'logistic', 'tanh', 'relu'}, default='relu'**

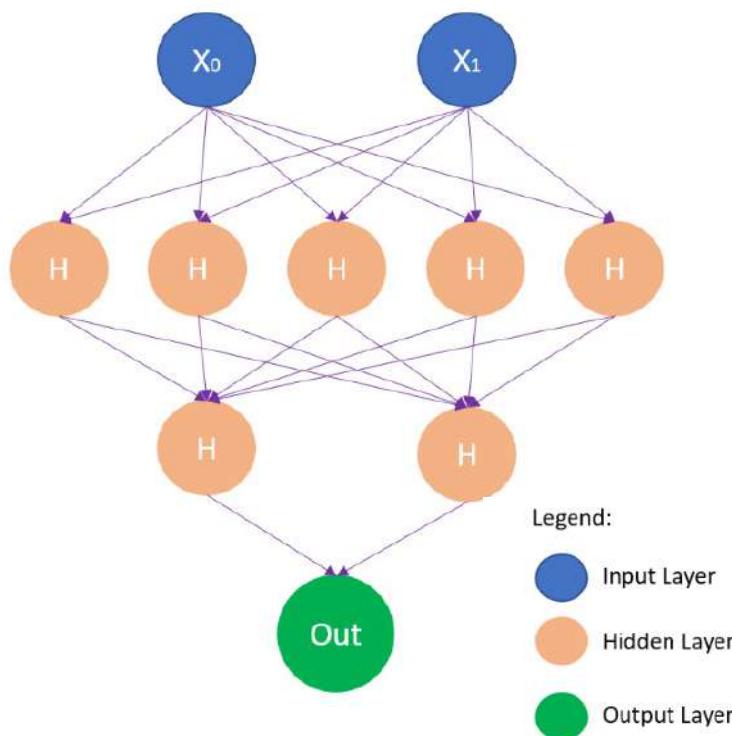
Activation function for the hidden layer.

- 'identity', no-op activation, useful to implement linear bottleneck, returns  $f(x) = x$
- 'logistic', the logistic sigmoid function, returns  $f(x) = 1 / (1 + \exp(-x))$ .
- 'tanh', the hyperbolic tan function, returns  $f(x) = \tanh(x)$ .
- 'relu', the rectified linear unit function, returns  $f(x) = \max(0, x)$

**solver : {'lbfgs', 'sgd', 'adam'}, default='adam'**

The solver for weight optimization.

# Example



**batch\_size : int, default='auto'**

Size of minibatches for stochastic optimizers. If the solver is 'lbfgs', the classifier will not use minibatch.

When set to "auto", `batch_size=min(200, n_samples)`.

**learning\_rate : {'constant', 'invscaling', 'adaptive'}, default='constant'**

Learning rate schedule for weight updates.

```
mlp_clf = MLPClassifier(hidden_layer_sizes=(5,2),  
                        max_iter = 300, activation = 'relu',  
                        solver = 'adam')
```

```
param_grid = {  
    'hidden_layer_sizes': [(150,100,50), (120,80,40), (100,50)],  
    'max_iter': [50, 100, 150],  
    'activation': ['tanh', 'relu'],  
    'solver': ['sgd', 'adam'],  
    'alpha': [0.0001, 0.05],  
    'learning_rate': ['constant','adaptive'],  
}
```

```
grid = GridSearchCV(mlp_clf, param_grid, n_jobs= -1, cv=5)  
grid.fit(trainX_scaled, trainY)
```

```
print(grid.best_params_)
```

+

4) kNN

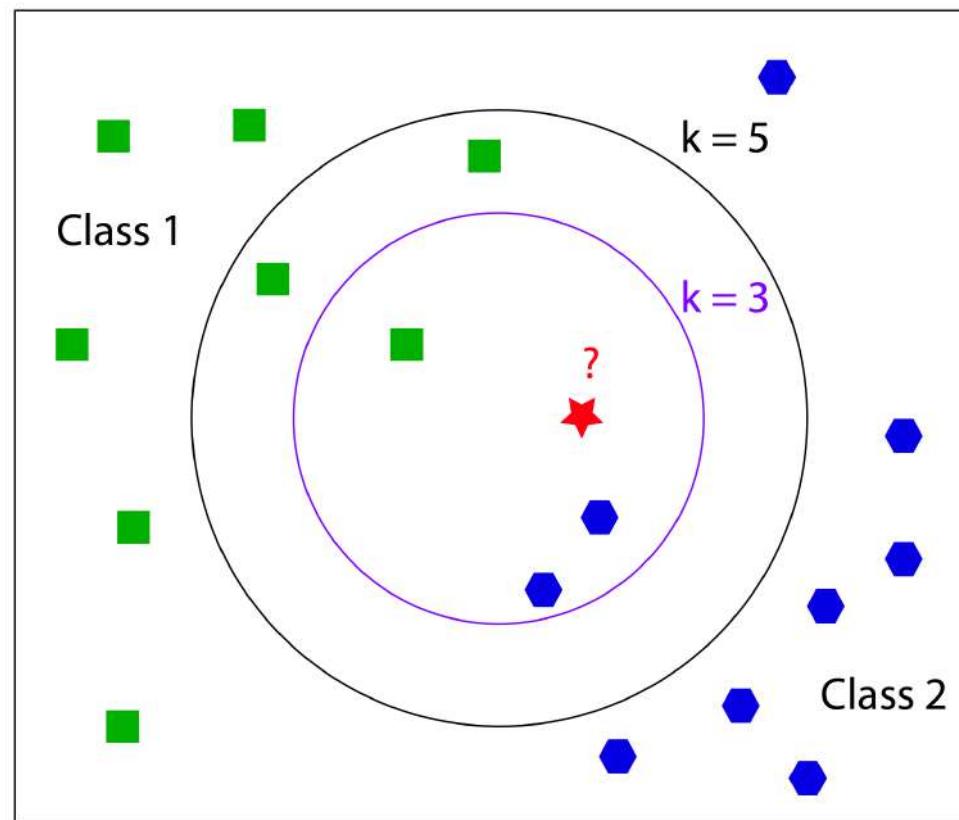


## 4) k-Nearest Neighbors (kNN)

- Memory based learning
- Suitable for small data sets
- Merge
  - Voting
  - Average
  - Maximum prob
- Cautions:
  - Support only numerical variables
  - Need to adjust variable range

Important Params:

- $k$
- Distance function





# Distance Function

## ■ Euclidean Distance

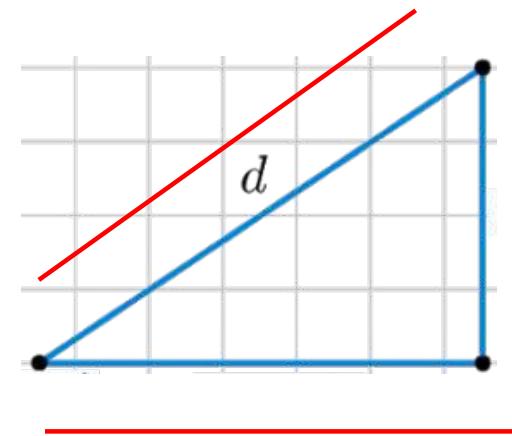
$$\sqrt{\sum_{i=1}^k (x_i - y_i)^2}$$

## ■ Manhattan Distance

$$\sum_{i=1}^k |x_i - y_i|$$

## ■ Minkowski Distance

$$\left( \sum_{i=1}^k (|x_i - y_i|)^q \right)^{1/q}$$



$q = 1$  is Manhattan Distance  
 $q = 2$  is Euclidean Distance



## Distance Function (cont.)

- Hamming distance: same (0) vs diff (1)
- It still supports only numeric variable.

$$D_H = \sum_{i=1}^k |x_i - y_i|$$

$x = y \Rightarrow D = 0$

$x \neq y \Rightarrow D = 1$

X	Y	Distance
Male	Male	0
Male	Female	1



# Nearest Neighbors

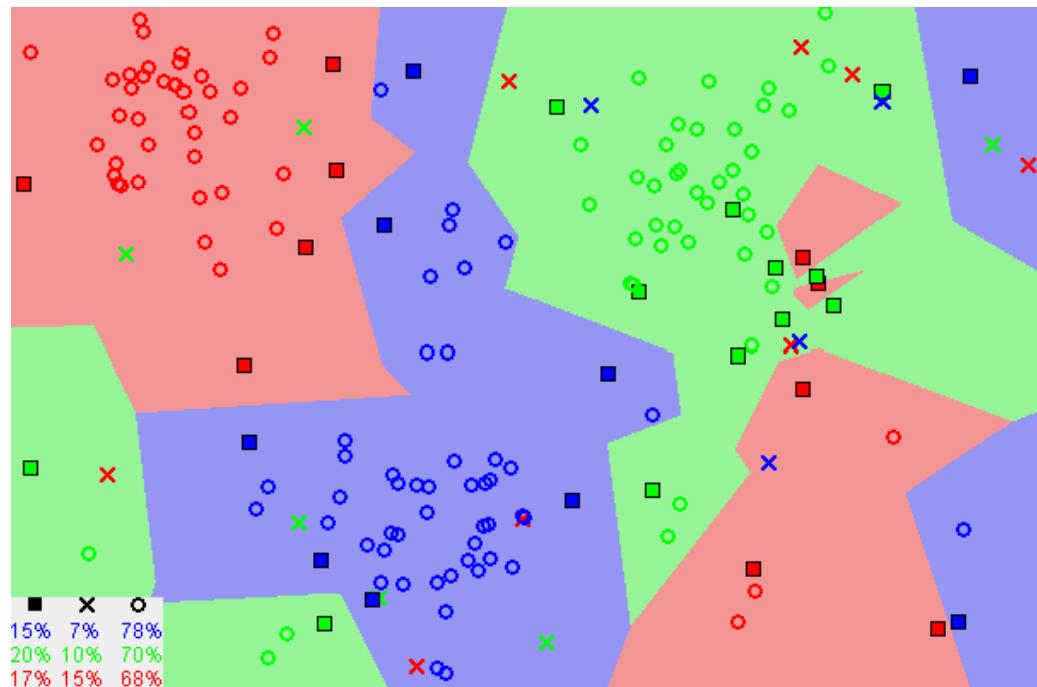


Image showing how similar data points typically exist close to each other

Source : <https://towardsdatascience.com/machine-learning-basics-with-the-k-nearest-neighbors-algorithm-6a6e71d01761>



Please [cite us](#) if you use the software.

[sklearn.neighbors.KNeighborsClassifier](#)  
Examples using  
[sklearn.neighbors.KNeighborsClassifier](#)

## sklearn.neighbors.KNeighborsClassifier

```
class sklearn.neighbors.KNeighborsClassifier(n_neighbors=5, weights='uniform', algorithm='auto', leaf_size=30, p=2,
metric='minkowski', metric_params=None, n_jobs=None, **kwargs)
```

[\[source\]](#)

Classifier implementing the k-nearest neighbors vote.

Read more in the [User Guide](#).

**Parameters:** **n\_neighbors : int, optional (default = 5)**

Number of neighbors to use by default for [kneighbors](#) queries.

**weights : str or callable, optional (default = 'uniform')**

weight function used in prediction. Possible values:

- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- [callable] : a user-defined function which accepts an array of distances, and returns an array of the same shape containing the weights.

**algorithm : {'auto', 'ball\_tree', 'kd\_tree', 'brute'}, optional**

Algorithm used to compute the nearest neighbors:

- 'ball\_tree' will use [BallTree](#)
- 'kd\_tree' will use [KDTree](#)
- 'brute' will use a brute-force search.

'auto' will attempt to decide the most appropriate algorithm based on the values passed to the method



## sklearn.neighbors.KNeighborsRegressor

```
class sklearn.neighbors.KNeighborsRegressor(n_neighbors=5, weights='uniform', algorithm='auto', leaf_size=30, p=2, metric='minkowski', metric_params=None, n_jobs=None, **kwargs)
```

[source]

Regression based on k-nearest neighbors.

The target is predicted by local interpolation of the targets associated of the nearest neighbors in the training set.

Read more in the [User Guide](#).

New in version 0.9.

**Parameters:**

**n\_neighbors : int, optional (default = 5)**

Number of neighbors to use by default for `kneighbors` queries.

**weights : str or callable**

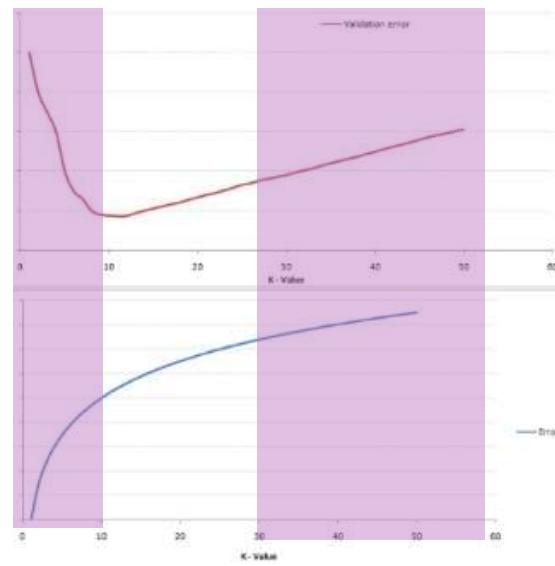
weight function used in prediction. Possible values:

- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- [callable] : a user-defined function which accepts an array of distances, and returns an array of the same shape containing the weights.

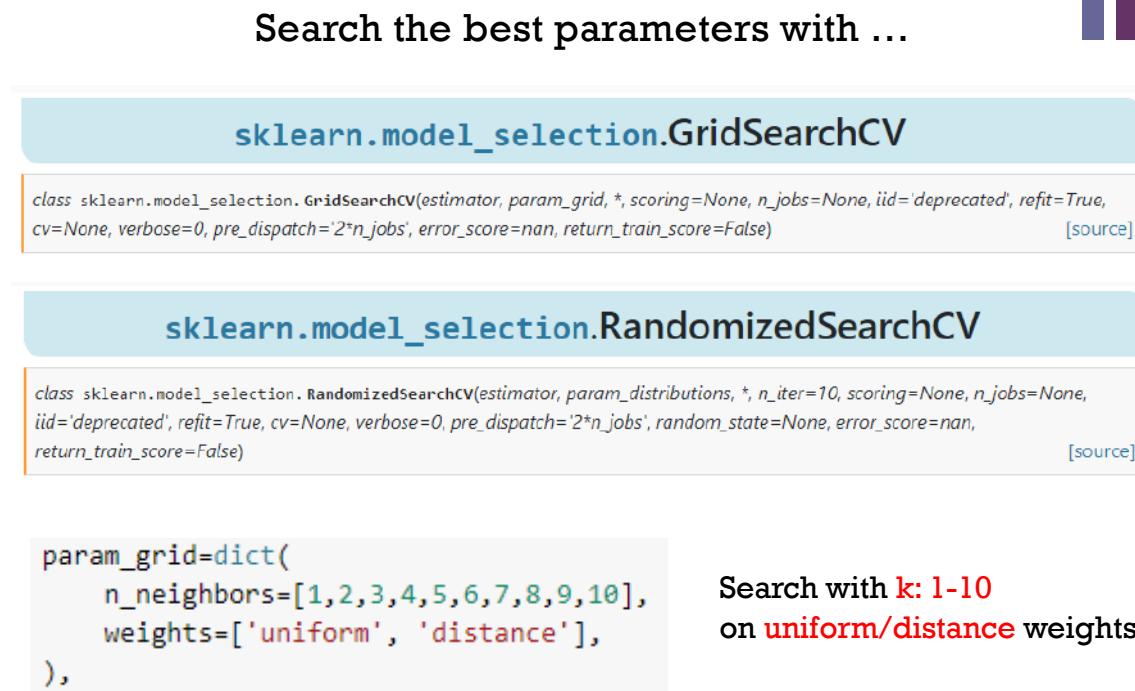
Uniform weights are used by default.

# Choosing the right value of K

Too Underfitted



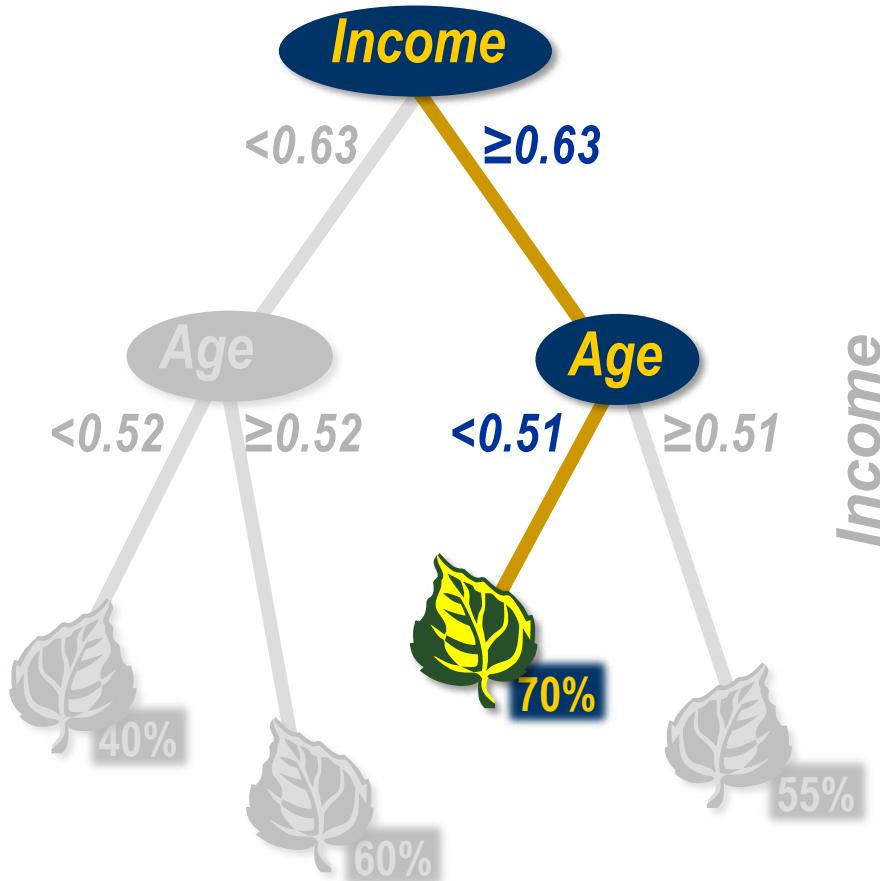
Too Overfitted



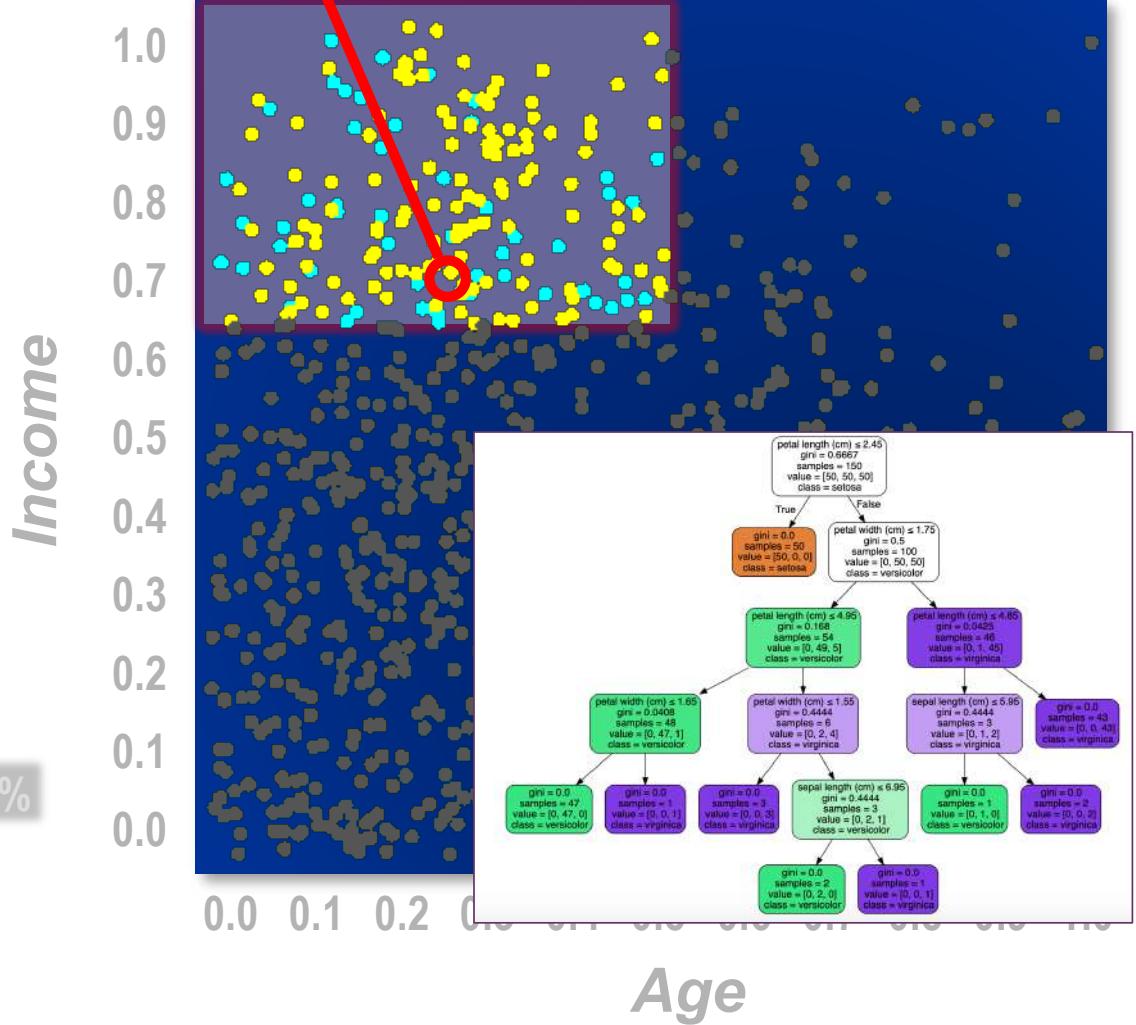


## Multiclass & Multi-Label

# 1) Decision Tree (recap)

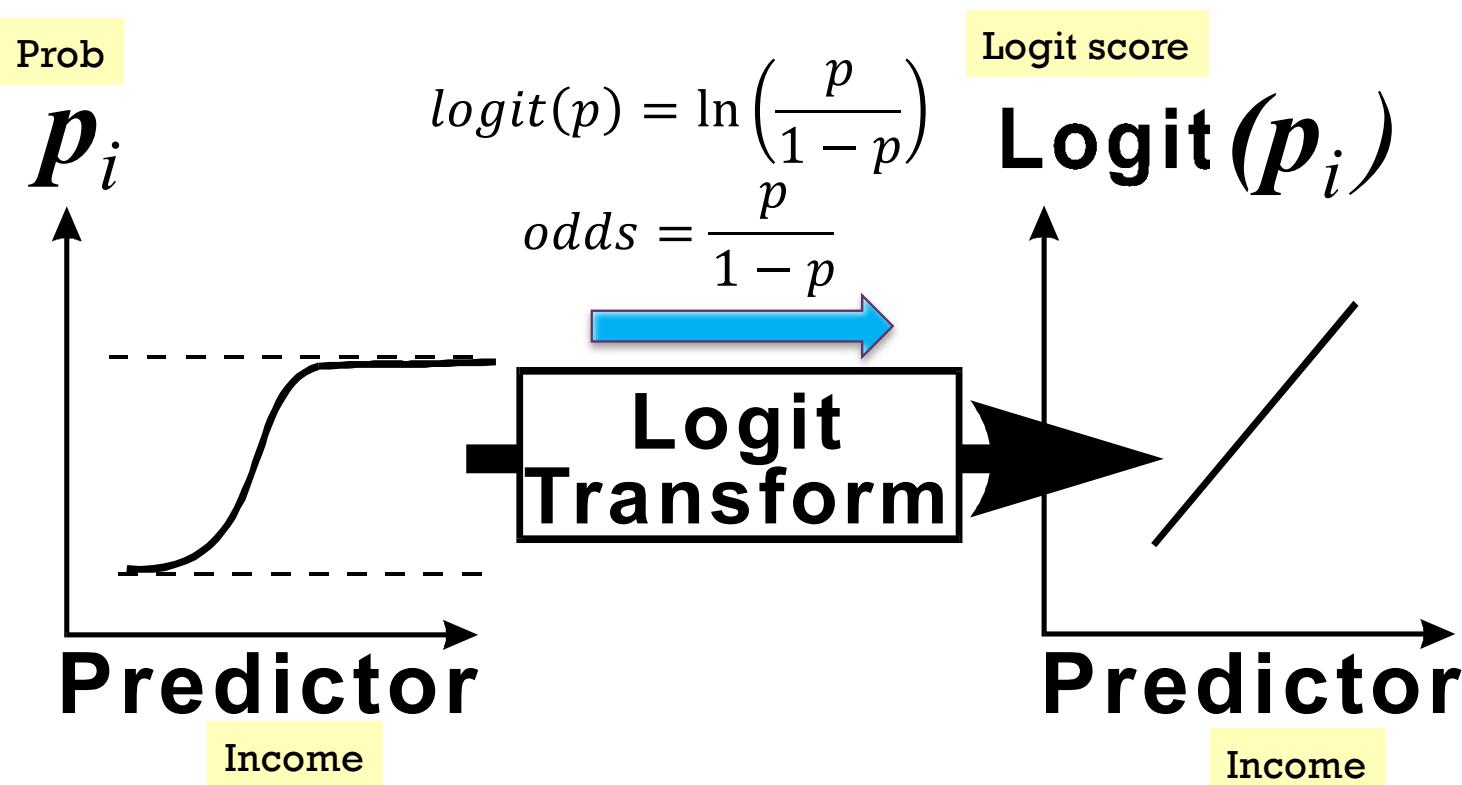


Predict: Decision = Estimate = 0.70

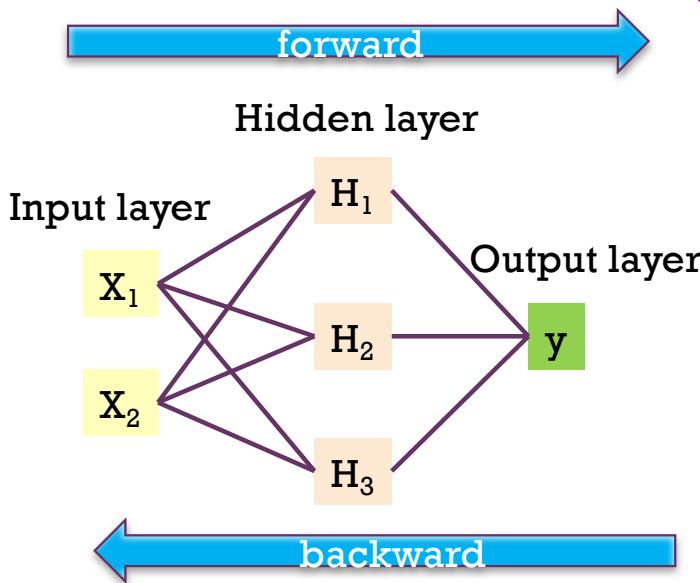




## 2) Regression (recap)



## 3) Neural Networks (recap)

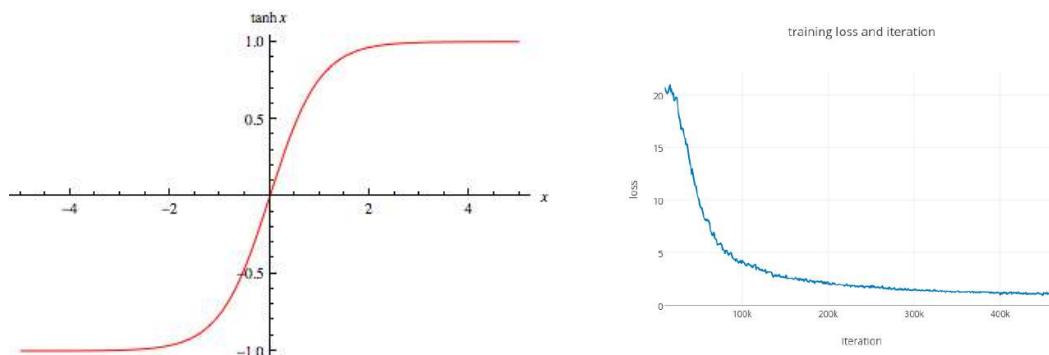


$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_0 + \hat{w}_1 H_1 + \hat{w}_2 H_2 + \hat{w}_3 H_3$$

$$H_1 = \tanh(\hat{w}_{10} + \hat{w}_{11}x_1 + \hat{w}_{12}x_2)$$

$$H_2 = \tanh(\hat{w}_{20} + \hat{w}_{21}x_1 + \hat{w}_{22}x_2)$$

$$H_3 = \tanh(\hat{w}_{30} + \hat{w}_{31}x_1 + \hat{w}_{32}x_2)$$



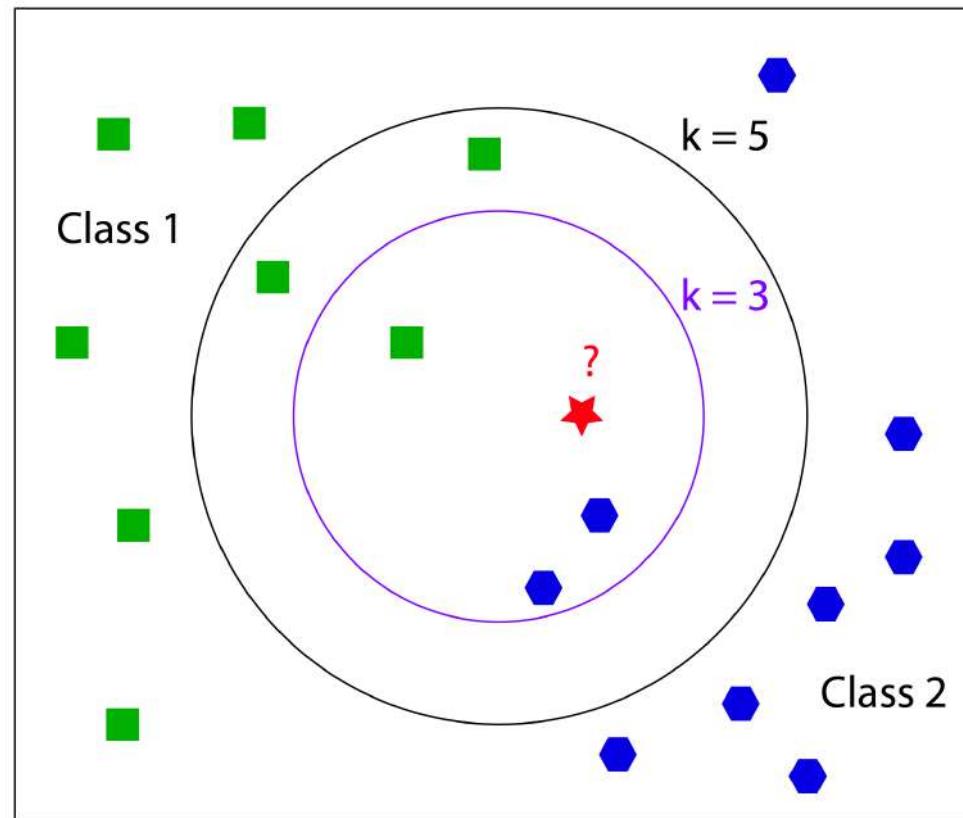
How to update weight

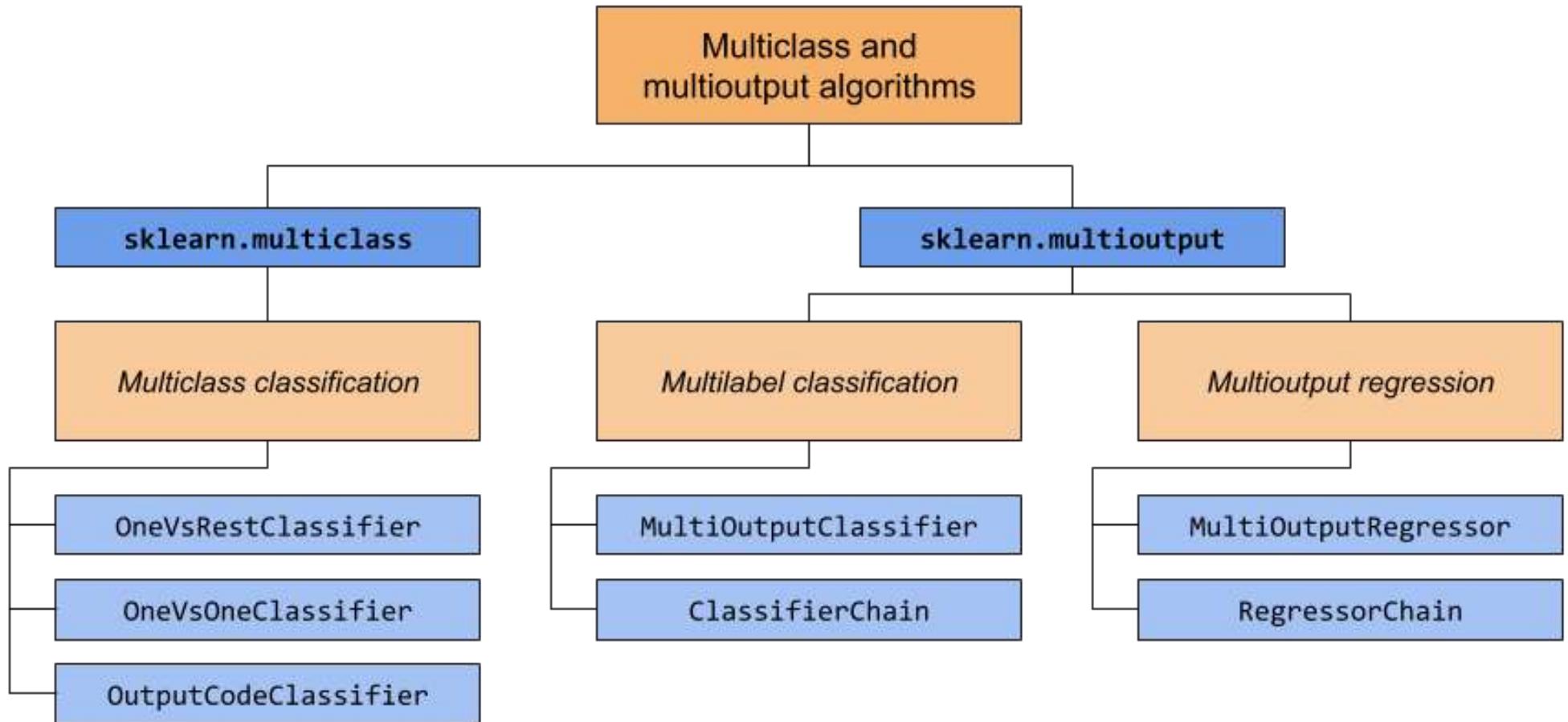
<https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/>



## 4) k-Nearest Neighbors (recap)

- Memory based learning
- Suitable for small data sets
- Merge
  - Voting
  - Average
  - Maximum prob
- Cautions:
  - Support only numerical variables
  - Need to adjust variable range







# Multiclass

- Inherently multiclass:

- `naive_bayes.BernoulliNB`
- `tree.DecisionTreeClassifier`
- `tree.ExtraTreeClassifier`
- `ensemble.ExtraTreesClassifier`
- `naive_bayes.GaussianNB`
- `neighbors.KNeighborsClassifier`
- `semi_supervised.LabelPropagation`
- `semi_supervised.LabelSpreading`
- `discriminant_analysis.LinearDiscriminantAnalysis`
- `svm.LinearSVC` (setting `multi_class="crammer_singer"`)
- `linear_model.LogisticRegression` (setting `multi_class="multinomial"`)
- `linear_model.LogisticRegressionCV` (setting `multi_class="multinomial"`)
- `neural_network.MLPClassifier`
- `neighbors.NearestCentroid`
- `discriminant_analysis.QuadraticDiscriminantAnalysis`
- `neighbors.RadiusNeighborsClassifier`
- `ensemble.RandomForestClassifier`
- `linear_model.RidgeClassifier`
- `linear_model.RidgeClassifierCV`

- Multiclass as One-Vs-One:

- `svm.NuSVC`
- `svm.SVC`
- `gaussian_process.GaussianProcessClassifier` (setting `multi_class = "one_vs_one"`)

- Multiclass as One-Vs-The-Rest:

- `ensemble.GradientBoostingClassifier`
- `gaussian_process.GaussianProcessClassifier` (setting `multi_class = "one_vs_rest"`)
- `svm.LinearSVC` (setting `multi_class="ovr"`)
- `linear_model.LogisticRegression` (setting `multi_class="ovr"`)
- `linear_model.LogisticRegressionCV` (setting `multi_class="ovr"`)
- `linear_model.SGDClassifier`
- `linear_model.Perceptron`
- `linear_model.PassiveAggressiveClassifier`

- Support multilabel:

- `tree.DecisionTreeClassifier`
- `tree.ExtraTreeClassifier`
- `ensemble.ExtraTreesClassifier`
- `neighbors.KNeighborsClassifier`
- `neural_network.MLPClassifier`
- `neighbors.RadiusNeighborsClassifier`
- `ensemble.RandomForestClassifier`
- `linear_model.RidgeClassifier`
- `linear_model.RidgeClassifierCV`

- Support multiclass-multioutput:

- `tree.DecisionTreeClassifier`
- `tree.ExtraTreeClassifier`
- `ensemble.ExtraTreesClassifier`
- `neighbors.KNeighborsClassifier`
- `neighbors.RadiusNeighborsClassifier`
- `ensemble.RandomForestClassifier`

<https://scikit-learn.org/stable/modules/multiclass.html>



# Multiclass Logistic Regression

## `sklearn.linear_model.LogisticRegression`

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True,
intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0,
warm_start=False, n_jobs=None, l1_ratio=None)
```

[source]

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi\_class' option is set to 'ovr', and uses the cross-entropy loss if the 'multi\_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs', 'sag', 'saga' and 'newton-cg' solvers.)

This class implements regularized logistic regression using the 'liblinear' library, 'newton-cg', 'sag', 'saga' and 'lbfgs' solvers.

**Note that regularization is applied by default.** It can handle both dense and sparse input. Use C-ordered arrays or CSR matrices containing 64-bit floats for optimal performance; any other input format will be converted (and copied).

### `multi_class : {'auto', 'ovr', 'multinomial'}, default='auto'`

If the option chosen is 'ovr', then a binary problem is fit for each label. For 'multinomial' the loss minimised is the multinomial loss fit across the entire probability distribution, even when the data is binary.

'multinomial' is unavailable when solver='liblinear'. 'auto' selects 'ovr' if the data is binary, or if solver='liblinear', and otherwise selects 'multinomial'.

*New in version 0.18:* Stochastic Average Gradient descent solver for 'multinomial' case.

# Wrapper (Multiclass)

## sklearn.multiclass.OneVsRestClassifier

```
class sklearn.multiclass.OneVsRestClassifier(estimator, *, n_jobs=None, verbose=0)
```

[\[source\]](#)

One-vs-the-rest (OvR) multiclass strategy.

Also known as one-vs-all, this strategy consists in fitting one classifier per class. For each classifier, the class is fitted against all the other classes. In addition to its computational efficiency (only `n_classes` classifiers are needed), one advantage of this approach is its interpretability. Since each class is represented by one and one classifier only, it is possible to gain knowledge about the class by inspecting its corresponding classifier. This is the most commonly used strategy for multiclass classification and is a fair default choice.

`OneVsRestClassifier` can also be used for multilabel classification. To use this feature, provide an indicator matrix for the target `y` when calling `.fit`. In other words, the target labels should be formatted as a 2D binary (0/1) matrix, where `[i, j] == 1` indicates the presence of label `j` in sample `i`. This estimator uses the binary relevance method to perform multilabel classification, which involves training one binary classifier independently for each label.

Read more in the [User Guide](#).

### Parameters:

`estimator : estimator object`

A regressor or a classifier that implements `fit`. When a classifier is passed, `decision_function` will be used in priority and it will fallback to `predict_proba` if it is not available. When a regressor is passed, `predict` is used.

`n_jobs : int, default=None`

The number of jobs to use for the computation: the `n_classes` one-vs-rest problems are computed in parallel.

`None` means 1 unless in a `joblib.parallel_backend` context. `-1` means using all processors. See [Glossary](#)

### See also:

[OneVsOneClassifier](#)

One-vs-one multiclass strategy.

[OutputCodeClassifier](#)

(Error-Correcting) Output-Code multiclass strategy.

[sklearn.multioutput.MultiOutputClassifier](#)

Alternate way of extending an estimator for multilabel classification.

[sklearn.preprocessing.MultiLabelBinarizer](#)

Transform iterable of iterables to binary indicator matrix.

## Examples

```
>>> import numpy as np
>>> from sklearn.multiclass import OneVsRestClassifier
>>> from sklearn.svm import SVC
>>> X = np.array([
...     [10, 10],
...     [8, 10],
...     [-5, 5.5],
...     [-5.4, 5.5],
...     [-20, -20],
...     [-15, -20]
... ])
>>> y = np.array([0, 0, 1, 1, 2, 2])
>>> clf = OneVsRestClassifier(SVC()).fit(X, y)
>>> clf.predict([-19, -20], [9, 9], [-5, 5])
array([2, 0, 1])
```



# MultiOutputClassifier #

```
class sklearn.multioutput.MultiOutputClassifier(estimator, *, n_jobs=None)
```

Multi target classification.

[\[source\]](#)

This strategy consists of fitting one classifier per target. This is a simple strategy for extending classifiers that do not natively support multi-target classification.

## Parameters:

### **estimator : estimator object**

An estimator object implementing [fit](#) and [predict](#). A [predict\\_proba](#) method will be exposed only if `estimator` implements it.

### **n\_jobs : int or None, optional (default=None)**

The number of jobs to run in parallel. [fit](#), passed estimator) will be parallelized for ea

When individual estimators are fast to train performance due to the parallelism overhead

`None` means `1` unless in a [joblib.parallel](#) processes / threads. See [Glossary](#) for more

## Examples

```
>>> import numpy as np
>>> from sklearn.datasets import make_multilabel_classification
>>> from sklearn.multioutput import MultiOutputClassifier
>>> from sklearn.linear_model import LogisticRegression
>>> X, y = make_multilabel_classification(n_classes=3, random_state=0)
>>> clf = MultiOutputClassifier(LogisticRegression()).fit(X, y)
>>> clf.predict(X[-2:])
array([[1, 1, 1],
       [1, 0, 1]])
```

# MultiOutputRegressor

```
class sklearn.multioutput.MultiOutputRegressor(estimator, *, n_jobs=None)
```

Multi target regression.

[\[source\]](#)

This strategy consists of fitting one regressor per target. This is a simple strategy for extending regressors that do not natively support multi-target regression.

! Added in version 0.18.

## Parameters:

**estimator : estimator object**

An estimator object implementing [fit](#) and [predict](#).

**n\_jobs : int or None, optional (default=None)**

The number of jobs to run in parallel. [fit](#), [predict](#)

passed estimator) will be parallelized for each target.

When individual estimators are fast to train or predict, this can result in performance due to the parallelism overhead.

**None** means 1 unless in a [joblib.parallel](#) context. The number of parallel processes / threads. See [Glossary](#) for more details.

## Examples

```
>>> import numpy as np
>>> from sklearn.datasets import load_linnerud
>>> from sklearn.multioutput import MultiOutputRegressor
>>> from sklearn.linear_model import Ridge
>>> X, y = load_linnerud(return_X_y=True)
>>> regr = MultiOutputRegressor(Ridge(random_state=123)).fit(X, y)
>>> regr.predict(X[[0]])
array([[176..., 35..., 57...]])
```



## Evaluation Measures



# Evaluation (Train/Test Split)

Training Data

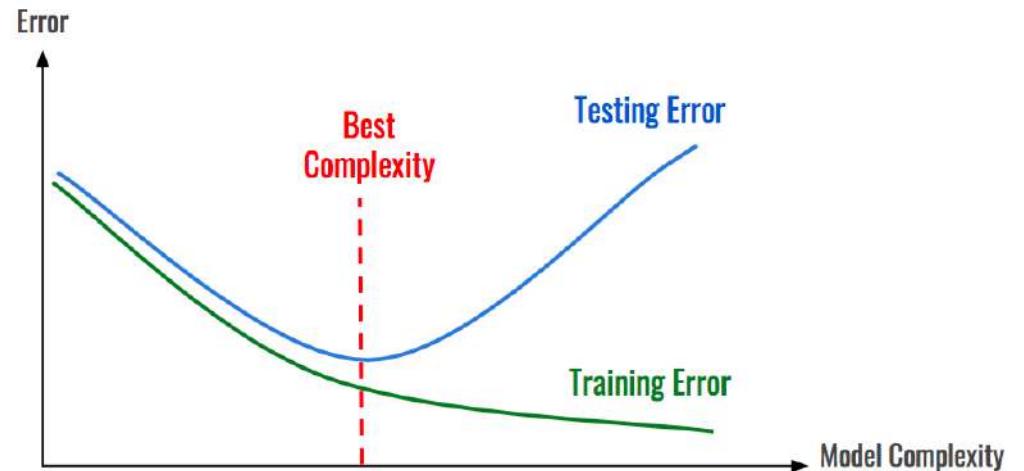


Age	Income	Purchase
25	25,000	Yes
35	50,000	Yes
32	35,000	No

Testing Data

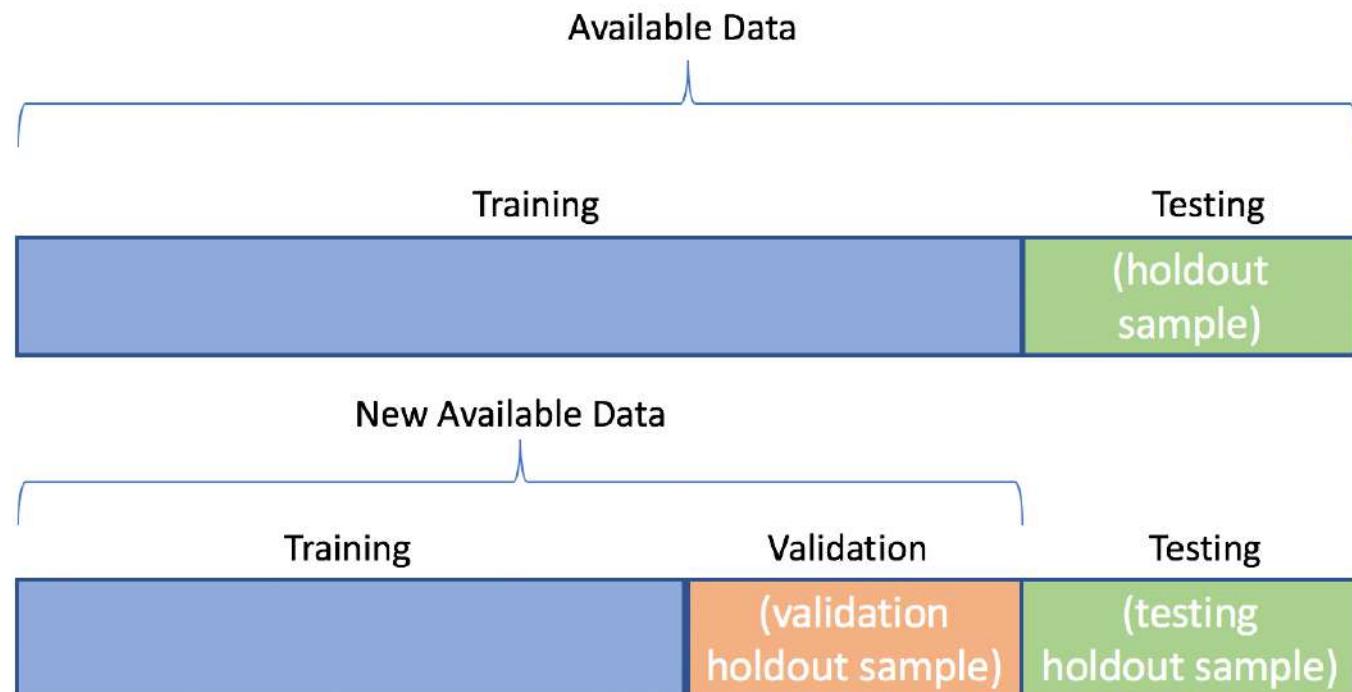


Age	Income	Purchase
27	35,000	Yes
23	20,000	No
45	34,000	No



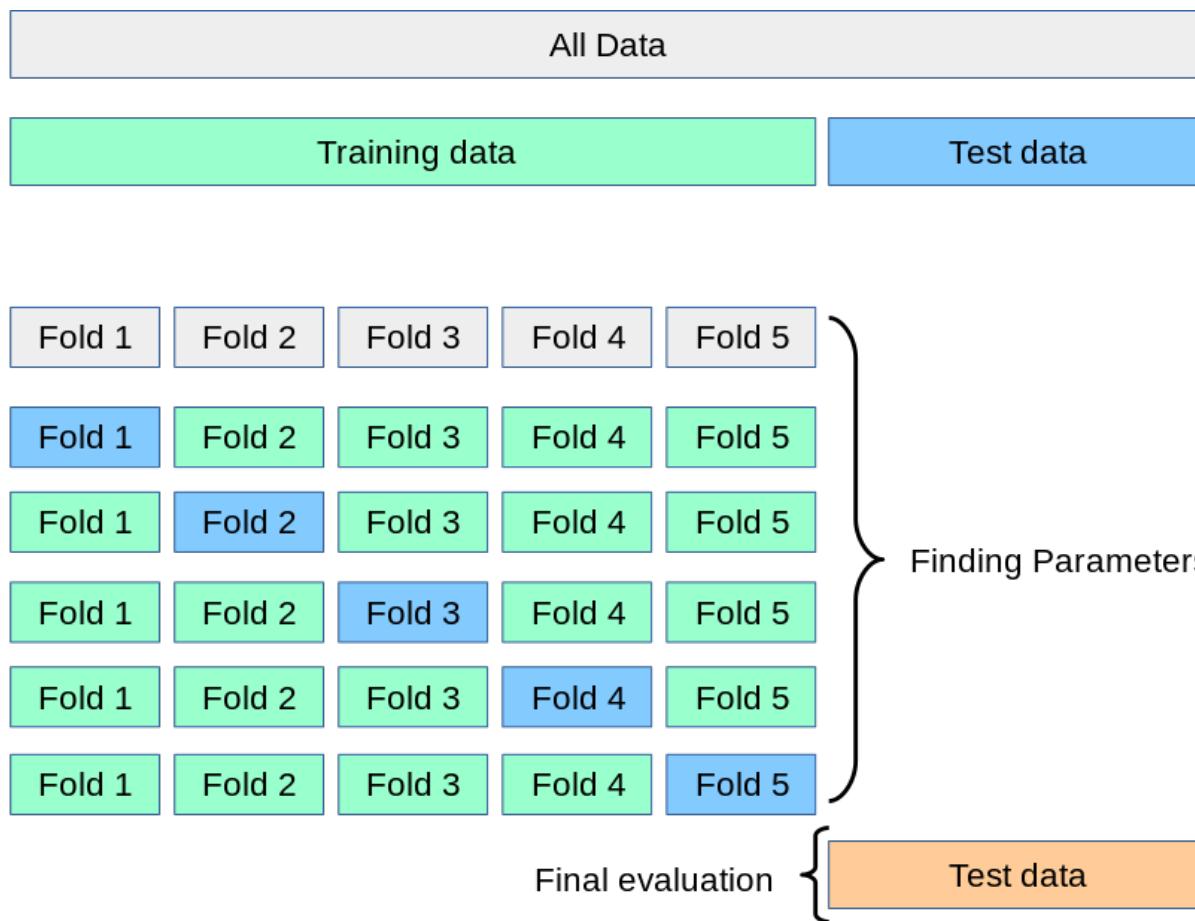
## + Train (Validation) & Test

- Training data = Textbook
- Validation data = Exercise
- Testing data = Final exam





# Single Validation → Cross Validation (CV)





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[sklearn.model\\_selection.train\\_test\\_split](#)

Examples using

[sklearn.model\\_selection.train\\_t](#)

[Toggle Menu](#)

## sklearn.model\_selection.train\_test\_split

`sklearn.model_selection.train_test_split(*arrays, **options)`

[\[source\]](#)

Split arrays or matrices into random train and test subsets

Quick utility that wraps input validation and `next(ShuffleSplit().split(X, y))` and application to input data into a single call for splitting (and optionally subsampling) data in a oneliner.

Read more in the [User Guide](#).

**Parameters:** *\*arrays : sequence of indexables with same length / shape[0]*

Allowed inputs are lists, numpy arrays, scipy-sparse matrices or pandas dataframes.

**test\_size : float, int or None, optional (default=None)**

If float, should be between 0.0 and 1.0 and represent the proportion of the dataset to include in the test split. If int, represents the absolute number of test samples. If None, the value is set to the complement of the train size. If `train_size` is also None, it will be set to 0.25.

**train\_size : float, int, or None, (default=None)**

If float, should be between 0.0 and 1.0 and represent the proportion of the dataset to include in the train split. If int, represents the absolute number of train samples. If None, the value is automatically set to the complement of the test size.

**random\_state : int, RandomState instance or None, optional (default=None)**

If int, `random_state` is the seed used by the random number generator; If RandomState instance, `random_state` is the random number generator; If None, the random number generator is the RandomState instance used by `np.random`.

# +

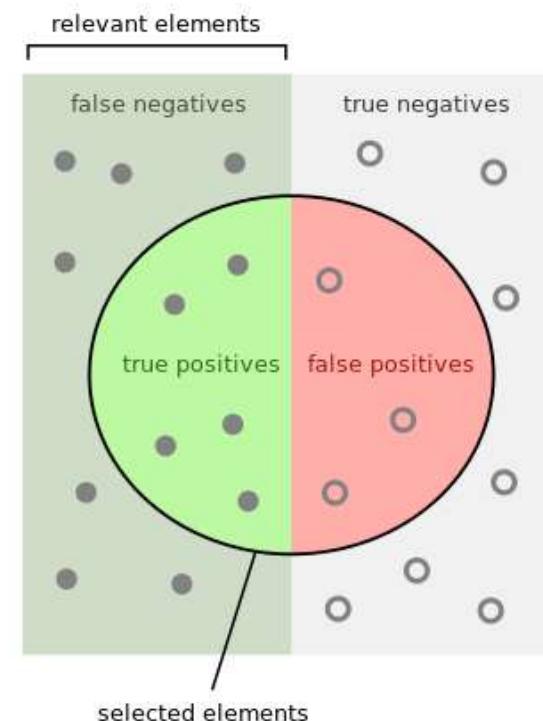
# Model Evaluation

- Regression
  - Sum Squared Error (SSE)
  - Average Squared Error (ASE)
- Classification
  - **Accuracy**
  - Misclassification
  - Precision
  - Recall
  - F1
- Graph
  - ROC Curve
  - Area Under ROC (c-statistic)
  - Lift
  - Gain
  - Response



# Precision, Recall, F1

n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	



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- Precision = correctly predict =  $TP / (TP + FP)$
- Recall = coverage =  $TP / (TP + FN)$
- F1 =  $(2 * \text{pre} * \text{rec}) / (\text{pre} + \text{rec})$

How many selected items are relevant?  
Precision =

How many relevant items are selected?  
Recall =

### 3.5.1. The scoring parameter: defining model evaluation rules

Model selection and evaluation using tools, such as `grid_search.GridSearchCV` and `cross_validation.cross_val_score`, take a `scoring` parameter that controls what metric they apply to estimators evaluated.

#### 3.5.1.1. Common cases: predefined values

For the most common usecases, you can simply provide a string as the `scoring` parameter. Possible values are:

Scoring	Function
<b>Classification</b>	
'accuracy'	<code>sklearn.metrics.accuracy_score</code>
'average_precision'	<code>sklearn.metrics.average_precision_score</code>
'f1'	<code>sklearn.metrics.f1_score</code>
'precision'	<code>sklearn.metrics.precision_score</code>
'recall'	<code>sklearn.metrics.recall_score</code>
'roc_auc'	<code>sklearn.metrics.roc_auc_score</code>
<b>Clustering</b>	
'adjusted_rand_score'	<code>sklearn.metrics.adjusted_rand_score</code>
<b>Regression</b>	
'mean_absolute_error'	<code>sklearn.metrics.mean_absolute_error</code>
'mean_squared_error'	<code>sklearn.metrics.mean_squared_error</code>
'r2'	<code>sklearn.metrics.r2_score</code>



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scikit-learn 0.22.1

[Other versions](#)Please [cite us](#) if you use the software.[sklearn.metrics.confusion\\_matrix](#)

Examples using

[sklearn.metrics.confusion\\_matrix](#)

## sklearn.metrics.confusion\_matrix

```
sklearn.metrics.confusion_matrix(y_true, y_pred, labels=None, sample_weight=None, normalize=None)
```

[\[source\]](#)

Compute confusion matrix to evaluate the accuracy of a classification.

By definition a confusion matrix  $C$  is such that  $C_{i,j}$  is equal to the number of observations known to be in group  $i$  and predicted to be in group  $j$ .

Thus in binary classification, the count of true negatives is  $C_{0,0}$ , false negatives is  $C_{1,0}$ , true positives is  $C_{1,1}$  and false positives is  $C_{0,1}$ .

Read more in the [User Guide](#).

Parameters: `y_true : array-like of shape (n_samples,)`

Ground truth (correct) target values.

```
>>> from sklearn.metrics import confusion_matrix
>>> y_true = [2, 0, 2, 2, 0, 1]
>>> y_pred = [0, 0, 2, 2, 0, 2]
>>> confusion_matrix(y_true, y_pred)
array([[2, 0, 0],
       [0, 0, 1],
       [1, 0, 2]])
```

`shape (n_samples,)`

is returned by a classifier.

`shape (n_classes), default=None`

Fix the matrix. This may be used to reorder or select a subset of labels. If `None` is given, those once in `y_true` or `y_pred` are used in sorted order.

`array-like of shape (n_samples,), default=None`

`normalize : {'true', 'pred', 'all'}, default=None`

Normalizes confusion matrix over the true (rows) : predicted (columns) conditions or all the population. If `None`, confusion matrix will not be normalized.

[https://scikit-learn.org/stable/modules/generated/sklearn.metrics.confusion\\_matrix.html](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.confusion_matrix.html)



## sklearn.metrics.classification\_report

```
sklearn.metrics.classification_report(y_true, y_pred, labels=None, target_names=None, sample_weight=None, digits=2,
output_dict=False, zero_division='warn')
```

[\[source\]](#)

Build a text report showing the main

### Examples

```
>>> from sklearn.metrics import classification_report
>>> y_true = [0, 1, 2, 2, 2]
>>> y_pred = [0, 0, 2, 2, 1]
>>> target_names = ['class 0', 'class 1', 'class 2']
>>> print(classification_report(y_true, y_pred, target_names=target_names))
          precision    recall  f1-score   support
  class 0       0.50      1.00      0.67      1
  class 1       0.00      0.00      0.00      1
  class 2       1.00      0.67      0.80      3

accuracy                           0.60      5
macro avg       0.50      0.56      0.49      5
weighted avg    0.70      0.60      0.61      5

>>> y_pred = [1, 1, 0]
>>> y_true = [1, 1, 1]
>>> print(classification_report(y_true, y_pred, labels=[1, 2, 3]))
          precision    recall  f1-score   support
  1       1.00      0.67      0.80      3
  2       0.00      0.00      0.00      0
  3       0.00      0.00      0.00      0

  micro avg       1.00      0.67      0.80      3
  macro avg       0.33      0.22      0.27      3
  weighted avg    1.00      0.67      0.80      3

```

Read more in the [User Guide](#).

**Parameters:**

**y\_true** : *1d array*

Ground truth (correct) labels.

**y\_pred** : *1d array*

Estimated targets as returned by a classifier.

**labels** : *array, shape (n\_labels,)*

Optional list of labels to include in the report.

**target\_names** : *list or None*

Optional display names for classes which can be used to identify the columns.

**sample\_weight** : *array-like, shape (n\_samples,)*

Sample weights.

**digits** : *int*

Number of digits displayed in the returned values.

The returned values are rounded to this number of digits.

[sklearn.metrics.classification\\_report](#)  
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[sklearn.metrics.classification\\_](#)



## Regression

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[sklearn.metrics.mean\\_absolut](#)  
[e\\_error](#)

“

# sklearn.metrics.mean\_absolute\_error

`sklearn.metrics.mean_absolute_error(y_true, y_pred, sample_weight=None)` ¶

Mean absolute error regression loss

**Parameters:** `y_true` : array-like of shape = [n\_samples] or [n\_samples, n\_outputs]

Ground truth (correct) target values.

`y_pred` : array-like of shape = [n\_samples] or [n\_samples, n\_outputs]

Estimated target values.

`sample_weight` : array-like of

Sample weights.

**Returns:** `loss` : float

A positive floating point

### Examples

```
>>> from sklearn.metrics import mean_absolute_error
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> mean_absolute_error(y_true, y_pred)
0.5
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> mean_absolute_error(y_true, y_pred)
0.75
```



## Regression

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[sklearn.metrics.mean\\_squared\\_error](#)

Examples using

[sklearn.metrics.mean\\_squared\\_error](#)

“

# sklearn.metrics.mean\_squared\_error

```
sklearn.metrics.mean_squared_error(y_true, y_pred, sample_weight=None)
```

Mean squared error regression loss

**Parameters:** `y_true` : array-like of shape = [n\_samples] or [n\_samples, n\_outputs]

Ground truth (correct) target values.

`y_pred` : array-like of shape = [n\_samples] or [n\_samples, n\_outputs]

Estimated target values.

`sample_weight` : array-like of shape =

Sample weights.

**Returns:** `loss` : float

A positive floating point value (the

### Examples

```
>>> from sklearn.metrics import mean_squared_error
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> mean_squared_error(y_true, y_pred)
0.375
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> mean_squared_error(y_true, y_pred)
0.708...
```



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[sklearn.metrics.r2\\_score](#)  
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## sklearn.metrics.r2\_score

`sklearn.metrics.r2_score(y_true, y_pred, sample_weight=None)`

R<sup>2</sup> (coefficient of determination) regression score function.

Best possible score is 1.0, lower values are worse.

**Parameters:** `y_true` : array-like of shape = [n\_samples] or [n\_samples, n\_outputs]

Ground truth (correct) target values.

`y_pred` : array-like of shape = [n\_samples] or [n\_samples, n\_outputs]

Estimated target values.

`sample_weight` : array-like of sh

Sample weights.

**Returns:** `z` : float

The R<sup>2</sup> score.

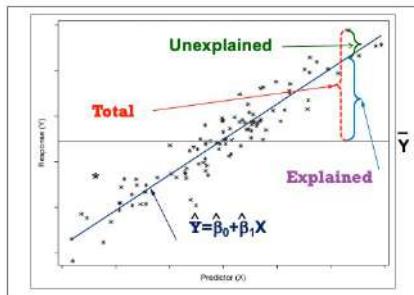
### Examples

```
>>> from sklearn.metrics import r2_score
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> r2_score(y_true, y_pred)
0.948...
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> r2_score(y_true, y_pred)
0.938...
```

# Coefficient of Determination

## Regression

```
'mean_absolute_error'    sklearn.metrics.mean_absolute_error
'mean_squared_error'    sklearn.metrics.mean_squared_error
'r2'                    sklearn.metrics.r2_score
```



$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSE}{SST}$$

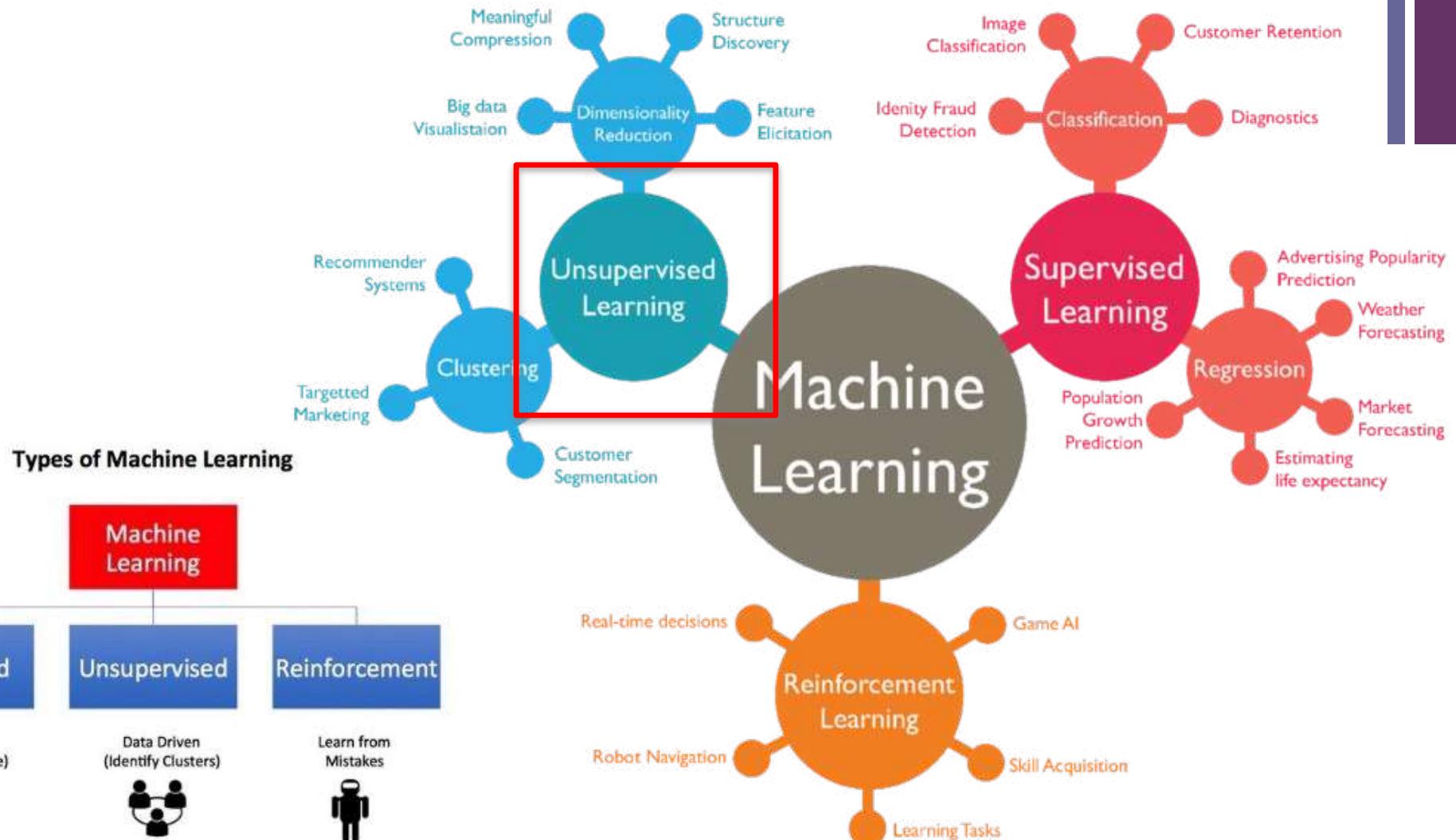
id	chol (x)	bp (y)	predict	error	squared error (SE)	guess	(y - y_bar )	squared total (ST)
1	437	194	196.1897	(2.1897)	4.7948	143.4286	50.5714	2,557.4694
2	264	121	141.4179	(20.4179)	416.8906	143.4286	(22.4286)	503.0408
3	249	131	136.6689	(5.6689)	32.1364	143.4286	(12.4286)	154.4694
4	297	159	151.8657	7.1343	50.8982	143.4286	15.5714	242.4694
5	243	123	134.7693	(11.7693)	138.5164	143.4286	(20.4286)	417.3265
6	272	161	143.9507	17.0493	290.6786	143.4286	17.5714	308.7551
7	161	115	108.8081	6.1919	38.3396	143.4286	(28.4286)	808.1837
average	274.7143	143.4286	SSE	972.2548	SST			4,991.7143
)			MSE	138.8935				
			RMSE	<b>11.7853</b>				
	<b>R^2</b>	<b>1 - (SSE/SST)</b>	<b>0.8052</b>					



## Part3: Unsupervised Learning (Descriptive Task)

# + Machine Learning (cont.)

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## Task2: Unsupervised learning (descriptive task)

Training Data



Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes
32	35,000	Male	Bangkok	No



Testing Data



Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	?





## Clustering

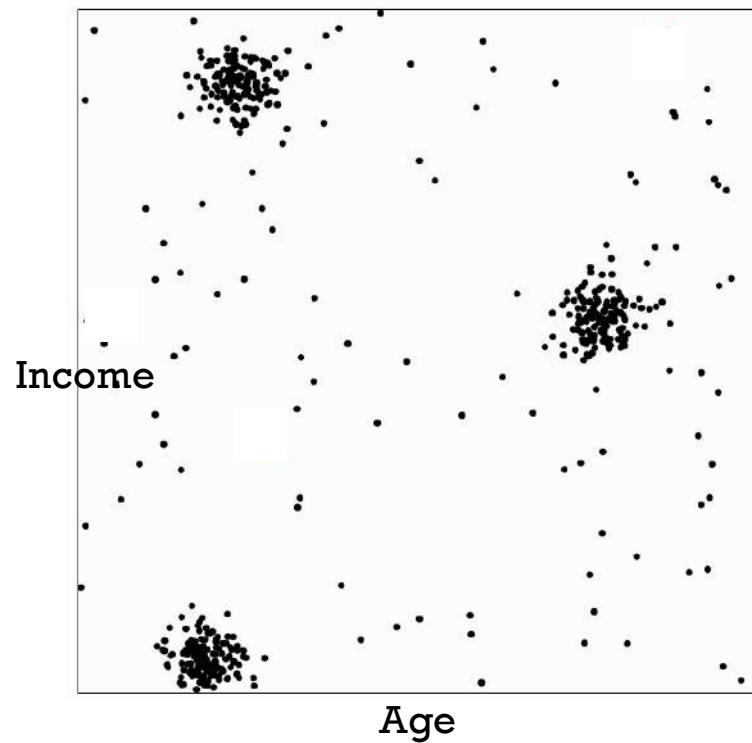


- In our class, there are many participants. Should we teach them using the same method?
- **May be not!** Since they may have different learning behaviors and backgrounds.
- Inputs
  - Education field
  - Level of English communication
  - Level of computer skills
  - Age range
  - Gender

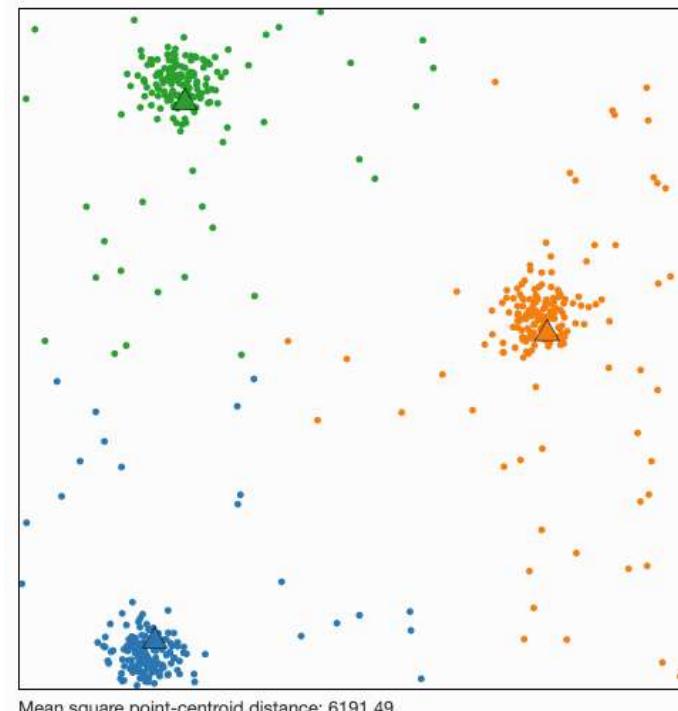


# K-means Clustering

- <http://web.stanford.edu/class/ee103/visualizations/kmeans/kmeans.html>



## Visualizing K-Means Clustering



The  $k$ -means algorithm is an iterative method for clustering a set of  $N$  points (vectors) into  $k$  groups or clusters of points.

### Algorithm

Repeat until convergence:

#### Find closest centroid

Find the closest centroid to each point, and group points that share the same closest centroid.

#### Update centroid

Update each centroid to be the mean of the points in its group.

[Update centroid](#)

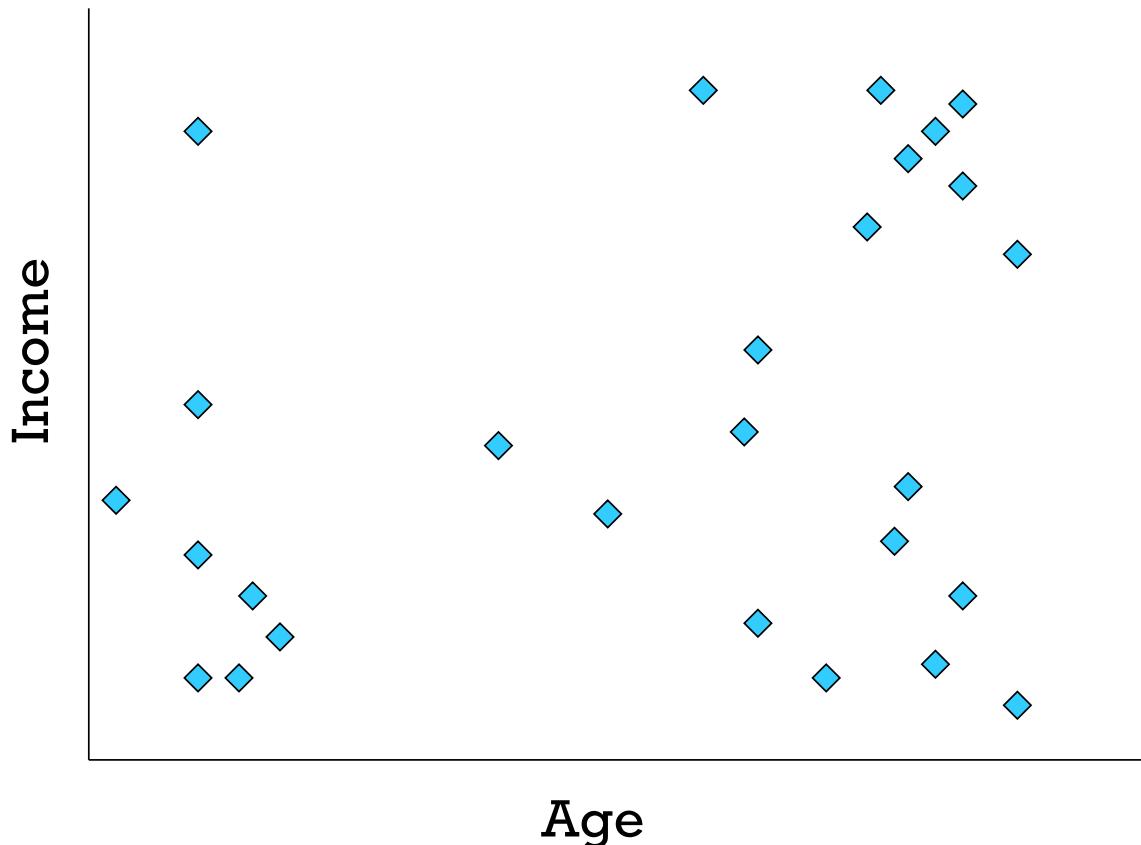
### Data

Clustered points  Random  
Number of clusters : 3  
Number of centroids: 3

[New points](#) [New centroids](#)

+

## K-means: Step0

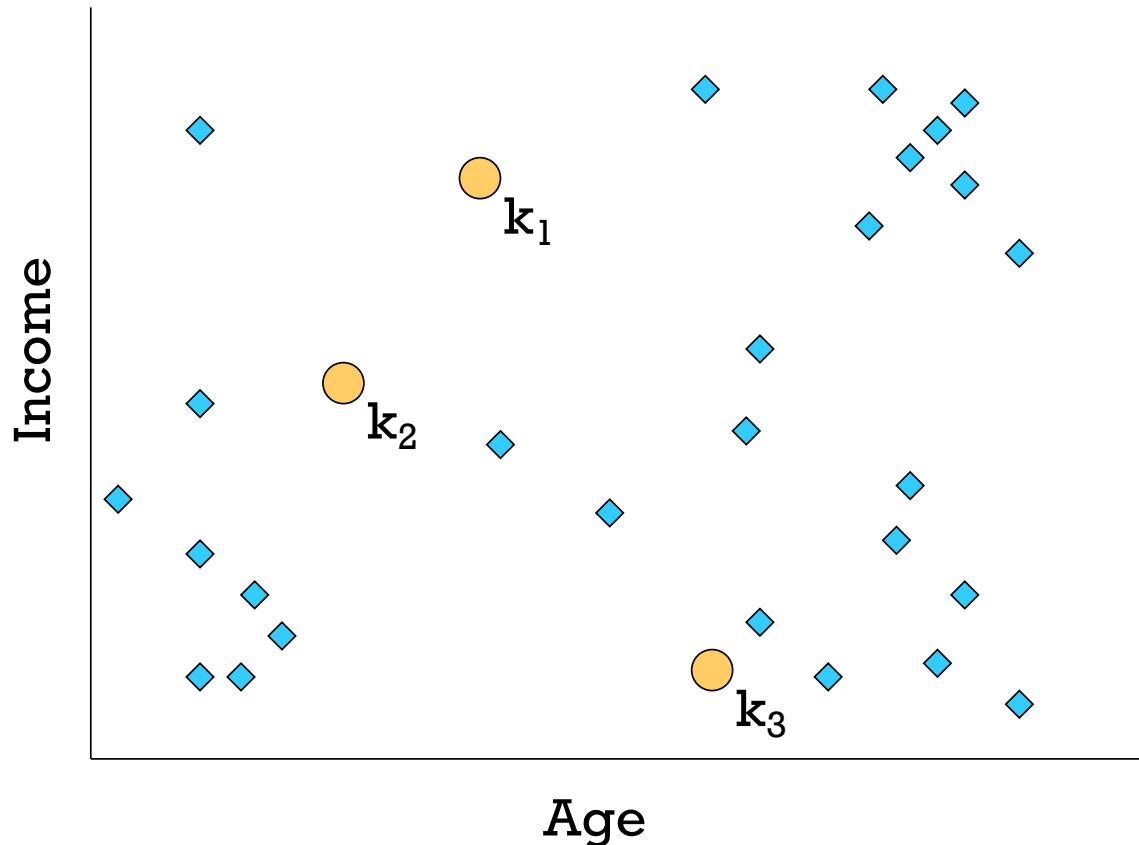


160



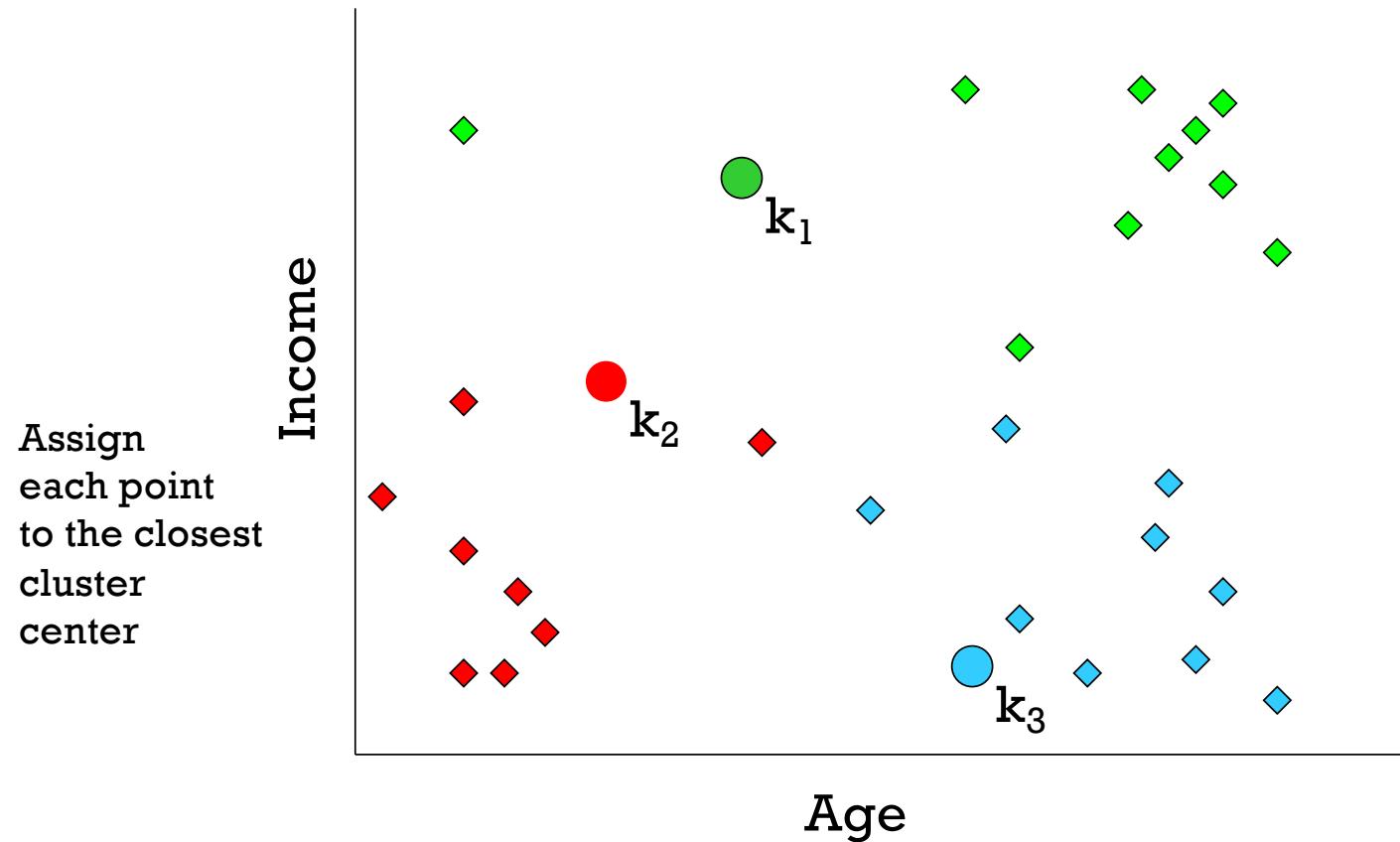
## K-means: Step 1

Pick 3  
initial  
cluster  
centers  
(randomly)





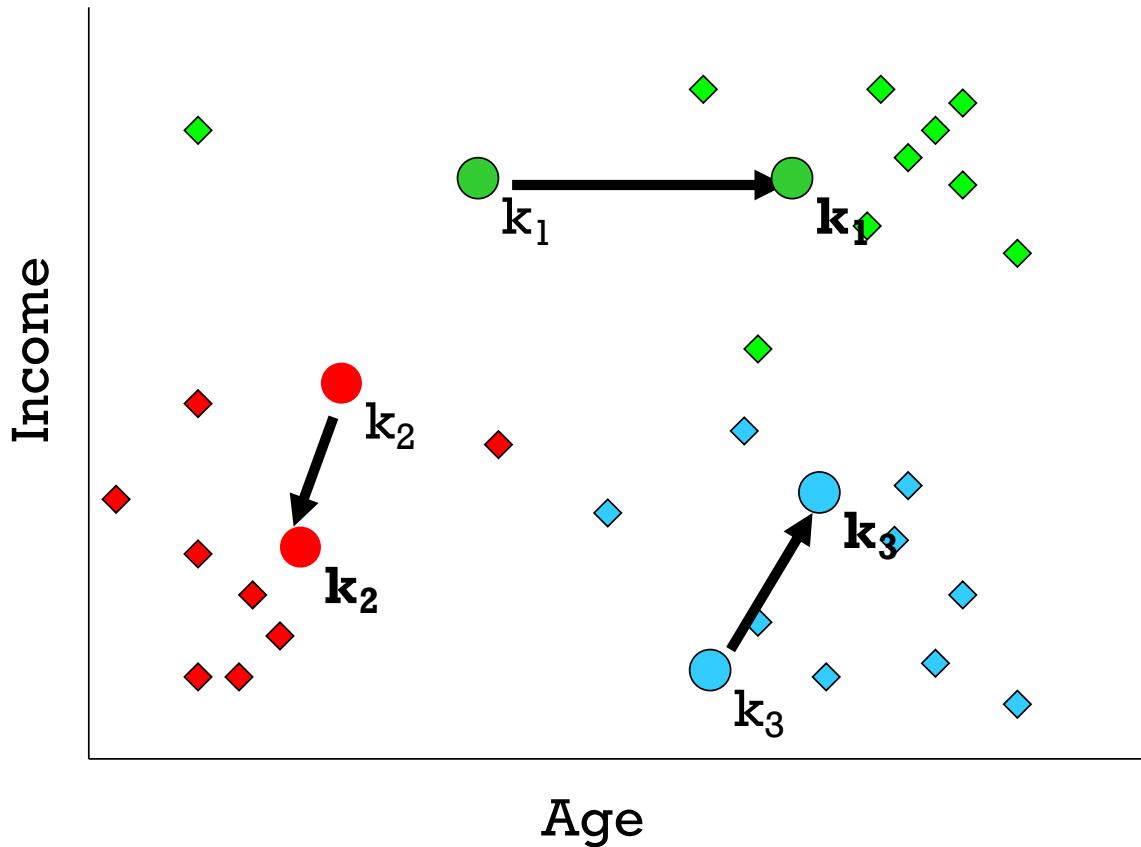
## K-means: Step2





## K-means: Step3

Move  
each cluster  
center  
to the mean  
of each cluster

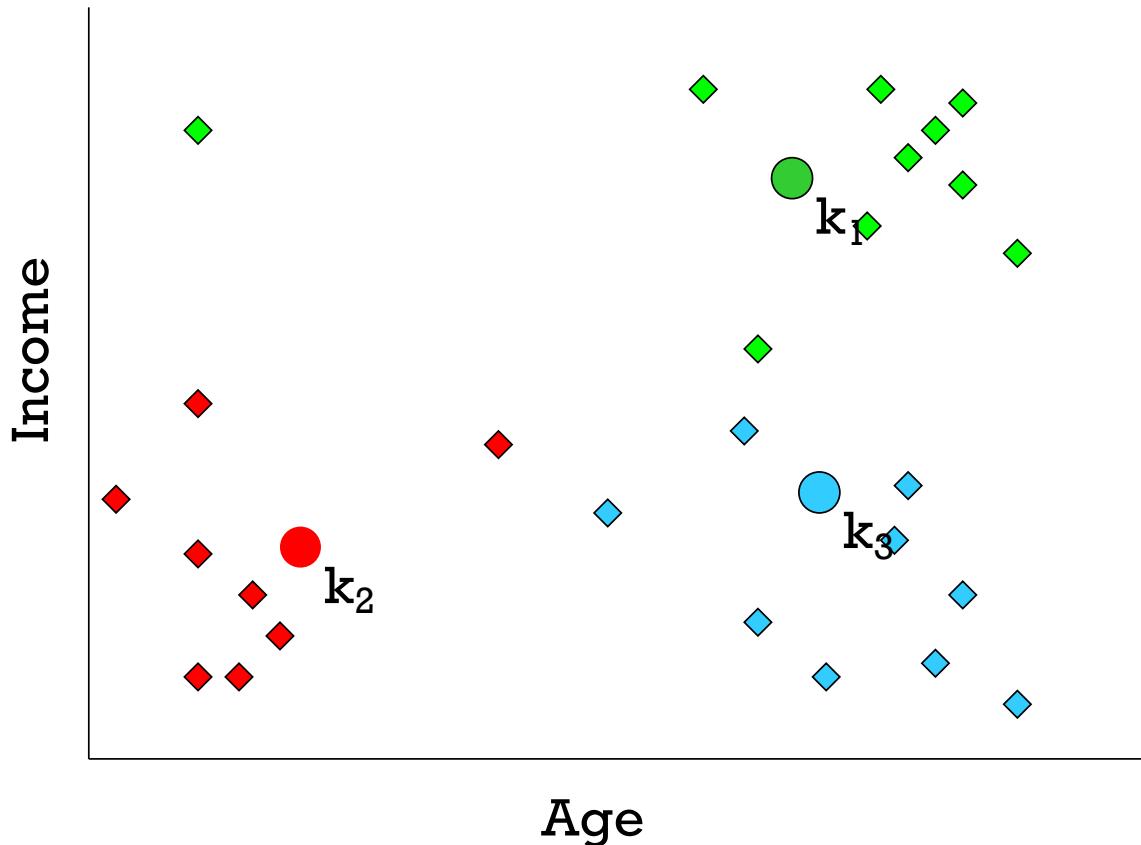




## K-means: Step4

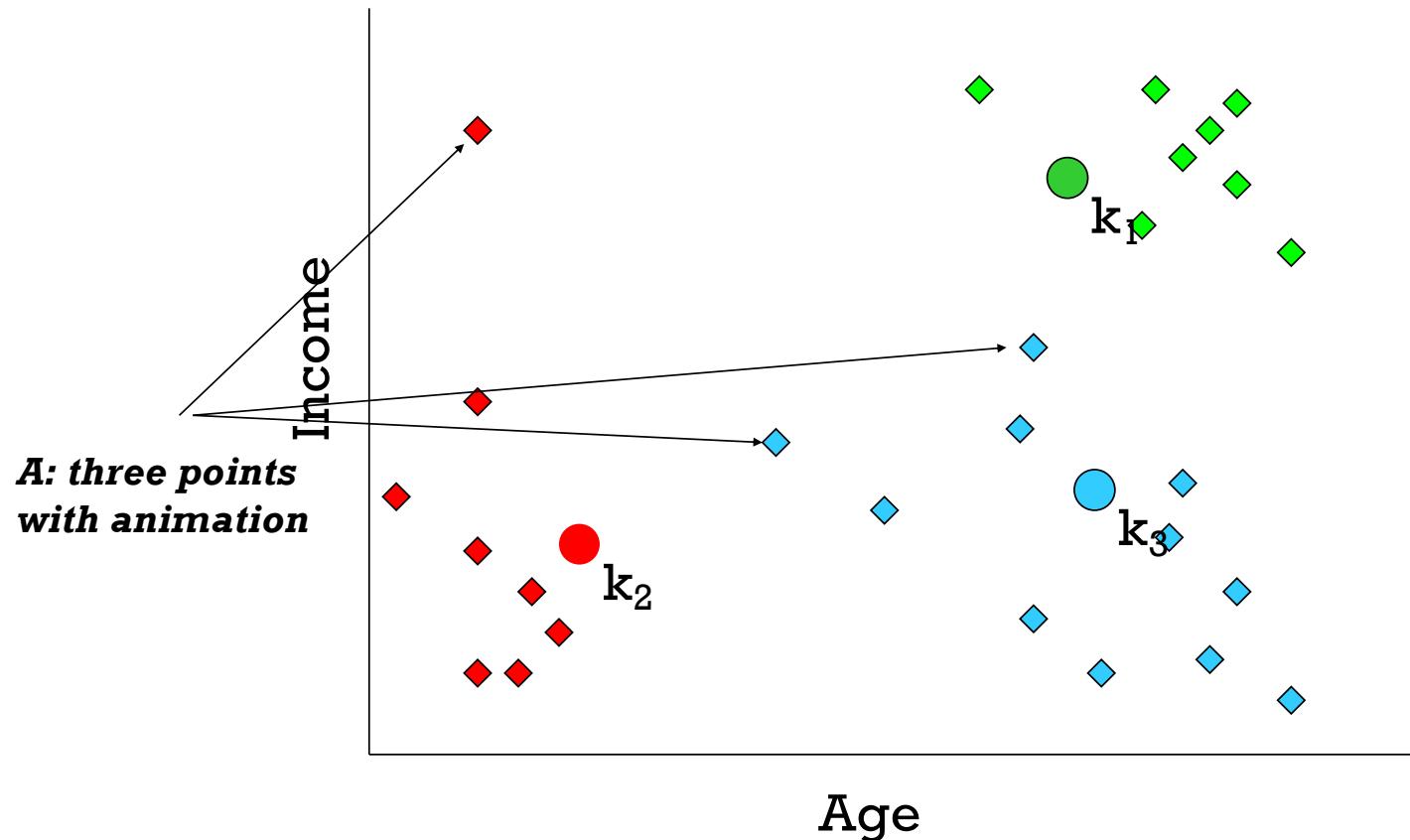
Reassign  
points  
closest to a  
different new  
cluster center

**Q: Which points  
are reassigned?**



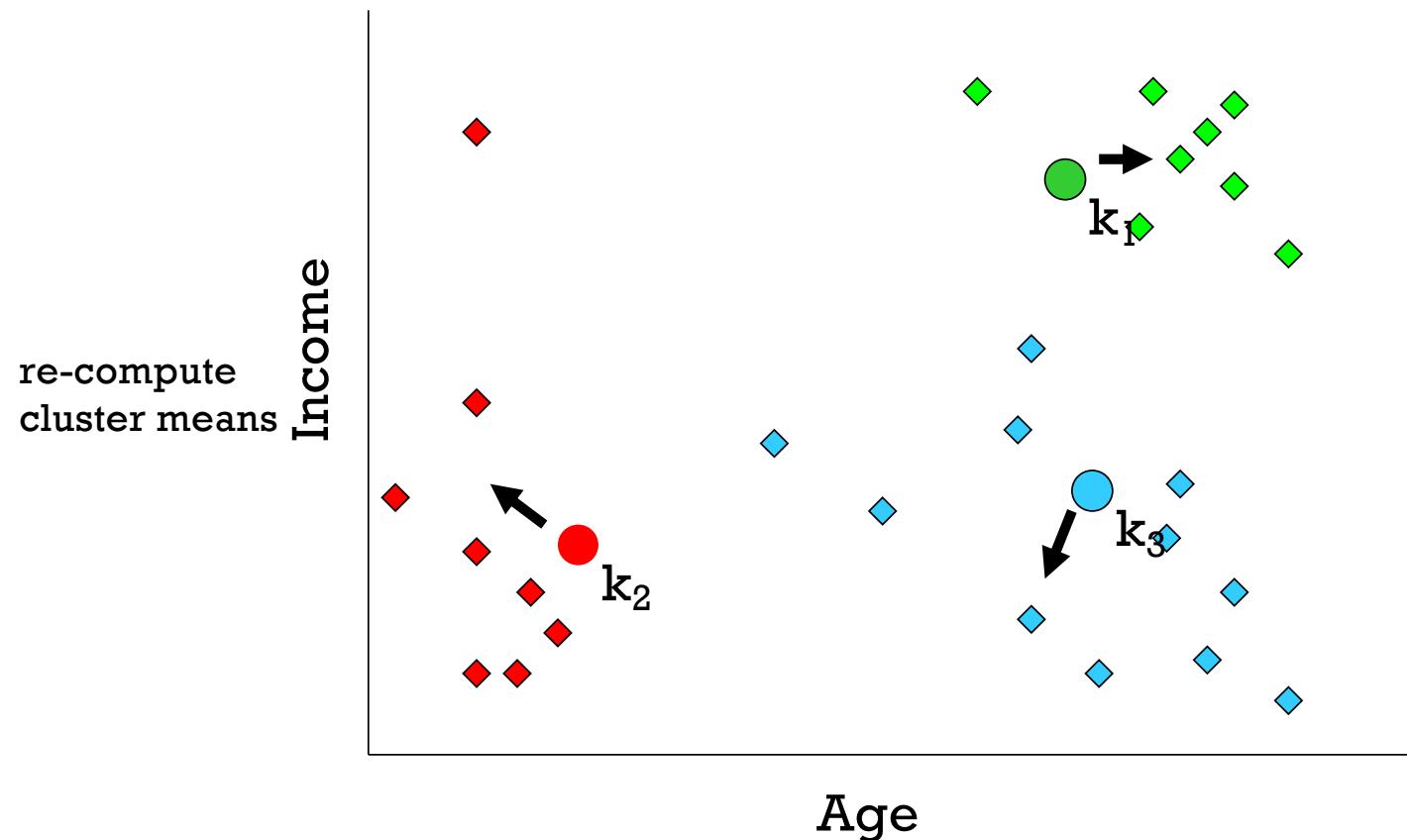


## K-means: Step4(a)





## K-means: Step5





## K-means: Step5(a)

### Cautions:

- Support only numerical variables
- Need to adjust variable range

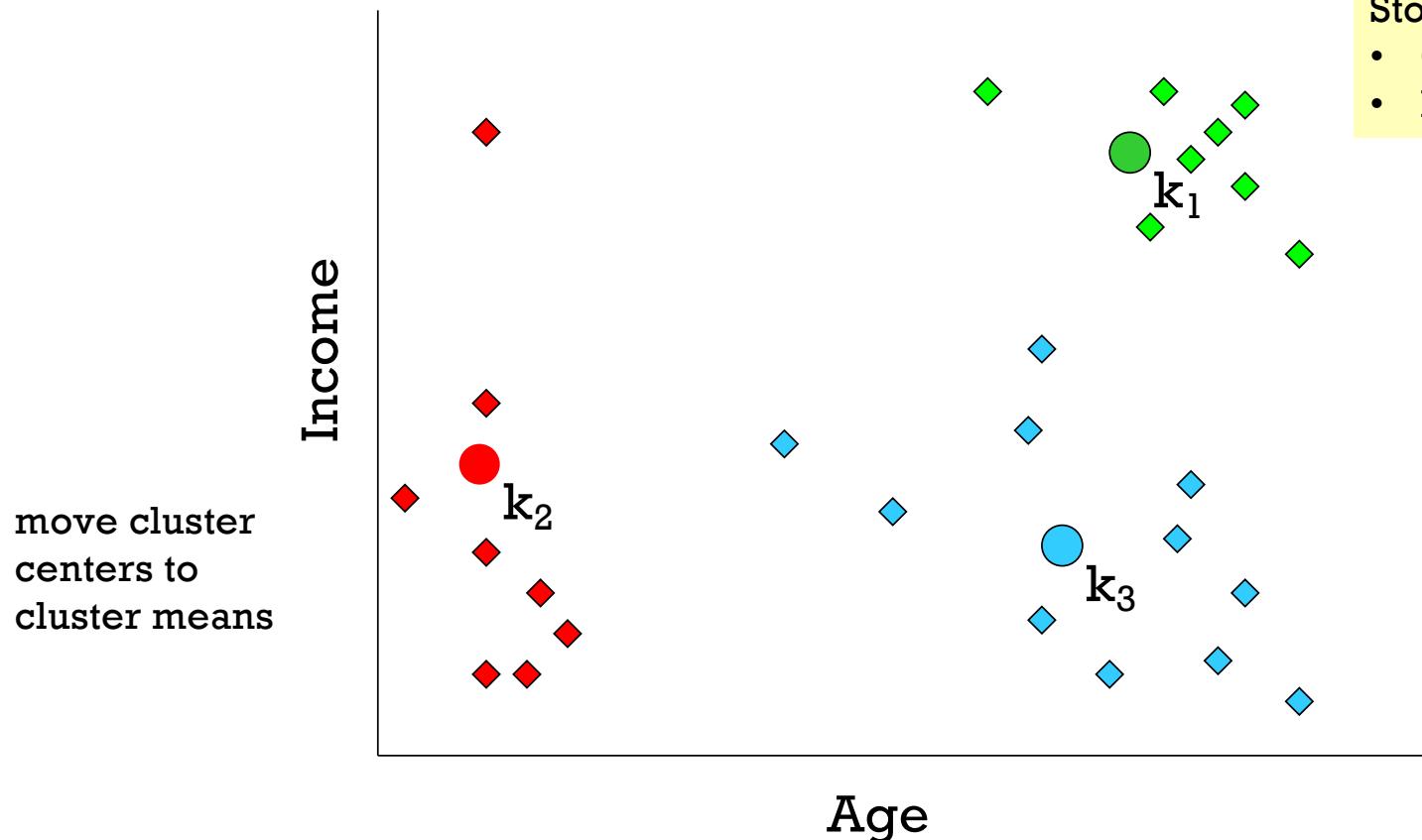
167

### Important Params:

- $k$ , Distance function
- Maximum epochs

### Stop

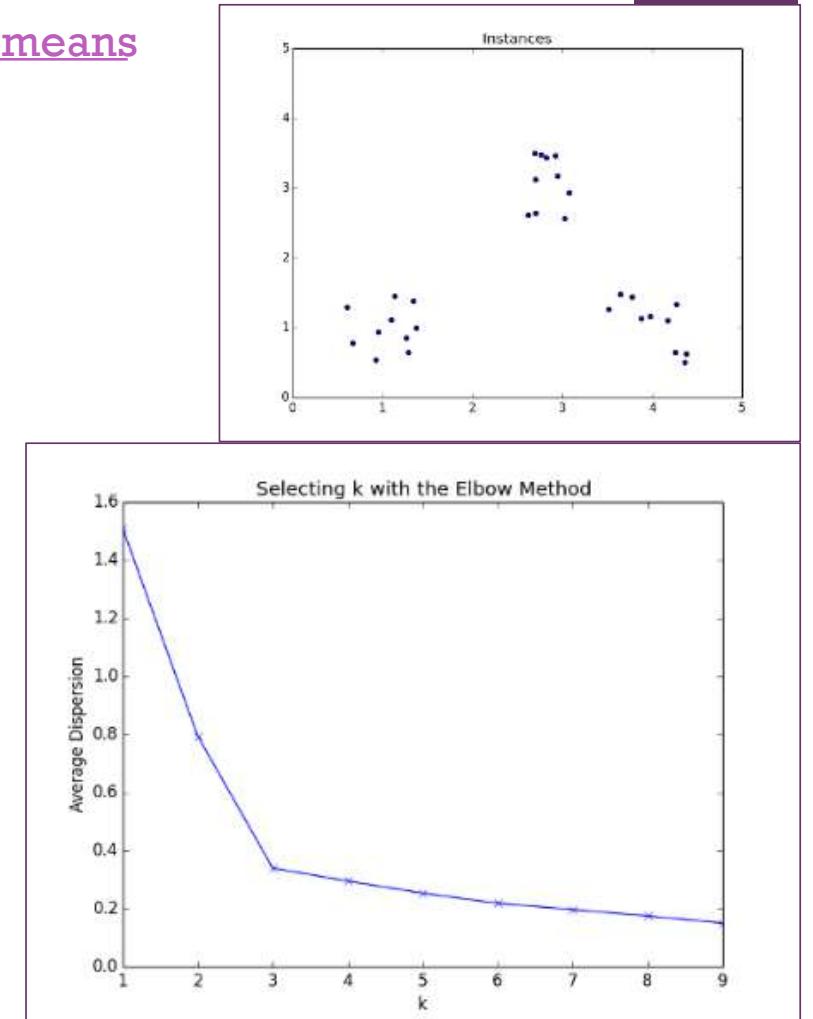
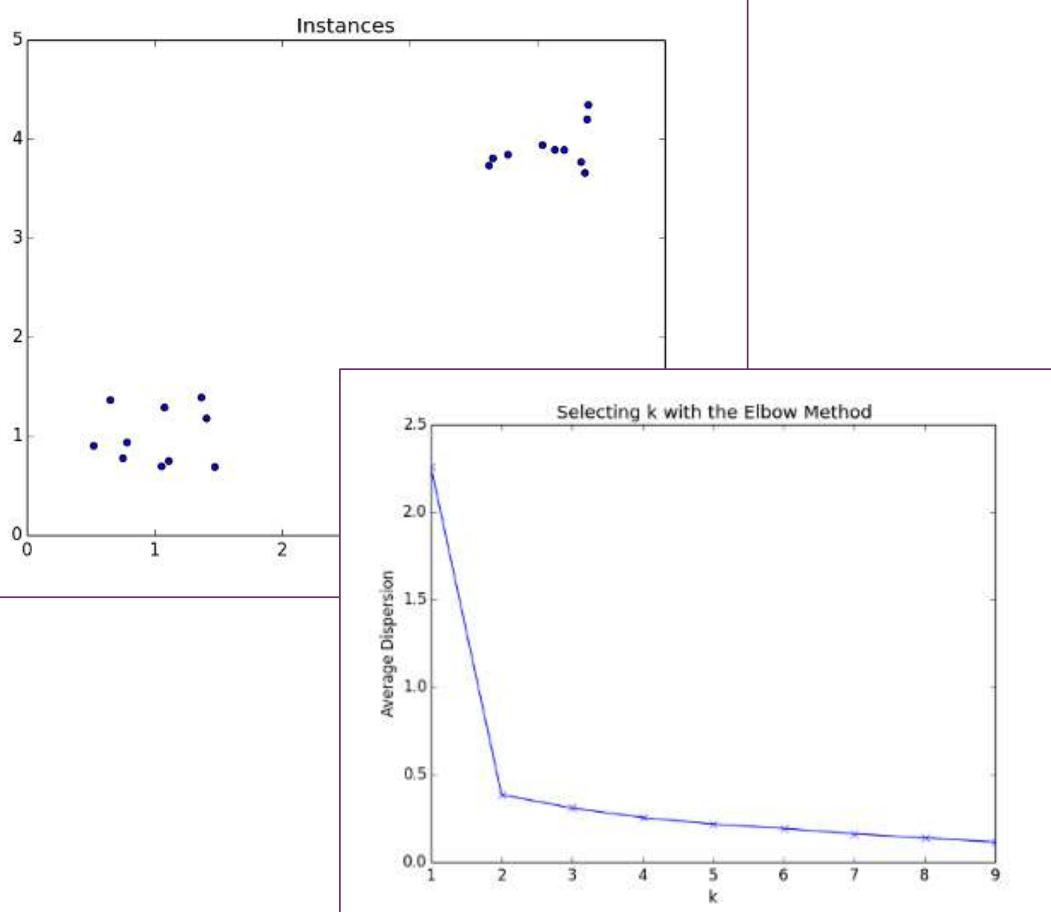
- Converge (no change)
- Maximum epochs





## Determine the number of $k$ : Elbow Method

<https://www.packtpub.com/books/content/clustering-k-means>





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Other versions

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Examples using

[sklearn.preprocessing.StandardScaler](#)

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## sklearn.preprocessing.StandardScaler

```
class sklearn.preprocessing.StandardScaler(copy=True, with_mean=True, with_std=True)
```

[source]

Standardize features by removing the mean and scaling to unit variance

The standard score of a sample  $x$  is calculated as:

$$z = (x - u) / s$$

where  $u$  is the mean of the training samples or zero if `with_mean=False`, and  $s$  is the standard deviation of the training samples or one if `with_std=False`.

Centering and scaling happen independently on each feature by computing the relevant statistics on the samples in the training set. Mean and standard deviation are then stored to be used on later data using `transform`.

Standardization of a dataset is a common requirement for many machine learning estimators: they might behave badly if the individual features do not more or less look like standard normally distributed data (e.g. Gaussian with 0 mean and unit variance).

For instance many elements used in the objective function of a learning algorithm (such as the RBF kernel of Support Vector Machines or the L1 and L2 regularizers of linear models) assume that all features are centered around 0 and have variance in the same order. If a feature has a variance that is orders of magnitude larger than others, it might dominate the objective function and make the estimator unable to learn from other features correctly as expected.

This scaler can also be applied to sparse CSR or CSC matrices by passing `with_mean=False` to avoid breaking the sparsity structure of the data.



# Clustering - K-means

```
>>> from sklearn.cluster import KMeans
>>> import numpy as np
>>> X = np.array([[1, 2], [1, 4], [1, 0],
...               [10, 2], [10, 4], [10, 0]])
>>> kmeans = KMeans(n_clusters=2, random_state=0).fit(X)
>>> kmeans.labels_
array([1, 1, 1, 0, 0, 0], dtype=int32)
>>> kmeans.predict([[0, 0], [12, 3]])
array([1, 0], dtype=int32)
>>> kmeans.cluster_centers_
array([[10.,  2.],
       [1.,  2.]])
```

## sklearn.cluster.KMeans

```
class sklearn.cluster.KMeans(n_clusters=8, *, init='k-means++', n_init=10, max_iter=300, tol=0.0001,
                             precompute_distances='deprecated', verbose=0, random_state=None, copy_x=True, n_jobs='deprecated', algorithm='auto') [source]
```

K-Means clustering.

Read more in the User Guide.

### Parameters:

#### **n\_clusters : int, default=8**

The number of clusters to form as well as the number of centroids to generate.

#### **init : {'k-means++', 'random', ndarray, callable}, default='k-means++'**

Method for initialization:

'k-means++' : selects initial cluster centers for k-mean clustering in a smart way to speed up convergence. See section Notes in k\_init for more details.

'random': choose `n_clusters` observations (rows) at random from data for the initial centroids.

If an ndarray is passed, it should be of shape (n\_clusters, n\_features) and gives the initial centers.

If a callable is passed, it should take arguments X, n\_clusters and a random state and return an initialization.

#### **n\_init : int, default=10**

Number of time the k-means algorithm will be run with different centroid seeds. The final results will be the best output of n\_init consecutive runs in terms of inertia.

#### **max\_iter : int, default=300**

Maximum number of iterations of the k-means algorithm for a single run.



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Other versions

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sklearn.metrics.silhouette\_score  
Examples using  
sklearn.metrics.silhouette\_score

For the whole cluster

## sklearn.metrics.silhouette\_score

```
sklearn.metrics.silhouette_score(X, labels, *, metric='euclidean', sample_size=None, random_state=None, **kwds)
```

[\[source\]](#)

Compute the mean Silhouette Coefficient of all samples.

The Silhouette Coefficient is calculated using the mean intra-cluster distance ( $a$ ) and the mean nearest-cluster distance ( $b$ ) for each sample. The Silhouette Coefficient for a sample is  $(b - a) / \max(a, b)$ . To clarify,  $b$  is the distance between a sample and the nearest cluster that the sample is not a part of. Note that Silhouette Coefficient is only defined if number of labels is  $2 \leq n\_labels \leq n\_samples - 1$ .

This function returns the mean Silhouette Coefficient over all samples. To obtain the values for each sample, use `silhouette_samples`.

The best value is 1 and the worst value is -1. Values near 0 indicate overlapping clusters. Negative values generally indicate that a sample has been assigned to the wrong cluster, as a different cluster is more similar.

Read more in the User Guide.

**Parameters:** `X : array-like of shape (n_samples_a, n_samples_a) if metric == "precomputed" or (n_samples_a, n_features) otherwise`

An array of pairwise distances between samples, or a feature array.

`labels : array-like of shape (n_samples,)`

Predicted labels for each sample.

`metric : str or callable, default='euclidean'`

The metric to use when calculating distance between instances in a feature array. If metric is a string, it must be one of the options allowed by `metrics.pairwise.pairwise_distances`. If `X` is the distance array itself, use `metric="precomputed"`.

`sample_size : int, default=None`

The size of the sample to use when computing the Silhouette Coefficient on a random subset of the data. If `sample_size is None`, no sampling is used.

[https://scikit-learn.org/stable/modules/generated/sklearn.metrics.silhouette\\_score.html](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.silhouette_score.html)

[Toggle Menu](#)



For each sample

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Examples using

[sklearn.metrics.silhouette\\_samp](#)

## sklearn.metrics.silhouette\_samples

```
sklearn.metrics.silhouette_samples(X, labels, *, metric='euclidean', **kwds)
```

[\[source\]](#)

Compute the Silhouette Coefficient for each sample.

The Silhouette Coefficient is a measure of how well samples are clustered with samples that are similar to themselves.

Clustering models with a high Silhouette Coefficient are said to be dense, where samples in the same cluster are similar to each other, and well separated, where samples in different clusters are not very similar to each other.

The Silhouette Coefficient is calculated using the mean intra-cluster distance ( $a$ ) and the mean nearest-cluster distance ( $b$ ) for each sample. The Silhouette Coefficient for a sample is  $(b - a) / \max(a, b)$ . Note that Silhouette Coefficient is only defined if number of labels is  $2 \leq n\_labels \leq n\_samples - 1$ .

This function returns the Silhouette Coefficient for each sample.

The best value is 1 and the worst value is -1. Values near 0 indicate overlapping clusters.

Read more in the [User Guide](#).

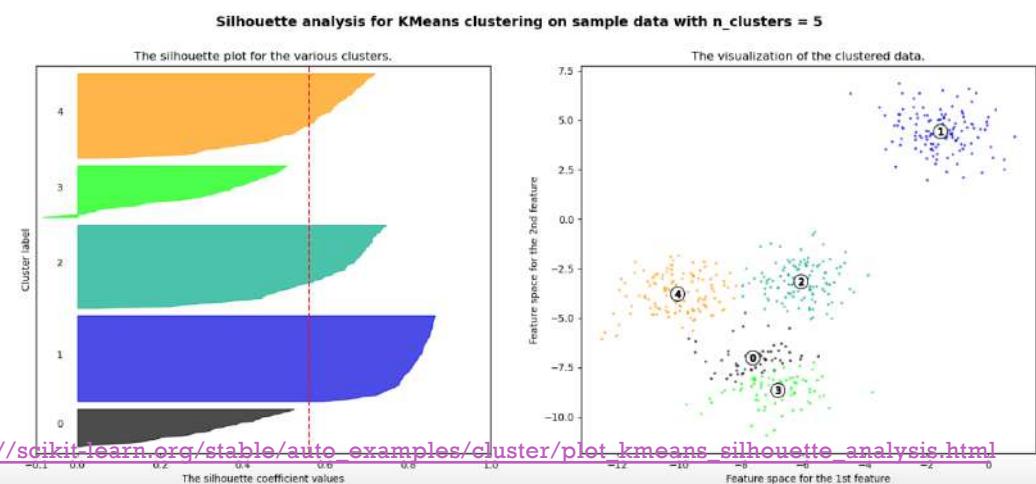
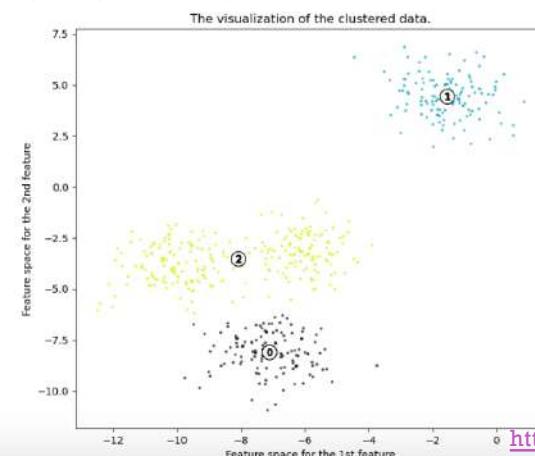
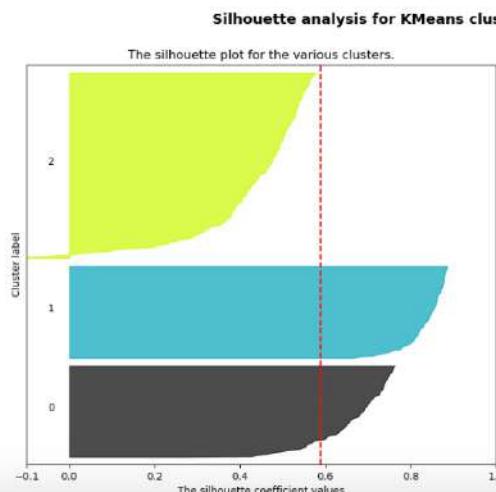
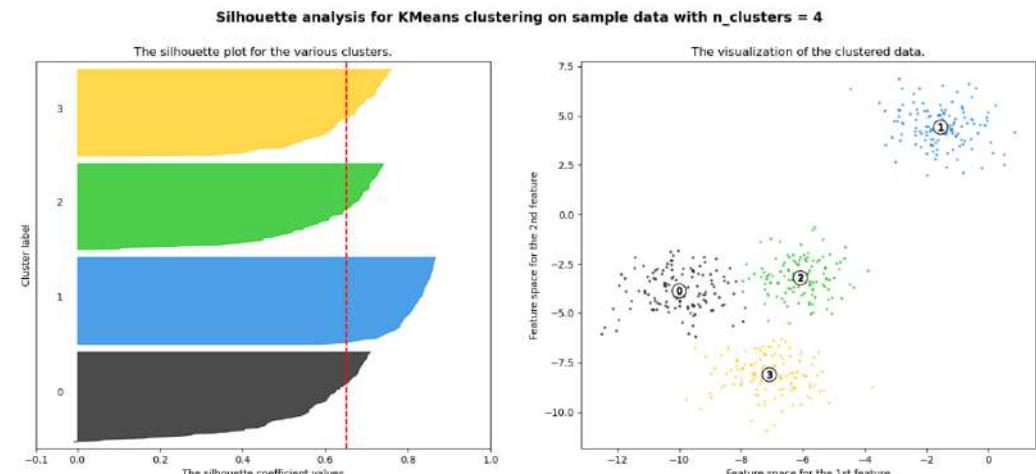
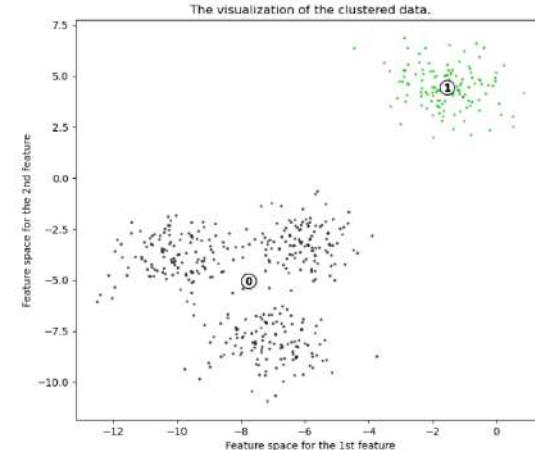
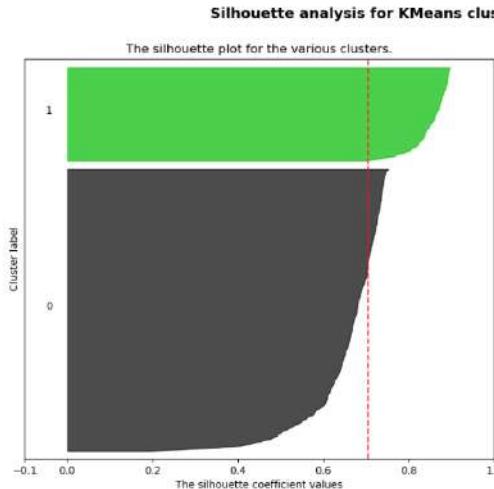
**Parameters:**  $X : \{array-like, sparse matrix\} of shape (n\_samples_a, n\_samples_a) if metric == "precomputed" or (n\_samples_a, n\_features) otherwise$

An array of pairwise distances between samples, or a feature array. If a sparse matrix is provided, CSR format should be favoured avoiding an additional copy.

# How to choose n\_clusters? Chosen is 2 or 4.

Out:

```
For n_clusters = 2 The average silhouette_score is : 0.7049787496083262
For n_clusters = 3 The average silhouette_score is : 0.5882004012129721
For n_clusters = 4 The average silhouette_score is : 0.6505186632729437
For n_clusters = 5 The average silhouette_score is : 0.561464362648773
For n_clusters = 6 The average silhouette_score is : 0.4857596147013469
```



[https://scikit-learn.org/stable/auto\\_examples/cluster/plot\\_kmeans\\_silhouette\\_analysis.html](https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html)



# Clustering

## - DBSCAN

- Density based algorithm
- **D**ensity-**B**ased **S**patial **C**lustering of **A**pplications with **N**oise
- It groups points that are closely packed together
- Then expanding clusters in any direction where there are nearby points
- this algorithm **does not requires** the **number of clusters** to be specified
- Can identify outliers as noises
- Doesn't perform well when the clusters are of varying density
- Can form any shape of cluster
- Expensive computation to high-dimensional data



# Clustering

## - DBSCAN

### Step

1. Initial starting point that has not been visited
2. All points which are within **the r distance (eps)** are neighborhood points
3. If (number of neighborhood points > **minPoints**)
  - Assign all neighborhood points to same cluster
  - Repeat step 2 – 3 on all neighborhood points
  - marked all of these point as “visited”

### Else

- the point will be labeled as noise
- marked all of these point as “visited”

4. Repeat step 1-3 until all points are visited

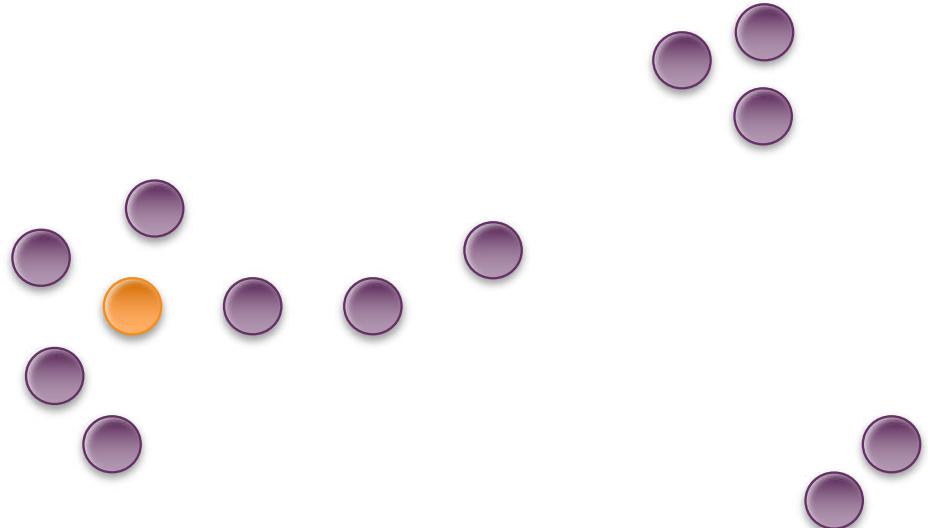


# Clustering - DBSCAN

Step

**minPoints = 3**

1. Initial starting point that has not been visited
2. All points which are within the  $r$  distance are neighborhood points
3. If (number of neighborhood points > minPoints)
  - Assign all neighborhood points to same cluster
  - Repeat step 2 – 3 on all neighborhood points
  - marked all of these point as “visited”
- Else
  - the point will be labeled as noise
  - marked all of these point as “visited”
4. Repeat step 1-3 until all points are visited





# Clustering - DBSCAN

Step

$\text{minPoints} = 3$

1. Initial starting point that has not been visited

2. All points which are within the  $r$  distance are neighborhood points

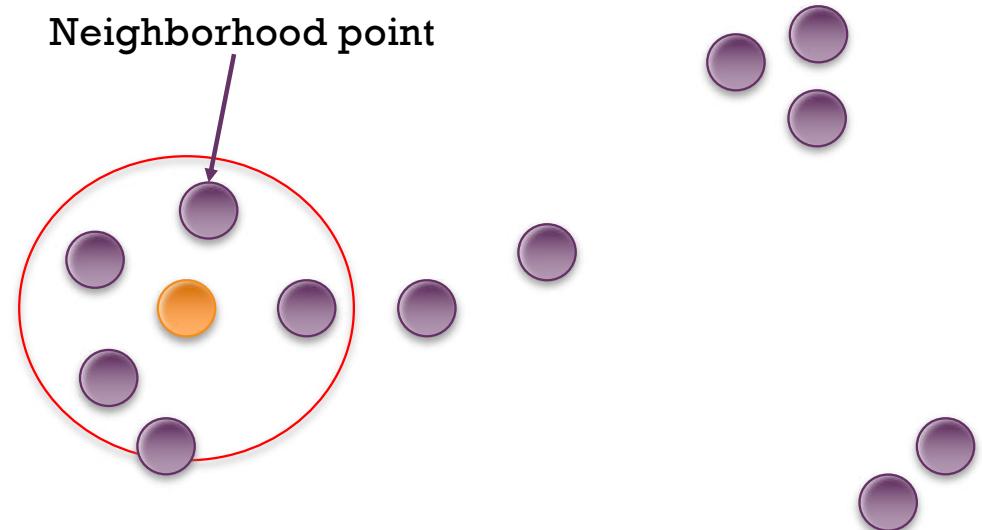
3. If (number of neighborhood points > minPoints)

- Assign all neighborhood points to same cluster
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- marked all of these point as “visited”

Else

- the point will be labeled as noise
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4. Repeat step 1-3 until all points are visited



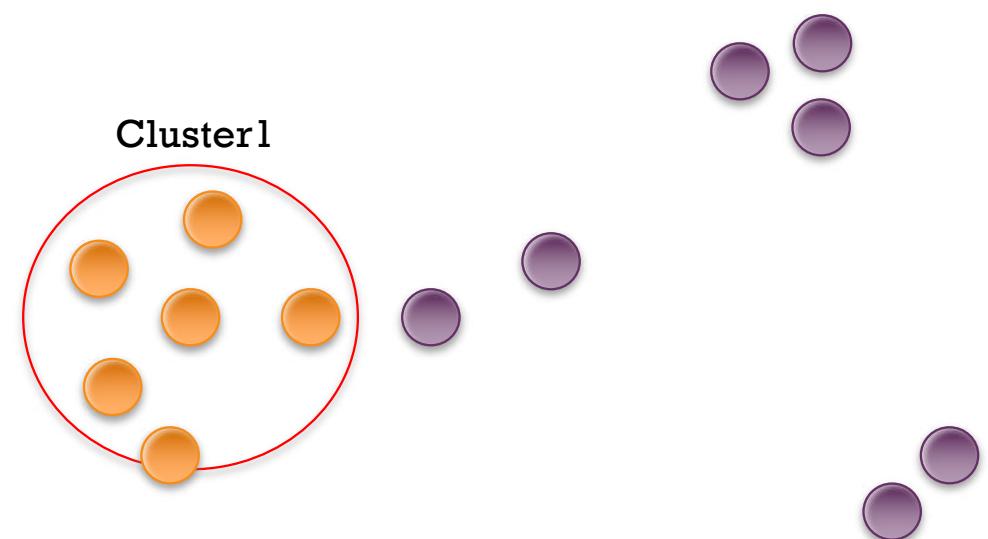


# Clustering - DBSCAN

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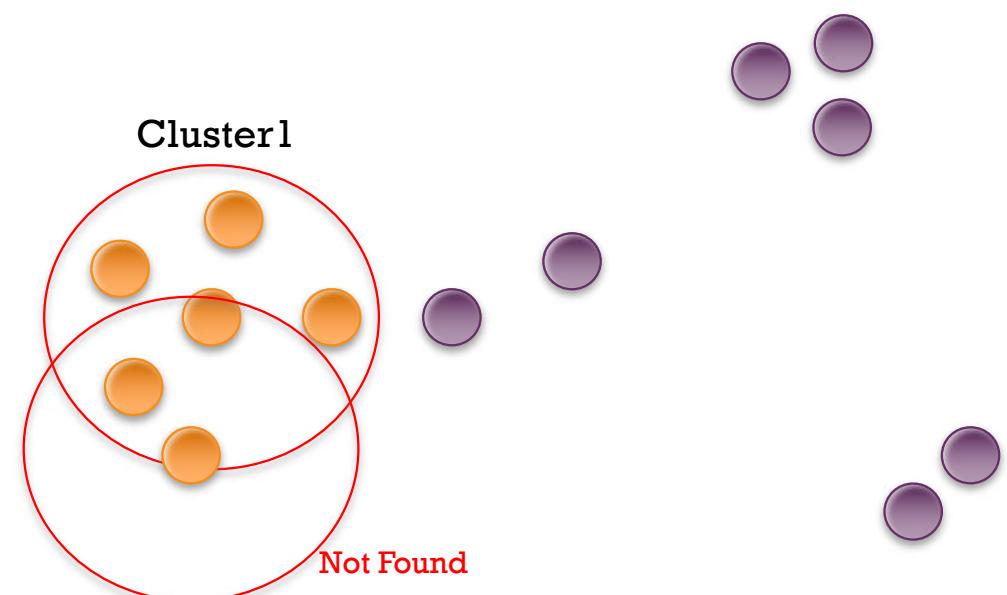


# Clustering - DBSCAN

Step

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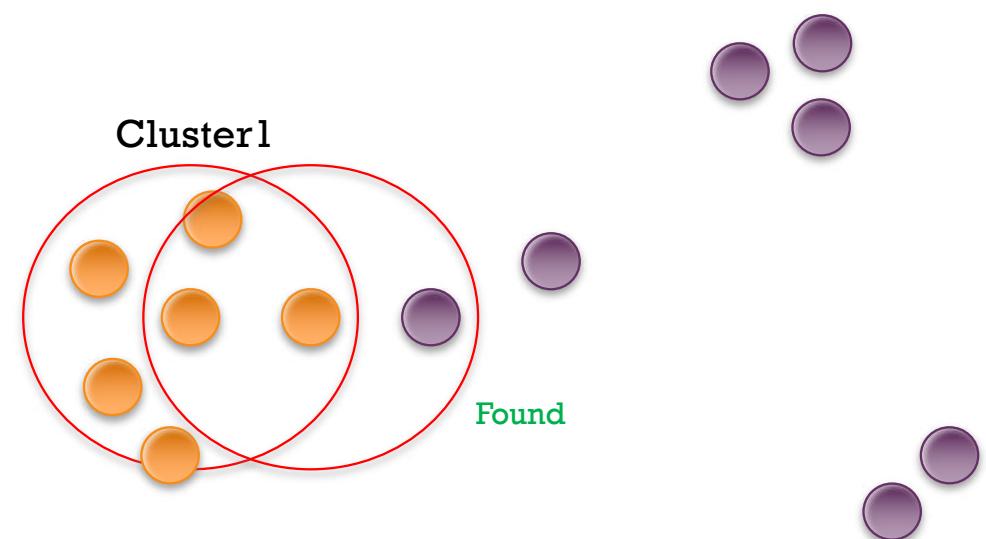


# Clustering - DBSCAN

Step

**minPoints = 3**

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4. Repeat step 1-3 until all points are visited



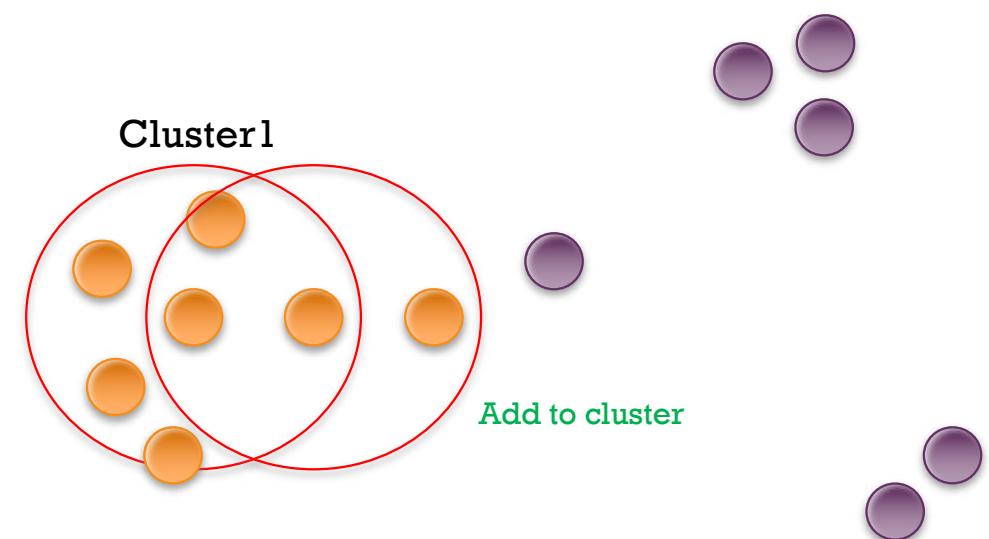


# Clustering - DBSCAN

Step

**minPoints = 3**

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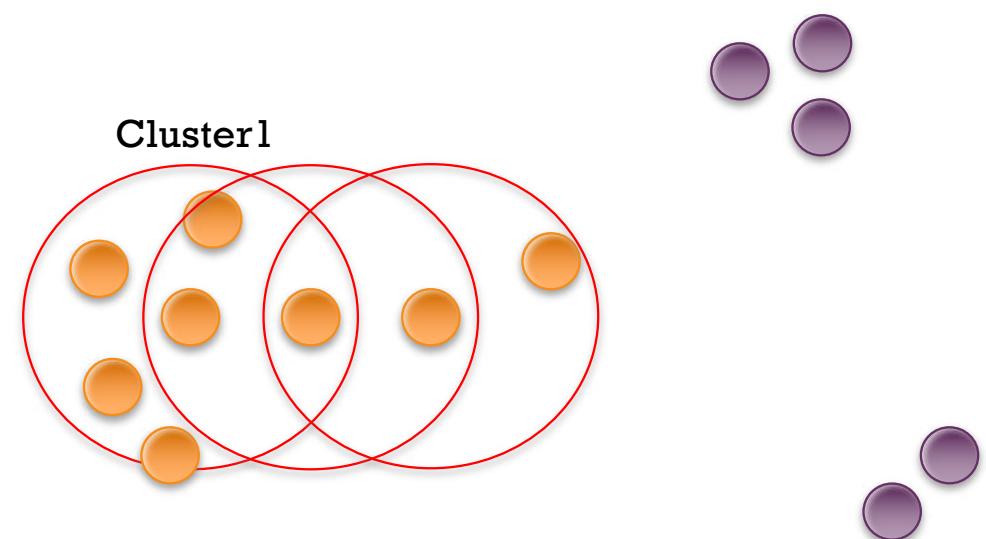


# Clustering - DBSCAN

Step

**minPoints = 3**

1. Initial starting point that has not been visited
2. All points which are within the  $r$  distance are neighborhood points
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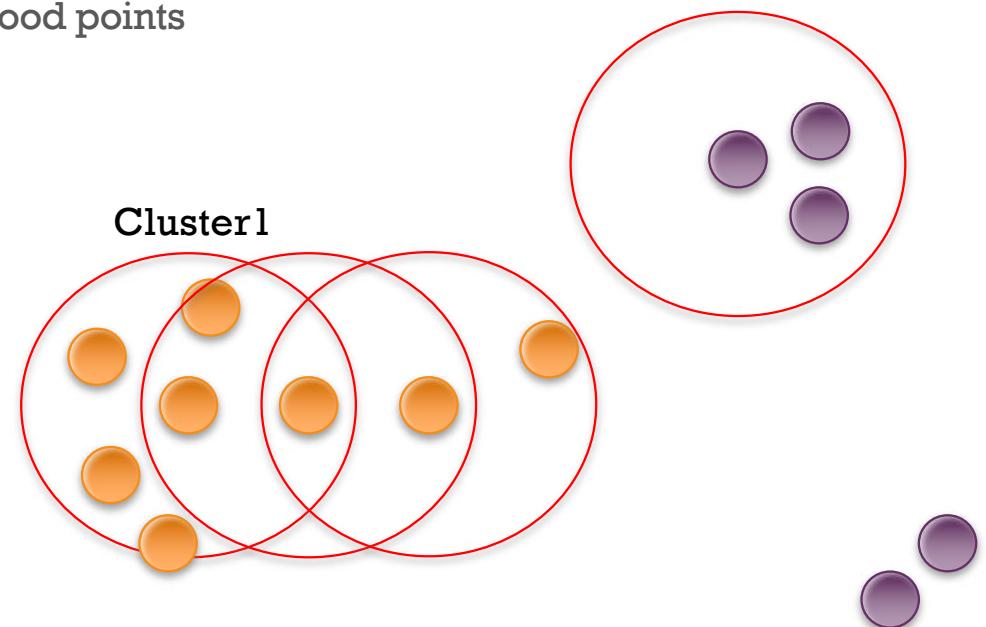


# Clustering - DBSCAN

Step

$\text{minPoints} = 3$

1. Initial starting point that has not been visited
2. All points which are within the  $r$  distance are neighborhood points
3. If (number of neighborhood points > minPoints)
  - Assign all neighborhood points to same cluster
  - Repeat step 2 – 3 on all neighborhood points
  - marked all of these point as “visited”
- Else
  - the point will be labeled as noise
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4. Repeat step 1-3 until all points are visited





# Clustering - DBSCAN

Step

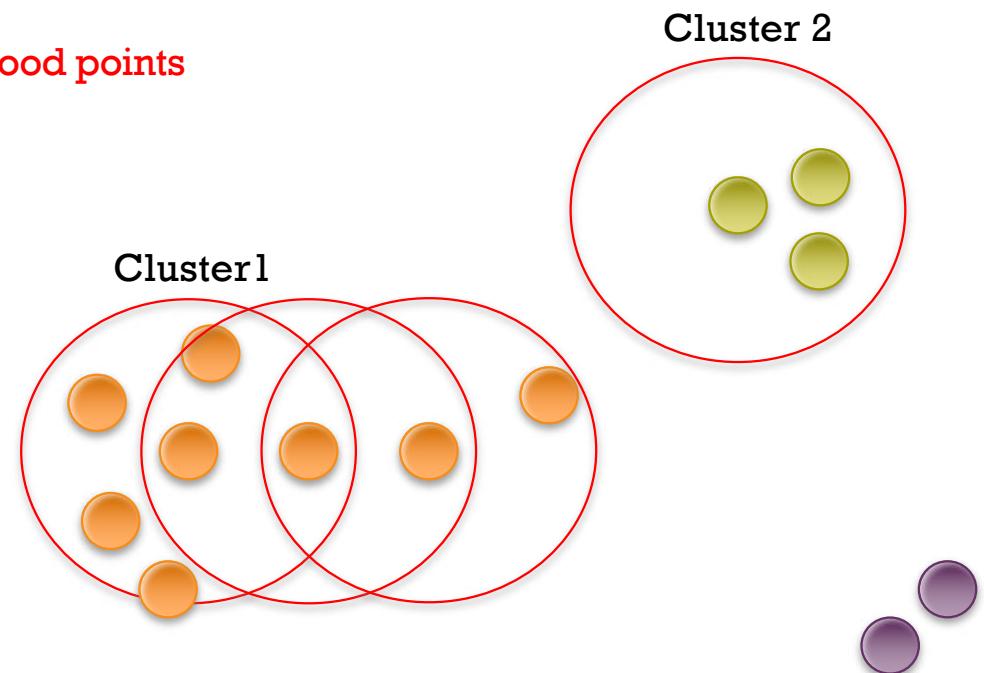
$\text{minPoints} = 3$

1. Initial starting point that has not been visited
2. All points which are within the  $r$  distance are neighborhood points
3. If ( $\text{number of neighborhood points} > \text{minPoints}$ )
  - Assign all neighborhood points to same cluster
  - Repeat step 2 – 3 on all neighborhood points
  - marked all of these point as “visited”

Else

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4. Repeat step 1-3 until all points are visited



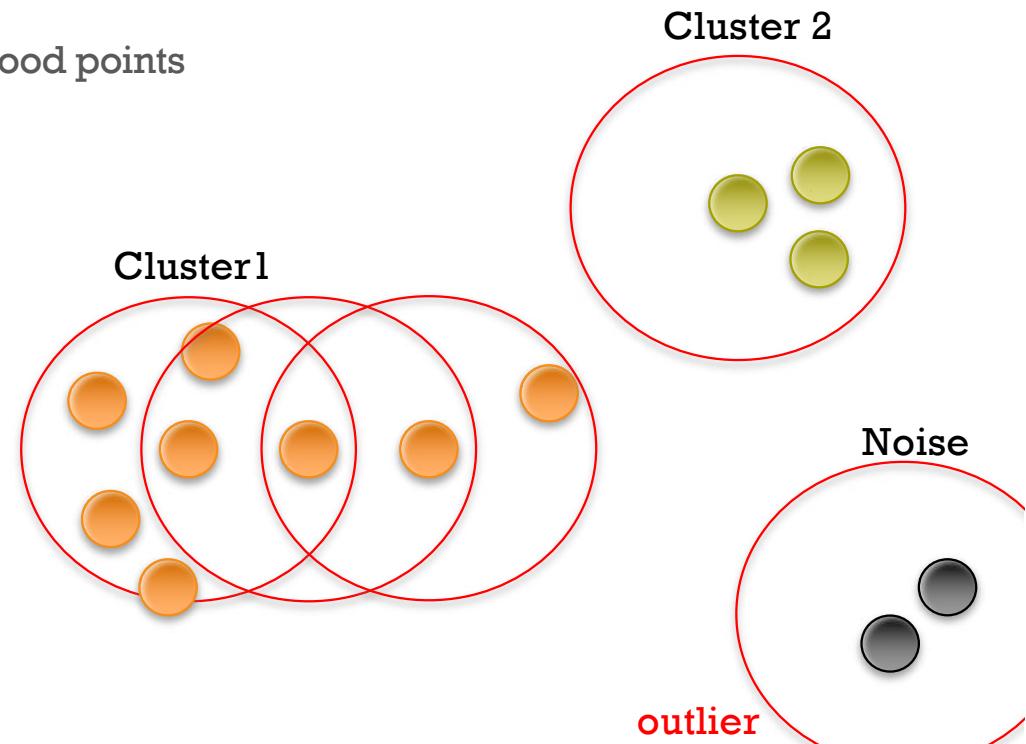


# Clustering - DBSCAN

Step

$\text{minPoints} = 3$

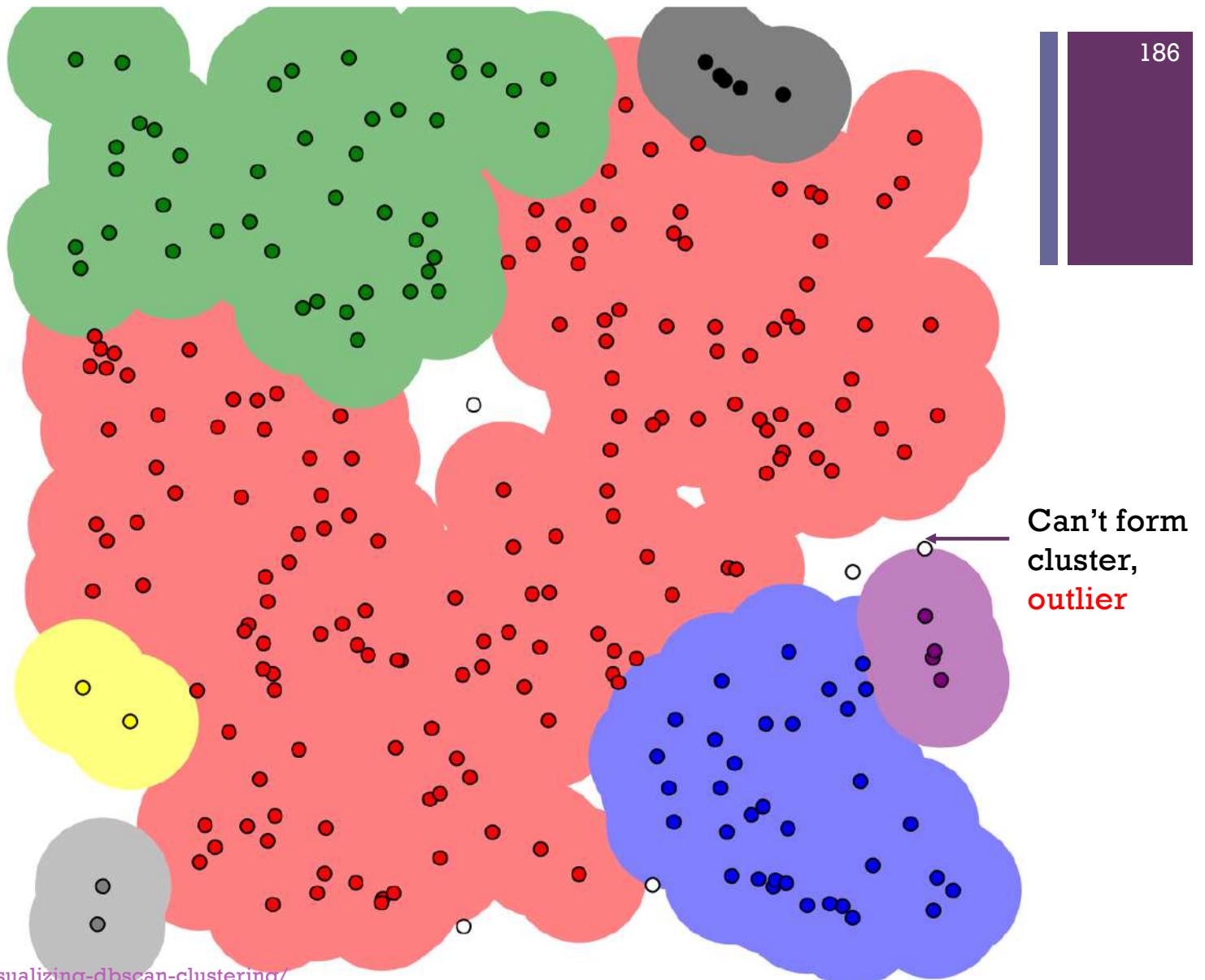
1. Initial starting point that has not been visited
2. All points which are within the  $r$  distance are neighborhood points
- 3. If (number of neighborhood points > minPoints)**
  - Assign all neighborhood points to same cluster
  - Repeat step 2 – 3 on all neighborhood points
  - marked all of these point as “visited”
- Else**
  - the point will be labeled as noise
  - marked all of these point as “visited”
- 4. Repeat step 1-3 until all points are visited**





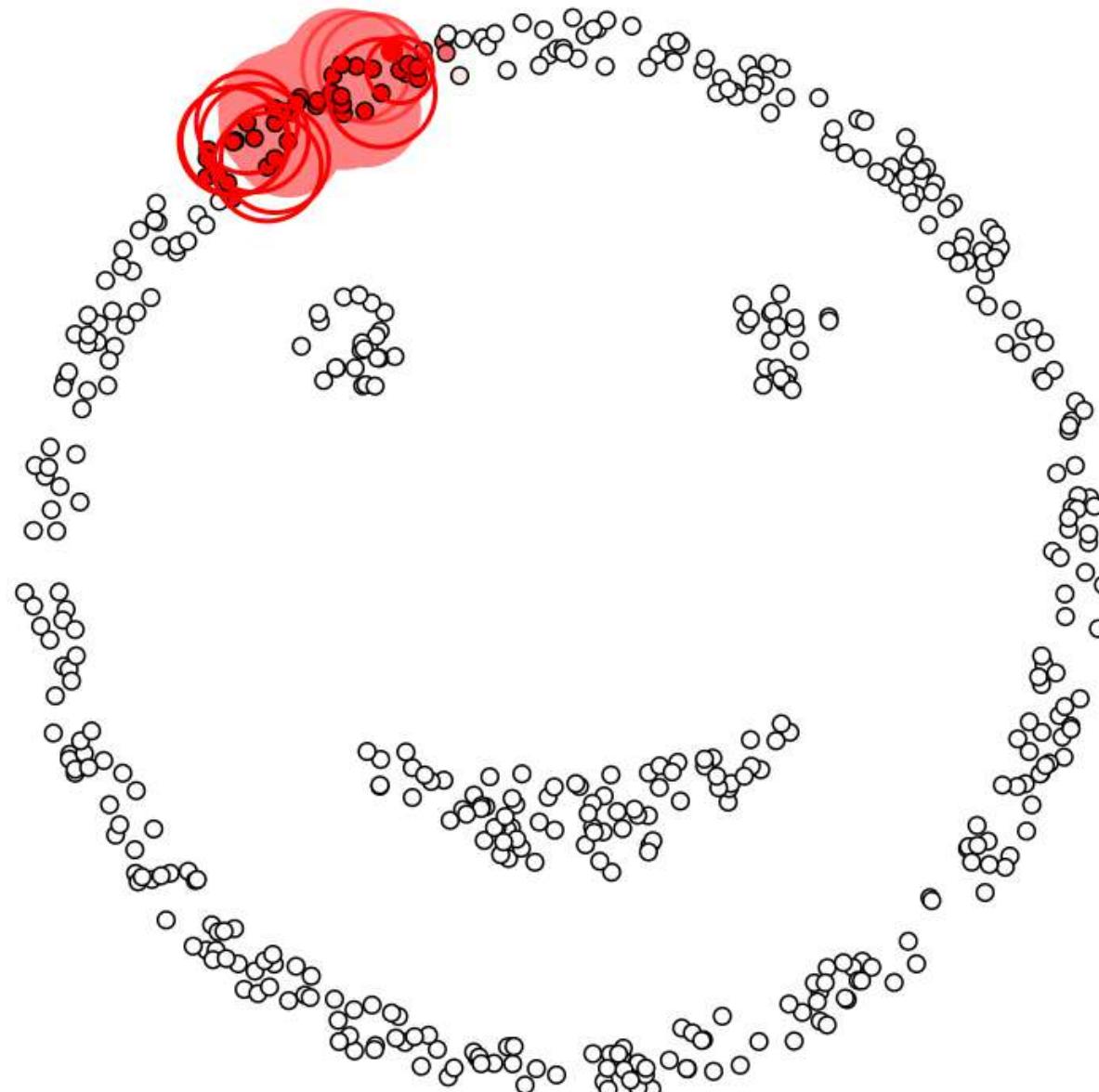
# Clustering - DBSCAN

- Try yourself
- Round 1
  - Epsilon = 1
  - minPoints = 4
- Round 1
  - Epsilon = 1
  - minPoints = 2
- Round 1
  - Epsilon = 1.5
  - minPoints = 4



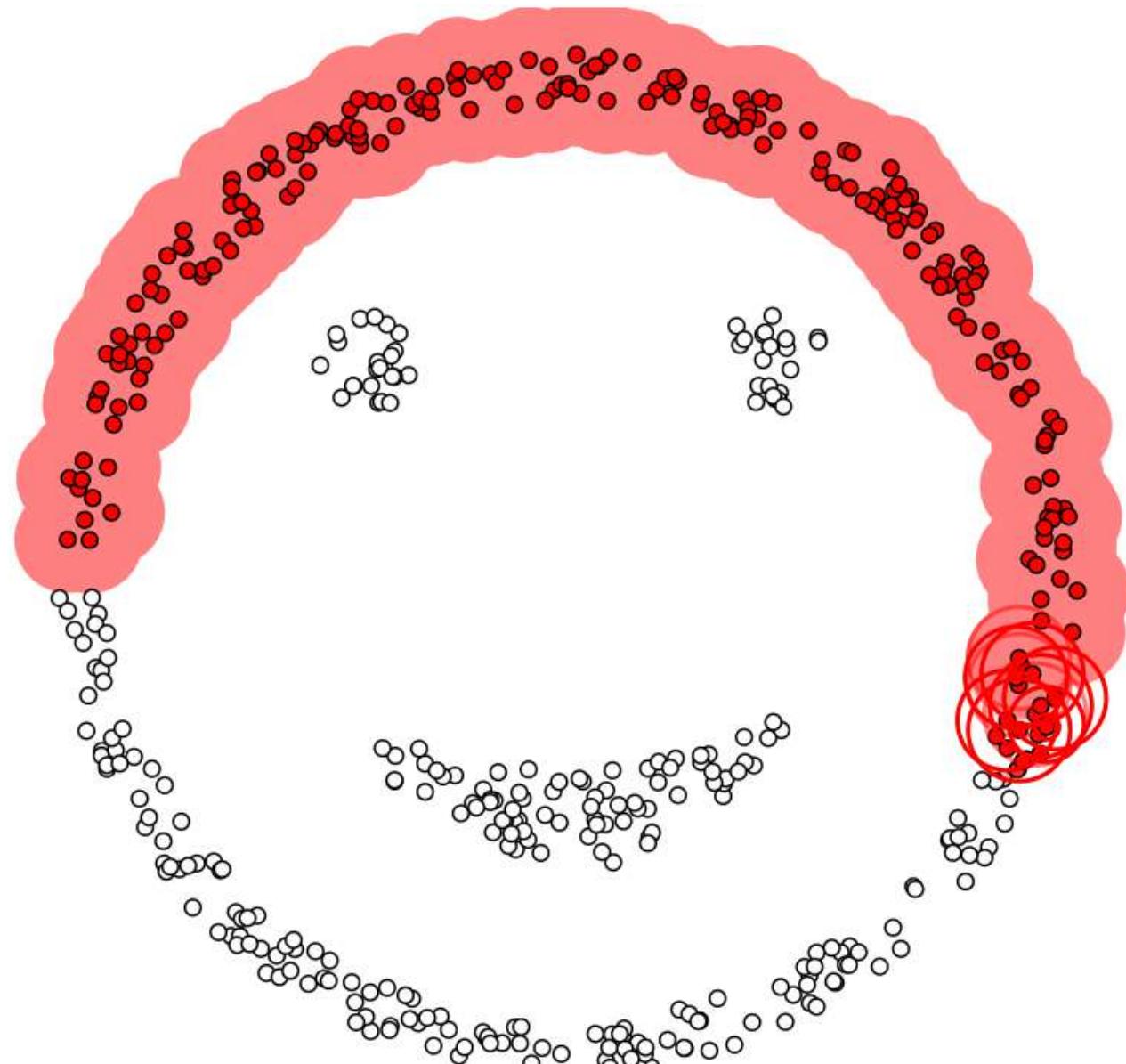


## Clustering - DBSCAN



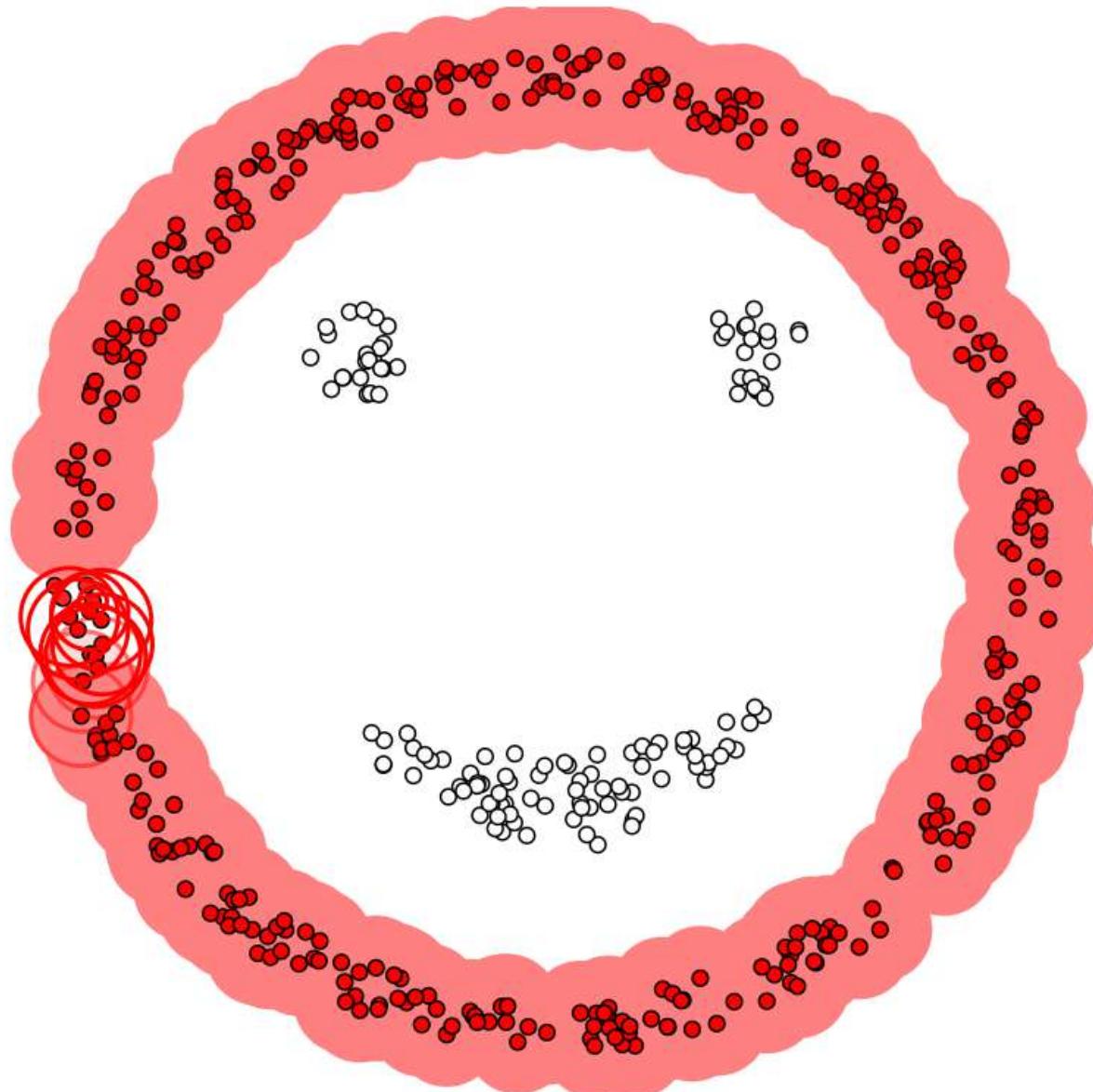
Reference : <https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/>

## + Clustering - DBSCAN



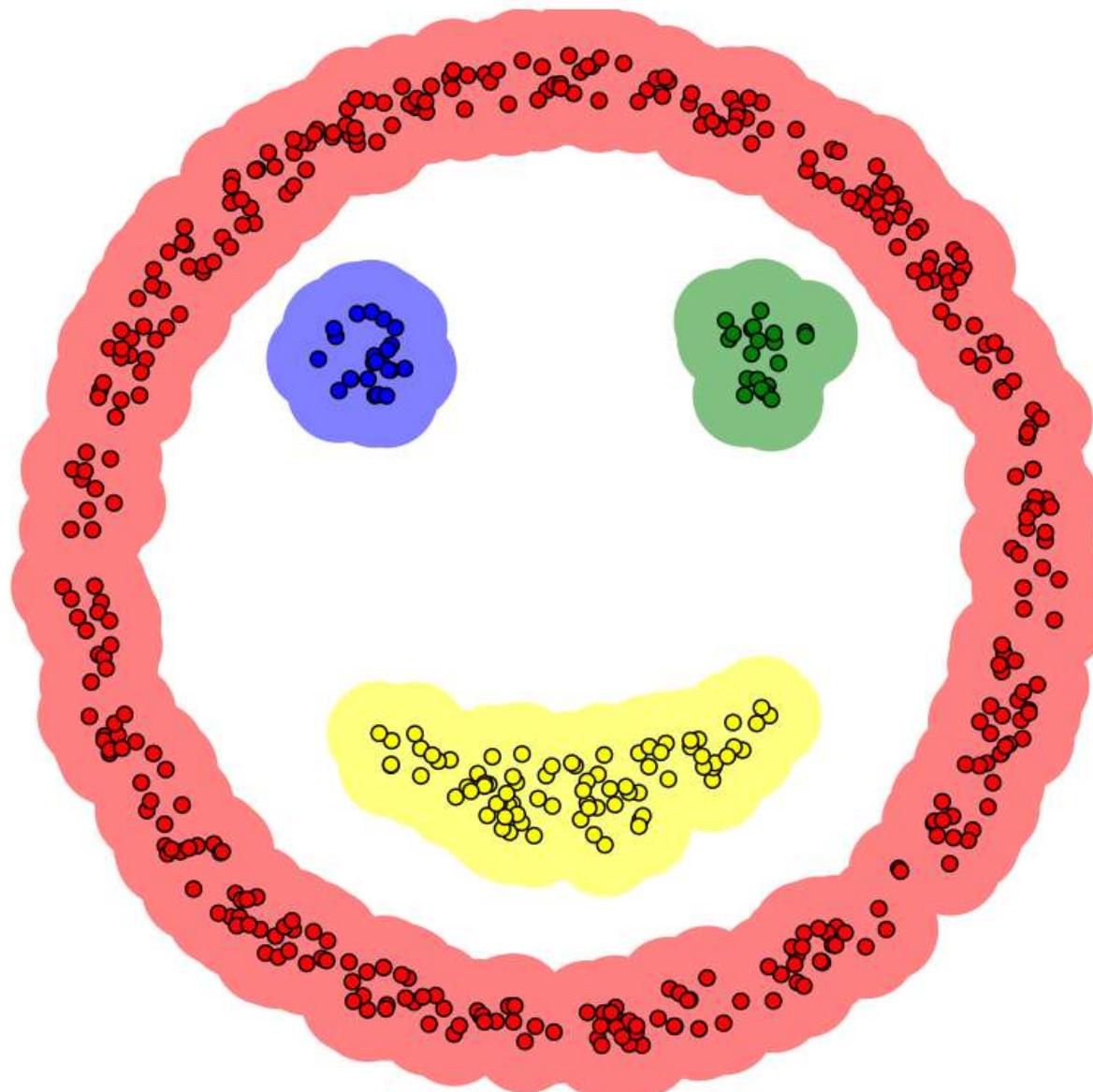
Reference : <https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/>

## + Clustering - DBSCAN



Reference : <https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/>

## + Clustering - DBSCAN



Reference : <https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/>



# Clustering - DBSCAN

## sklearn.cluster.DBSCAN

```
class sklearn.cluster.DBSCAN(eps=0.5, *, min_samples=5, metric='euclidean', metric_params=None, algorithm='auto',  
leaf_size=30, p=None, n_jobs=None)
```

[\[source\]](#)

Perform DBSCAN clustering from vector array or distance matrix.

DBSCAN - Density-Based Spatial Clustering of Applications with Noise. Finds core samples of high density and expands clusters from them. Good for data which contains clusters of similar density.

Read more in the [User Guide](#).

### Parameters:

#### **eps : float, default=0.5**

The maximum distance between two samples for one to be considered as in the neighborhood of the other. This is not a maximum bound on the distances of points within a cluster. This is the most important DBSCAN parameter to choose appropriately for your data set and distance function.

#### **min\_samples : int, default=5**

The number of samples (or total weight) in a neighborhood for a point to be considered as a core point. This includes the point itself.

#### **metric : string, or callable, default='euclidean'**

The metric to use when calculating distance between instances in a feature array. If metric is a string or callable, it must be one of the options allowed by `sklearn.metrics.pairwise_distances` for its metric parameter. If metric is "precomputed", X is assumed to be a distance matrix and must be square. X may be a [Glossary](#), in which case only "nonzero" elements may be considered neighbors for DBSCAN.

*New in version 0.17:* metric `precomputed` to accept precomputed sparse matrix.

#### **metric\_params : dict, default=None**

Additional keyword arguments for the metric function.

*New in version 0.19.*

#### **algorithm : {'auto', 'ball\_tree', 'kd\_tree', 'brute'}, default='auto'**

The algorithm to be used by the NearestNeighbors module to compute pointwise distances and find nearest neighbors. See `NearestNeighbors` module documentation for details.



# Market Basket Analysis



- Discover associations between items
- Count combinations of items that occur together frequently in transactions

$$\text{Support}(\{X\} \rightarrow \{Y\}) = \frac{\text{Transactions containing both } X \text{ and } Y}{\text{Total number of transactions}}$$

$$\text{Confidence}(\{X\} \rightarrow \{Y\}) = \frac{\text{Transactions containing both } X \text{ and } Y}{\text{Transactions containing } X}$$

$$\text{Lift}(\{X\} \rightarrow \{Y\}) = \frac{(\text{Transactions containing both } X \text{ and } Y) / (\text{Transactions containing } X)}{\text{Fraction of transactions containing } Y}$$

# Market Basket Analysis (Association Rule Mining)



Rule	Support	Confidence
Apple => Donut	2/5	2/3
Coconut => Apple	2/5	2/4
Apple => Coconut	2/5	2/3
Banana & Coconut => Donut	1/5	1/3



## Association Rule Mining (cont.)

- Wal-Mart customers who purchase Barbie dolls have a 60% likelihood of also purchasing one of three types of candy bars [Forbes, Sept 8, 1997]
- Strategies?
  1. Put them closer together in the store.
  2. Put them far apart in the store.
  3. Package candy bars with the dolls.
  4. Package Barbie + candy + poorly selling item.
  5. Raise the price on one and lower it on the other.
  6. Offer Barbie accessories for proofs of purchase.
  7. Do not advertise candy and Barbie together.
  8. Offer candies in the shape of a Barbie doll.





## Caution in Association Rule Mining



- Basket size: per bill, customer, day
- Item level: SKU, product category



mlxtend version: 0.17.2

[apriori](#)[association\\_rules](#)[fpgrowth](#)[fpmax](#)

# apriori

`apriori(df, min_support=0.5, use_colnames=False, max_len=None, verbose=0, low_memory=False)`

Get frequent itemsets from a one-hot DataFrame

## Parameters

- `df` : pandas DataFrame

pandas DataFrame the encoded format. Also supports DataFrames with sparse data; for more info, please see ([https://pandas.pydata.org/pandas-docs/stable/user\\_guide/sparse.html#sparse-data-structures](https://pandas.pydata.org/pandas-docs/stable/user_guide/sparse.html#sparse-data-structures))

Please note that the old pandas SparseDataFrame format is no longer supported in mlxtend >= 0.17.2.

The allowed values are either 0/1 or True/False. For example,

	Apple	Bananas	Beer	Chicken	Milk	Rice
0	True	False	True	True	False	True
1	True	False	True	False	False	True
2	True	False	True	False	False	False

[apriori](#)[association\\_rules](#)[fpgrowth](#)[fpmax](#)

# association\_rules

`association_rules(df, metric='confidence', min_threshold=0.8, support_only=False)`

Generates a DataFrame of association rules including the metrics 'score', 'confidence', and 'lift'

## Parameters

- `df` : pandas DataFrame

pandas DataFrame of frequent itemsets with columns ['support', 'itemsets']

- `metric` : string (default: 'confidence')

Metric to evaluate if a rule is of interest. **Automatically set to 'support' if `support_only=True`.**

Otherwise, supported metrics are 'support', 'confidence', 'lift',

'leverage', and 'conviction'. These metrics are computed as follows:

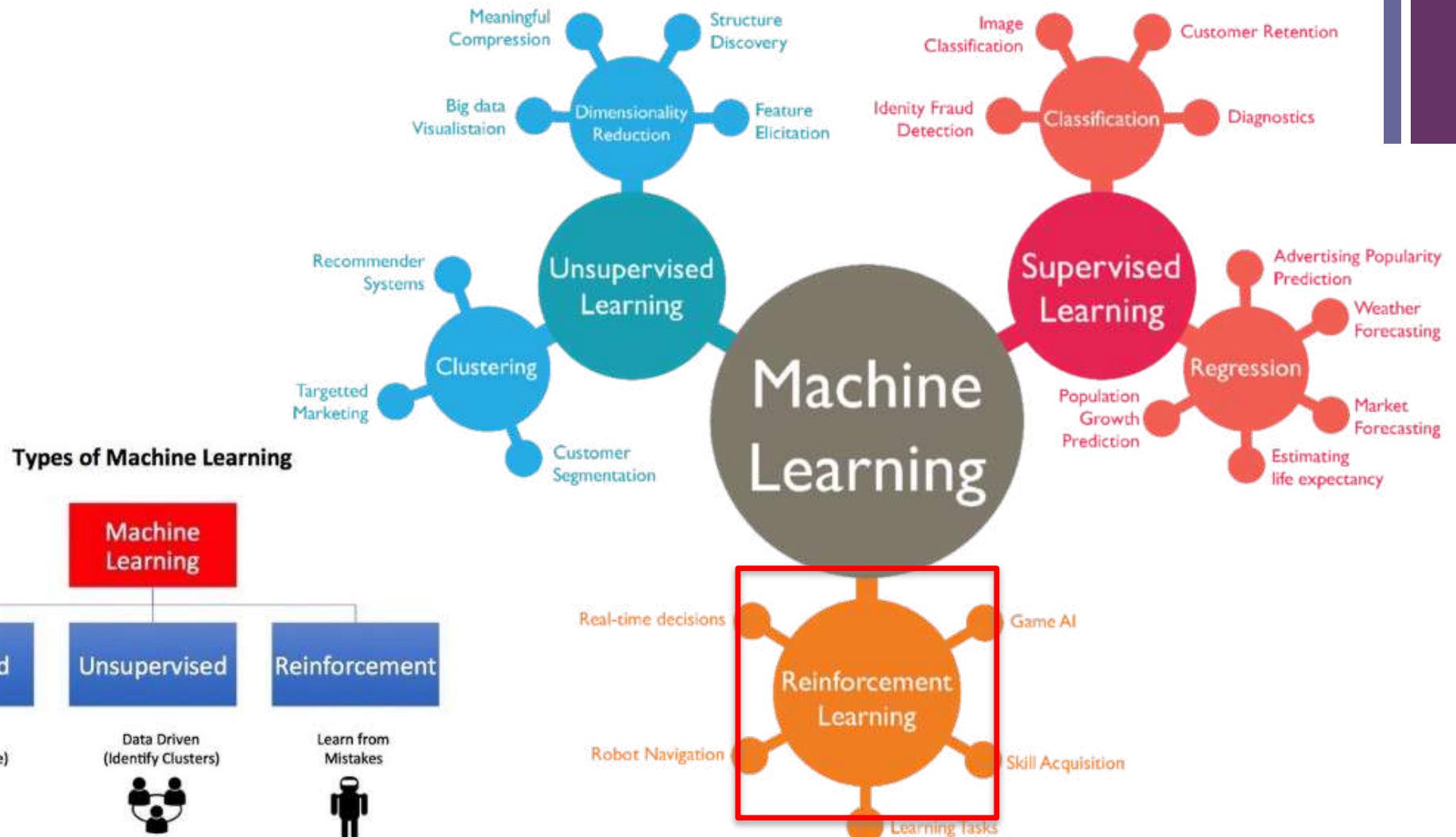
- `support(A->C) = support(A+C) [aka 'support']`, range: [0, 1]
- `confidence(A->C) = support(A+C) / support(A)`, range: [0, 1]
- `lift(A->C) = confidence(A->C) / support(C)`, range: [0, inf]
- `leverage(A->C) = support(A->C) - support(A)*support(C)`,  
range: [-1, 1]
- `conviction = [1 - support(C)] / [1 - confidence(A->C)]`,

+

## Part4: Reinforcement Learning (RL)

## + Task3: Reinforcement learning (optimization task)

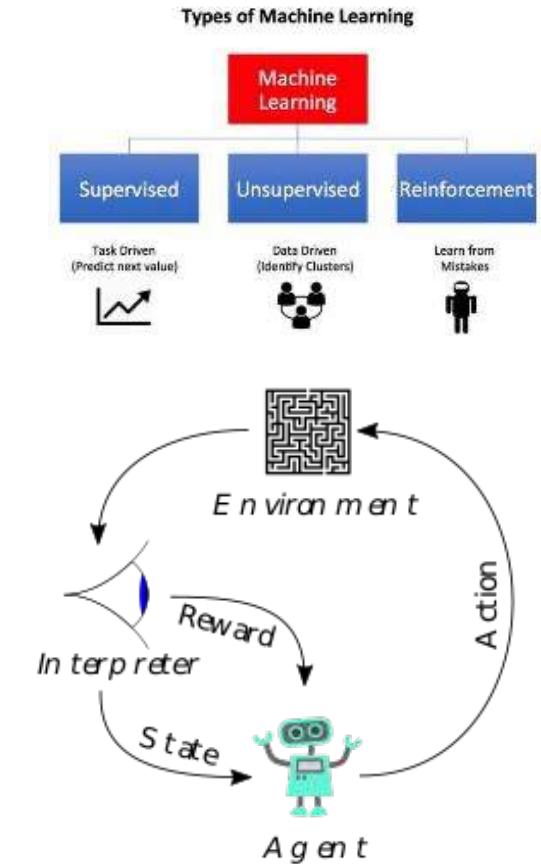
199





## Task3: Reinforcement Learning (cont.)

<https://www.youtube.com/watch?v=fiQsmdwEGT8>





## Reinforcement Learning (cont.)

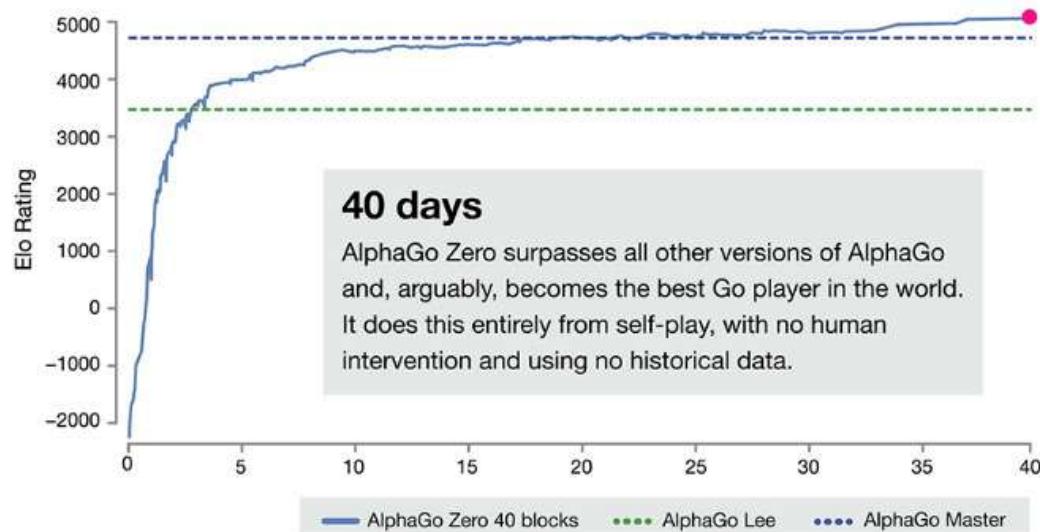
### DeepMind AlphaGo Zero learns on its own without meatbag intervention

The latest iteration of DeepMind's Go-playing AI has taught itself and bested other versions of AlphaGo.



By Chris Duckett | October 19, 2017 -- 00:44 GMT (08:44 GMT+08:00) | Topic: Innovation

Is AlphaGo Zero a scientific breakthrough – step towards AGI?

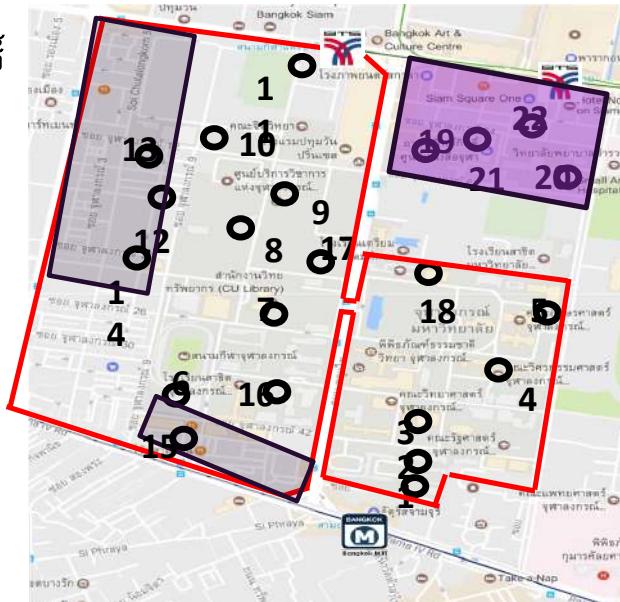


## การออกแบบระบบ Relocation สำหรับ CU TOYOTA Ha:mo

พื้นที่การให้บริการ 22 สถานี 60 ช่องจอด

ครอบคลุมบริเวณมหาวิทยาลัย ศูนย์การค้า และ สยามสแควร์

- |                              |                       |
|------------------------------|-----------------------|
| 1) ทางออกไปจามจุรีสแควร์     | 12) ระเบียงจามจุรี    |
| 2) เศรษฐศาสตร์               | 13) สวนหลวงสแควร์     |
| 3) ศาลาพระเกี้ยว             | 14) แมงพาร์ค          |
| 4) วิศวกรรมศาสตร์            | 15) ยู เช็นเตอร์      |
| 5) อักษรศาสตร์               | 16) นิเทศศาสตร์       |
| 6) จามจุรี 9                 | 17) สำนักงานทรัพย์สิน |
| 7) จามจุรี 5                 | 18) อาคารศิลปวัฒนธรรม |
| 8) หอพักวิทยนิเวศน์          | 19) เกษชศาสตร์        |
| 9) จามจุรี 10                | 20) สัตวแพทยศาสตร์    |
| 10) จุฬาพัฒน์ 14             | 21) อาคารวิทยกิตติ์   |
| 11) บีทีเอส สนามกีฬาแห่งชาติ | 22) สยามสแควร์ ซอย 8  |



เปิดให้บริการ

อัตราค่าบริการ

การใช้บริการ

ค่าลงทะเบียนสมาชิก

วิธีชำระค่าบริการ

จันทร์ - ศุกร์ 7.00-19.00

30 บาท / 20 นาทีแรก เกินจากนั้นนาทีละ 2 บาท

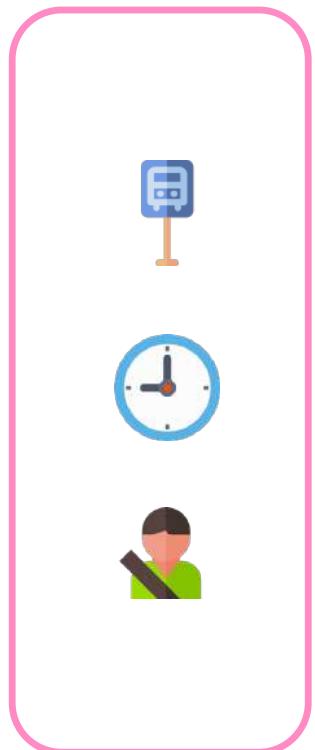
100 บาท (คืนเป็นคะแนนให้ 100 pt.)

ผ่านระบบอิเล็กทรอนิก ด้วยบัตรเครดิต/เดบิต





# Machine Learning



Demand Forecasting

Deep Learning

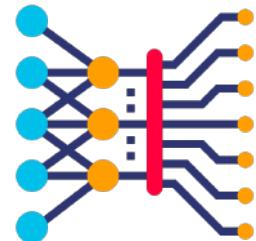
*Research Article*

**Recurrent Neural-Based Vehicle Demand Forecasting and Relocation Optimization for Car-Sharing System: A Real Use Case in Thailand**

Peerapon Vateekul ,<sup>1</sup> Panyawut Sri-iesaranusorn ,<sup>1,2</sup> Pawit Aiemvaravutigul ,<sup>1</sup> Adsadawut Chanakitkarnchok ,<sup>1</sup> and Kultida Rojviboonchai ,<sup>1</sup>

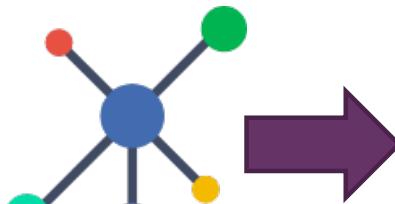
<sup>1</sup>Chulalongkorn University Big Data Analytics and IoT Center (CUBIC), Department of Computer Engineering,  
Faculty of Engineering, Chulalongkorn University, Bangkok, Thailand

<sup>2</sup>Division of Information Science, Nara Institute of Science and Technology, Nara, Japan



Relocation Optimization

Min Cost Max-Flow



Relocation  
Optimization  
System

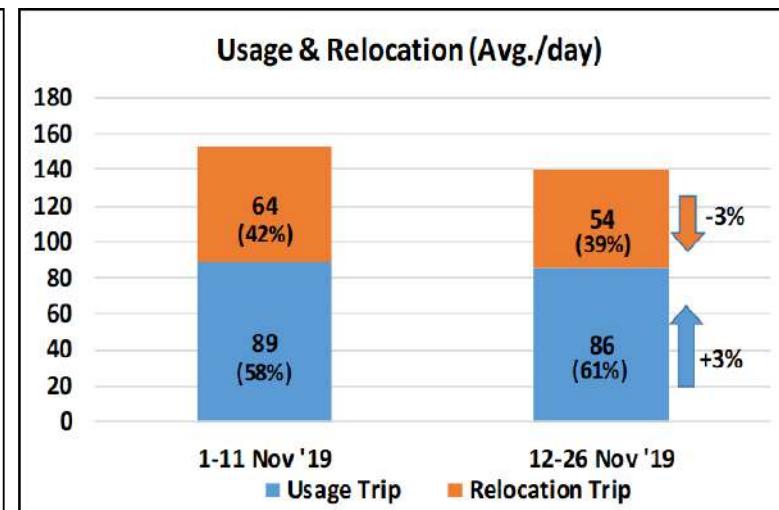
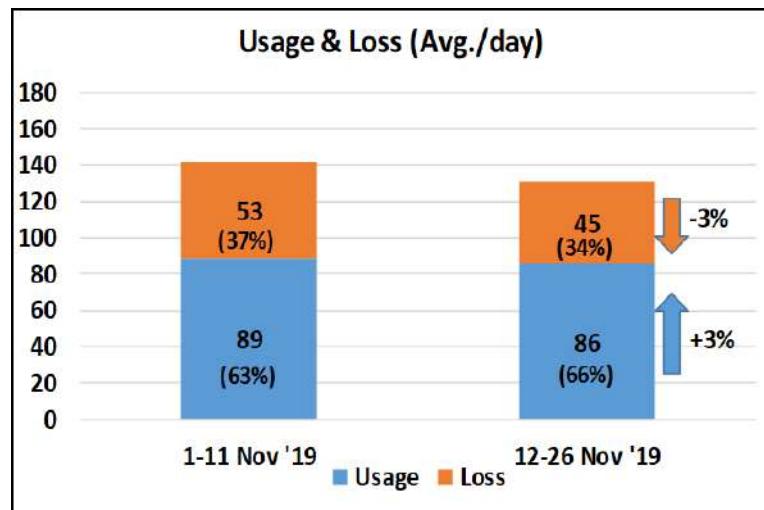
# Project 3 : System Design for Vehicle Relocation

## 4) Service Result :

- Opportunity Loss = 34% (-3%)
- Relocation job reduction = 39% (-3%)
- Reduction of manual job (loss analysis & demand forecasting) = 17 MH/Week

## 5) Conclusion :

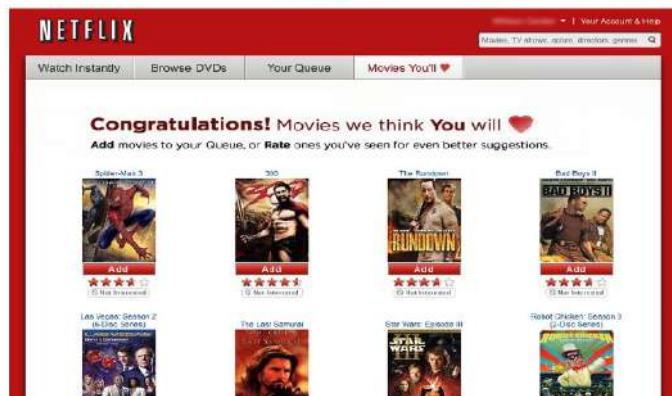
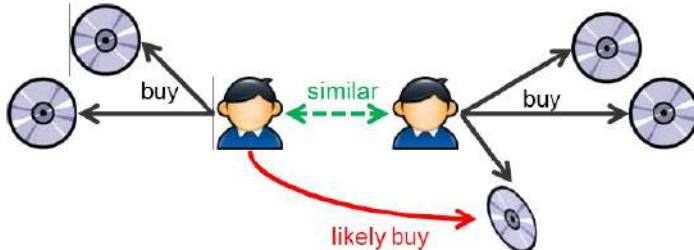
- Our AI assisted system can achieve lower opportunity loss (3%), lower relocation job (3%), and reduce human relocation effort (17 MH/Week).





## Part4: Special Tasks

# Special task



**65.00%**

- @Kobkorn\_ ดูนี้ต้องไม่ลืมซื้อ " //
- 5555555 ยังคงทำให้หัวใจบั่น腾 ~~
- คนไม่TOP ใช้เวลาอ่านบัญชีดีกว่า แต่ใช้เวลาอ่านข้อความบันเทิงมากกว่าคนไม่ใช้เวลาอ่านบัญชีดีกว่าคนที่ไม่ใช้เวลาอ่านบัญชี ~~~~ พากย์ ~~
- พี่น้อง 3
- @PAWma\_teabooth ขออภัยด้วยนะครับ แต่ปีนี้ จึงต้อง หยุดงาน D
- ข้อมูลนี้ต้องหักภาษี นะครับ ~
- @Zinger\_XNika ดูแลเรื่อง ภาระน้ำ อยู่แล้วก็ ภาระน้ำ ~~
- @BubbleBubble @richiehme หักเรื่อง ~~

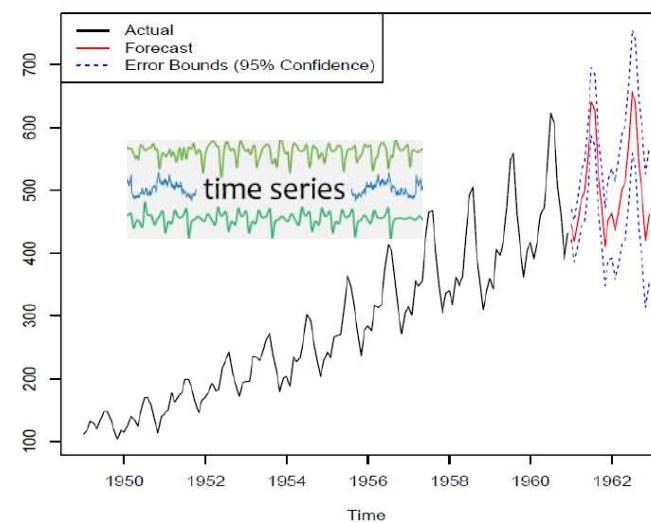
**35.00%**

- เงินเดือน ~ // ลิ้งค์ http://t.co/tUyrgXJUD
- ห้ามใช้ภาษาไทยในห้องเรียน ~~
- บ้านของฉัน 3 ห้องนอนห้องน้ำ 2 ห้องน้ำห้องน้ำ ห้องน้ำ ~~
- บ้านของฉัน 3 ห้องน้ำห้องน้ำ ~~
- สีฟ้า ห้องน้ำห้องน้ำ ~~
- เมืองไทยจะหายไป ญี่ปุ่น ~- #men 555
- สีฟ้า ห้องน้ำห้องน้ำ ~~
- บ้านของฉัน 3 ห้องน้ำห้องน้ำห้องน้ำห้องน้ำ ~~
- บ้านของฉัน 3 ห้องน้ำห้องน้ำห้องน้ำ ~~

SEARCH

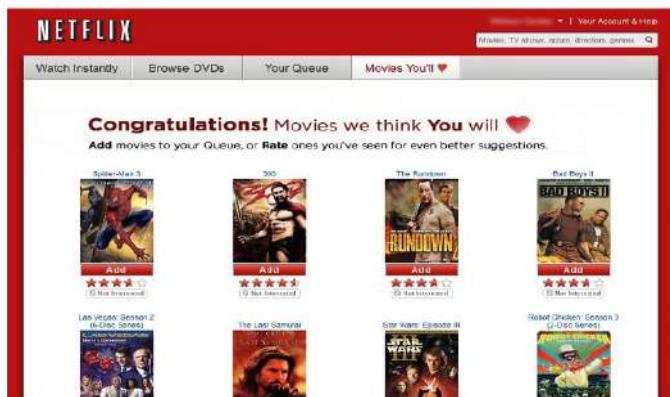
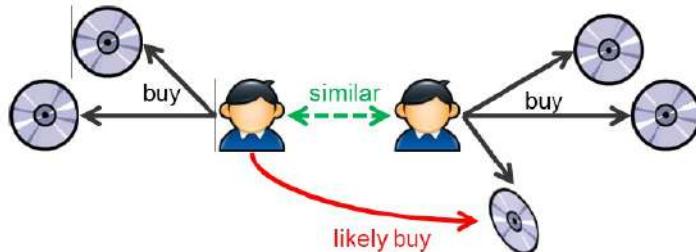
POWERED BY S-SENSE

SPT NECTEC





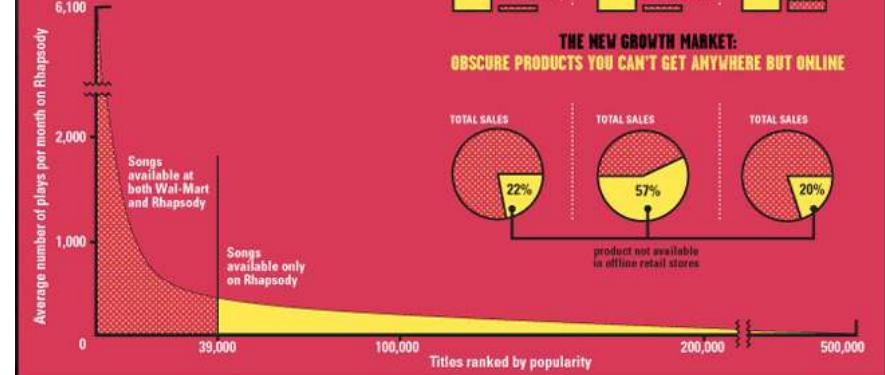
# Recommendation system



	Harry potter	X-Men	Hobbit	Argo	Pirates
101	5	2	4	?	?
102	?	?	5	2	?
103	1	2	?	?	3
104					
105					
...					

## ANATOMY OF THE LONG TAIL

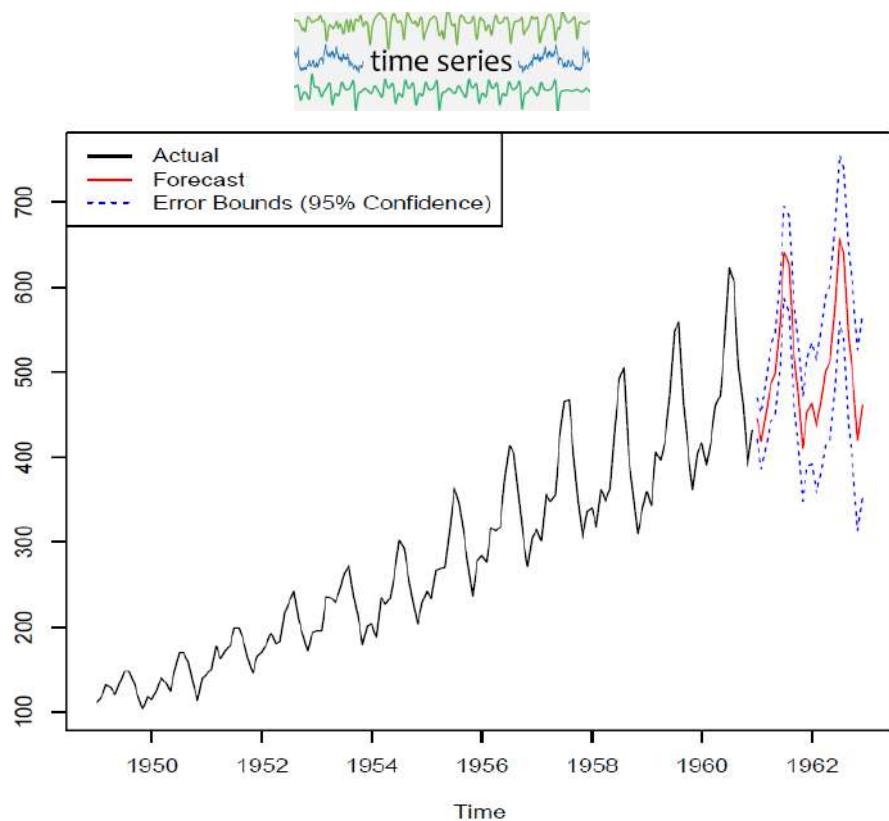
Online services carry far more inventory than traditional retailers. Rhapsody, for example, offers 18 times as many songs as Wal-Mart's stock of 39,000 tunes. The appetite for Rhapsody's more obscure tunes (charted below in yellow) makes up the so-called Long Tail. Meanwhile, even as consumers flock to mainstream books, music, and films (right), there is real demand for niche fare found only online.



	Harry potter	X-Men	Hobbit	Argo	Pirates
101	5	2	4	1	3
102	4	1	5	2	3
103	1	2	4	1	3
104					
105					
...					



# Time Series Analysis (Trend Forecasting)



- Techniques
  - ARIMA (Autoregressive integrated moving average)
  - Exponential Smoothing
  - Neural Networks
  - Deep Learning
- Sample Applications
  - Customer trend forecasting
  - Revenue trend forecasting
  - Rainfall forecasting
  - Remaining useful life forecasting (preventive maintenance)



# Text Mining

<https://ischool.syr.edu/infospace/2013/04/23/what-is-text-mining/>



- Text mining, which is sometimes referred to “text analytics” is one way to make qualitative or “unstructured” data **usable by a computer**.
- Convert from unstructured to structured data

NBC Nightly News @nbcnightlynews America's #1 evening news broadcast. Tweets by @newsdel & @braddjaffy. Join us on Facebook <http://facebook.com/nbcnightlynews>

NBC News @NBCNews A leading source of global news and information for more than 75 years. Have a news tip or question? Ask @rozzy, @lou\_dubois, @baicata or @anthonyquintano.

CNN Breaking News @cnnblk CNN.com is among the world's leaders in online news and information delivery.



Comments	Good	Like	Hate	Sentiment
Tweet1	7	8	0	😊
Tweet2	1	0	10	😢
Tweet3	2	9	1	😊



# Text Mining (cont.): Sentiment Analysis

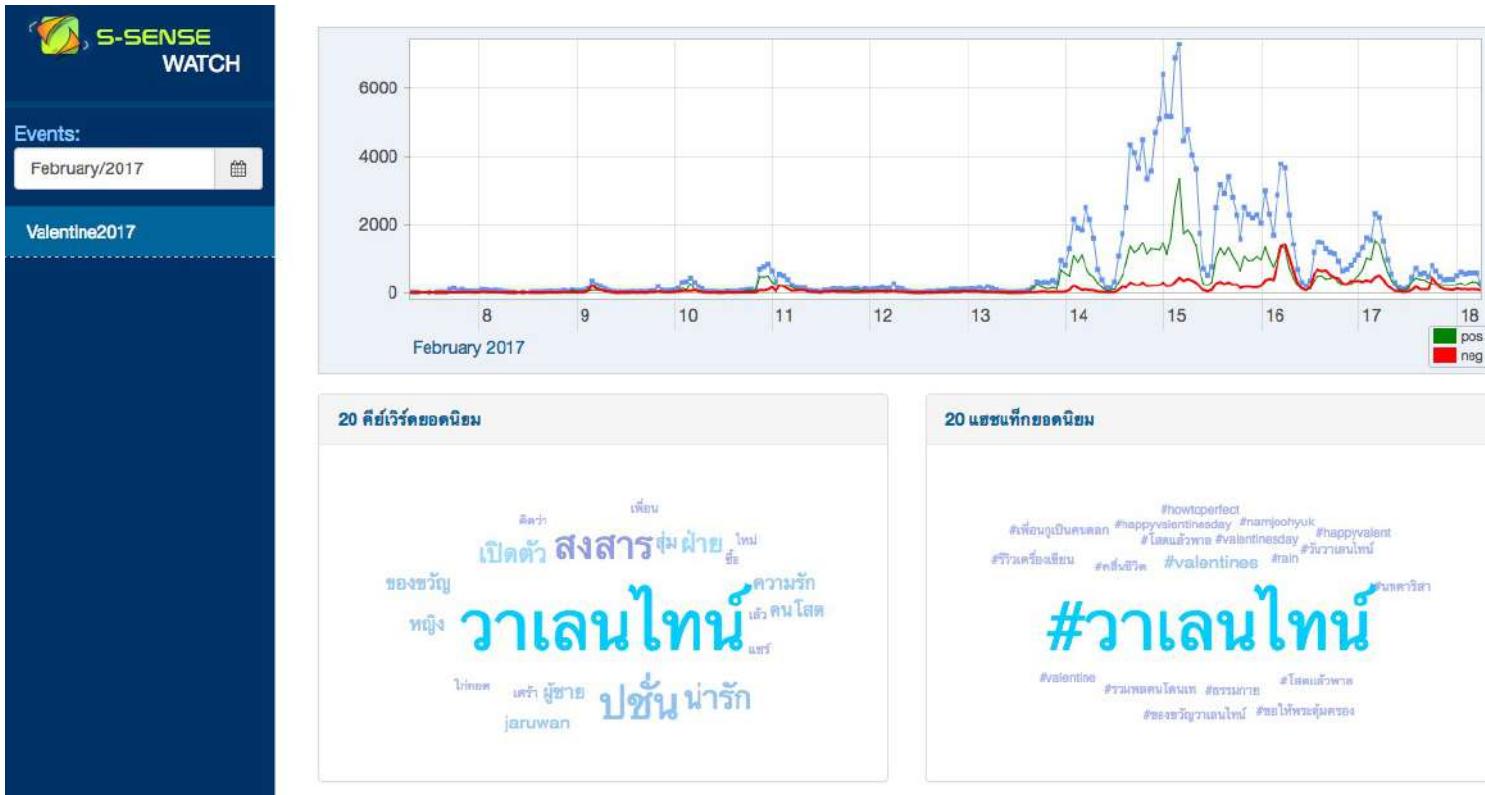
<http://pop.ssense.in.th/>



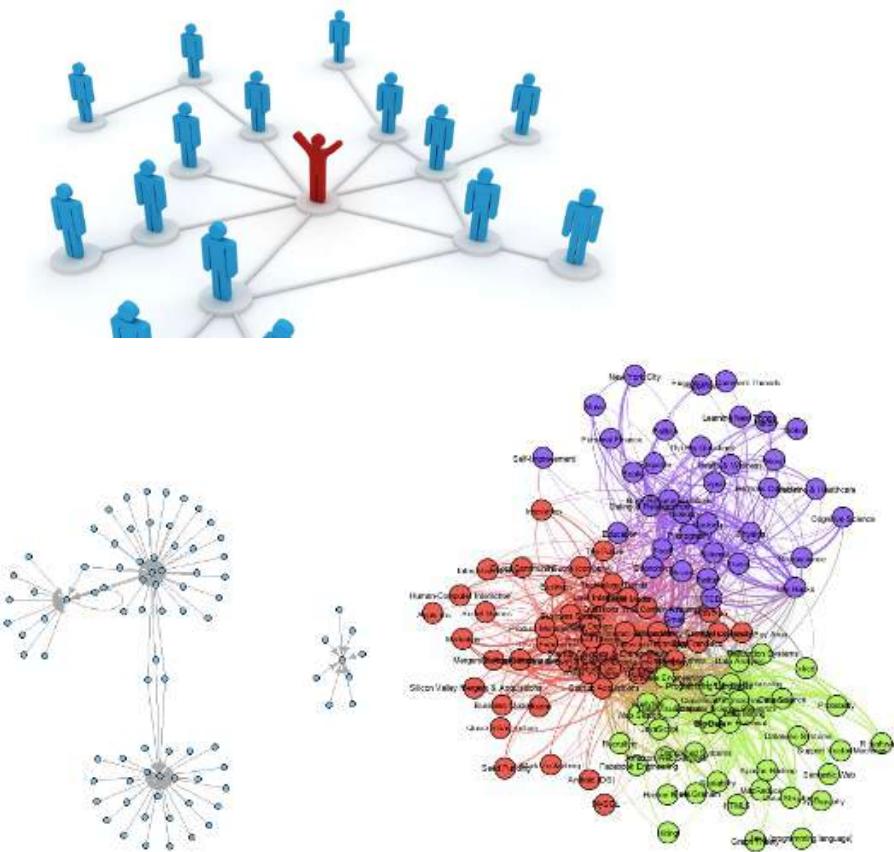
+

# Text Mining (cont.): Emerging Trend Analysis

<http://www.ssense.in.th/watch/>



# Social Network Analysis



- Techniques
    - Centrality: degree, closeness, betweenness, transitivity
    - Community detection
    - Graph Clustering
  - Sample Applications
    - Influencer detection
    - Community detection

+ Thank you  
& any questions