Machine Learning

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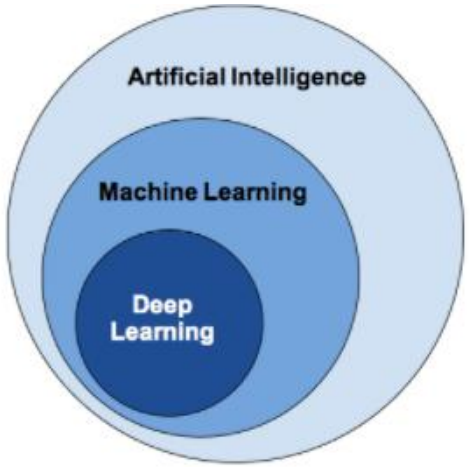
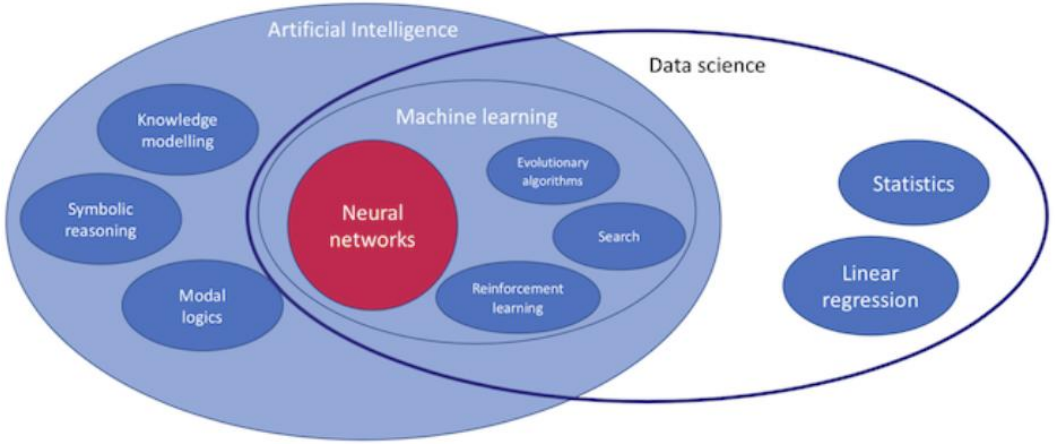
Contents

1. Introduction to Machine Learning

Machine Learning

- What is ML
  - the study of computer algorithms that improve automatically through experience and by the use of data. It is seen as a part of artificial intelligence. [wikipedia]
  - ML algorithms build a model based on sample data (training data) in order to make predictions or decisions without being explicitly programmed to do so.





[ref] https://ictinstitute.nl/ai-machine-learning-and-neural-networks-explained/

Machine Learning

- Machine Learning approaches
  - Supervised learning: inputs(features) and outputs(labels) are both given (by a teacher) to learn a general rule to map features to labels
    - Regression : labels are continuous values
    - Classification: labels are categorical values
  - Unsupervised learning: no labels are given, and to discover hidden patterns or features in data
    - Dimension reduction: PCA(Principal Component Analysis)
    - Clustering (or grouping)
  - Semi-supervised learning: large unlabeled data with small labeled data
  - Reinforcement learning: interacts with environment by producing actions and discovers errors or rewards (trial and error search, delayed reward)
    - Model-based RL (like control theory)
    - Model-free RL: Policy-iteration (Policy gradient, A3C) and value-iterations (Q-learning)

2. Data and Models

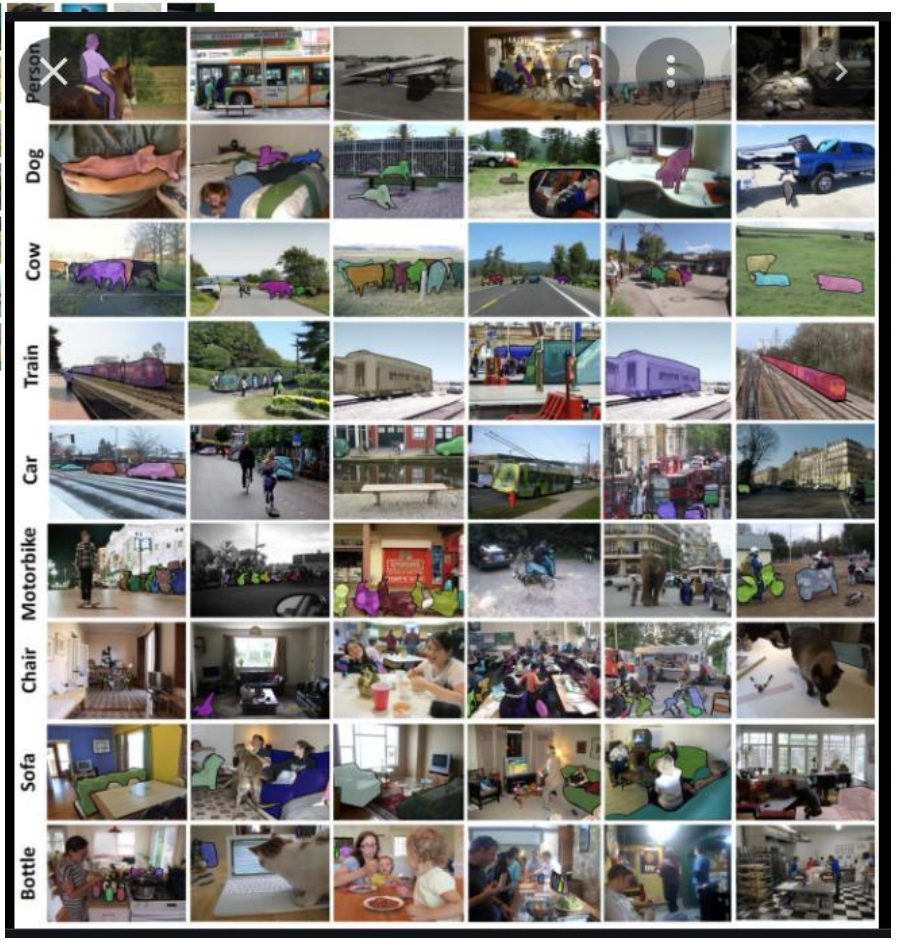
Datasets for Machine Learning

- Iris dataset
  - 4-column features, 150 samples
  - Target: 3 classes
- MNIST(Modified National Institute of Standards and Technology dataset)
  - 28*28 grayscale pixels, 60,000 train, 10,000 test set
  - Target: single digits 0 ~ 9
- Fashion MNIST
  - 28*28 pixels, 60,000 train set, 10,000 test set
  - Target:10 categories
- Many more in Kaggle.com

Fashion MNIST

Datasets for Machine Learning

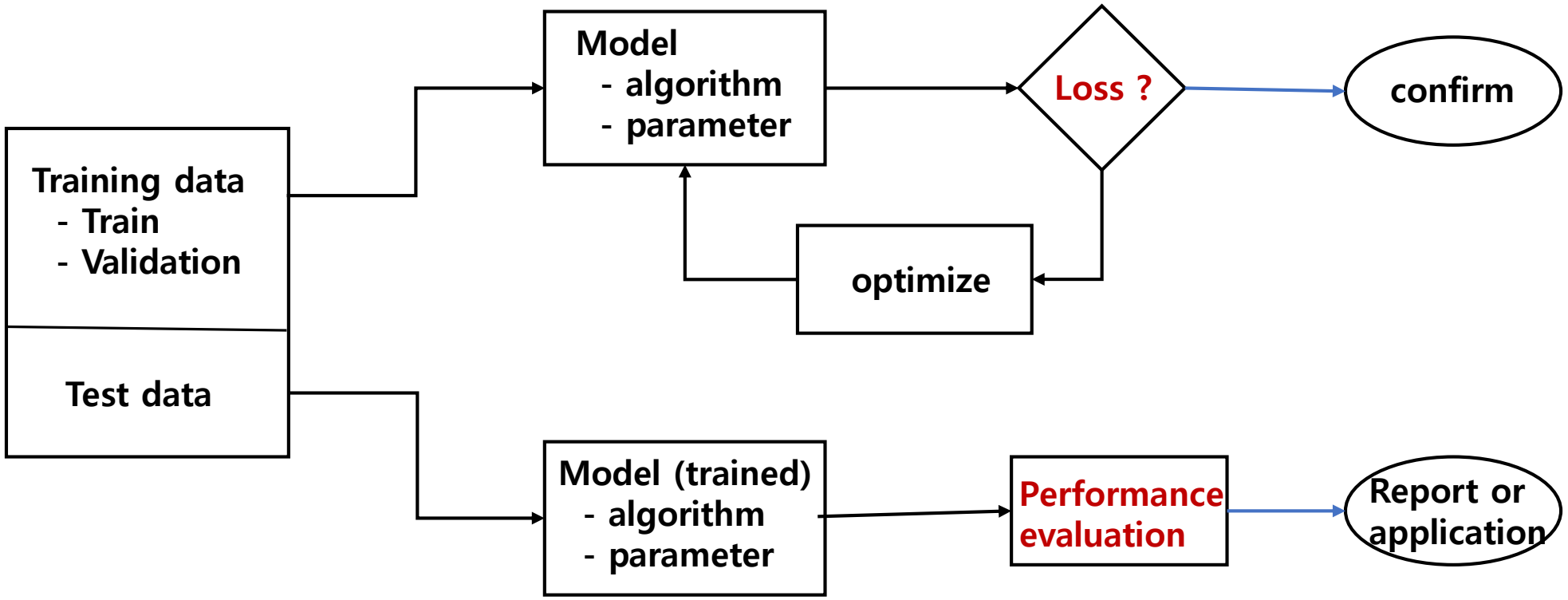
- Cifar-10 (Canadian institute for advanced research)
  - 32*32 color images in 10 classes, with 6,000 per class
  - 50,000 training, and 10,000 test images
  - Bigger dataset (Cifar-100)
- Microsoft COCO (common objects in Context)
  - Large image recognition/classification, object detection, segmentation, and captioning dataset
  - 330K images (200K+ annotated), more than 2M instances in 80 object categories
  - 5 captions per image, and 250,000 people with key points



Datasets for Machine Learning

- **ImageNet**
  - largest image dataset for computer vision, used in ILSVRC(ImageNet Large Scale Visual Recognition Challenge) for image classification and object detection (150 GB)
  - 469*387 resolution in average (usually cropped to 256*256 or 224*224 before usage)
  - More than 14 million images with more than 21,000 groups(classes)
  - More than 1 million images have bounding box annotations
- **ILSVRC**
  - To evaluate algorithms for object detection and image classification (and localization) at large scale
  - To measure the progress of computer vision for large scale image indexing for retrieval and annotation
  - Uses smaller portion of the ImageNet (1,000 categories with 1.3 million train images, 50,000 validation images, and 1,00,000 test images
  - Available in Kaggle
  - 2010 ~ 2017

Machine Learning Model (supervised)

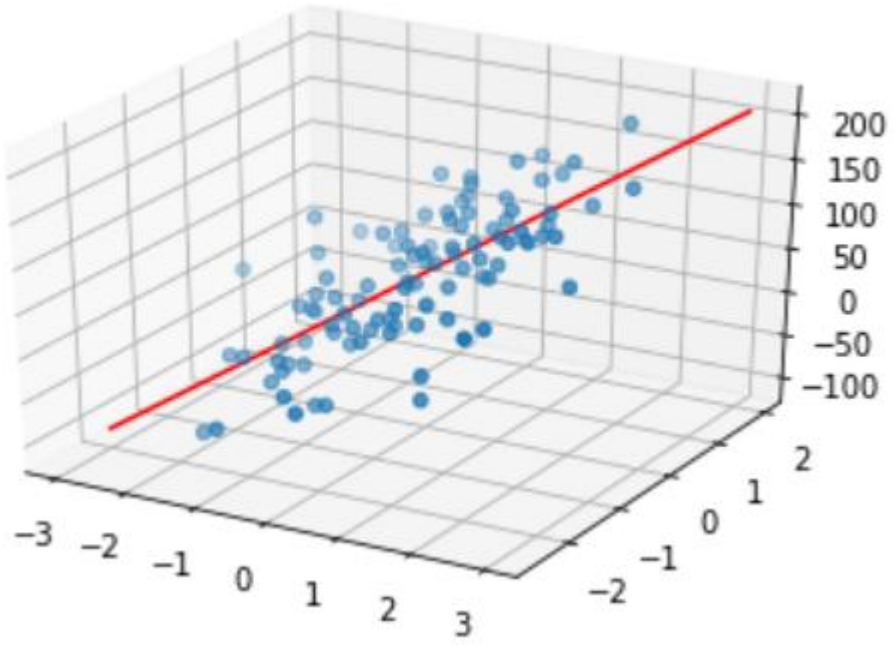


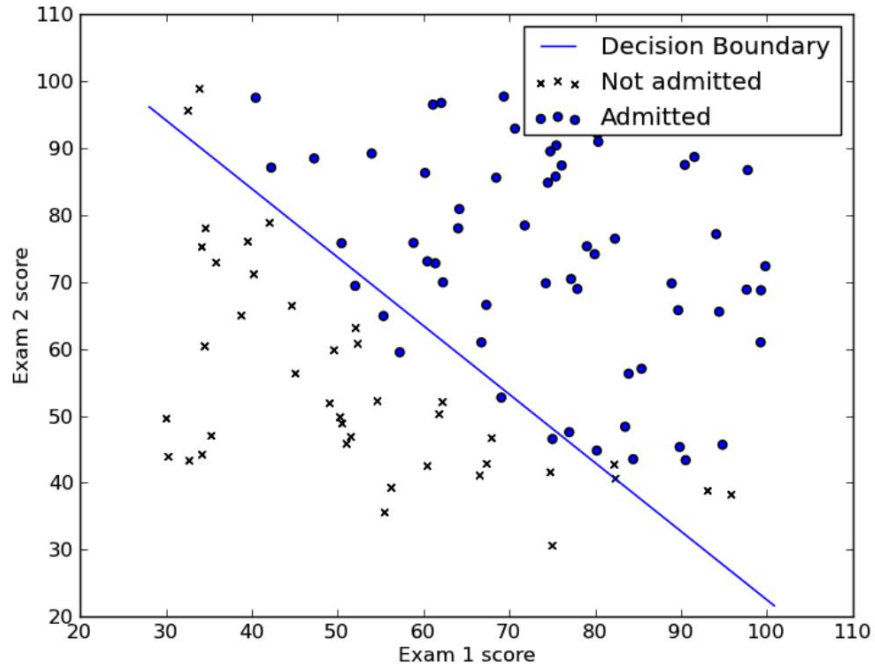
- (model) Parameter: estimated from the dataset (learned during training from the historical data sets)
- Hyper-parameter: external to the model (defined manually before the model training by trial-error)

3. Supervised Learning

Supervised Learning

- **Linear Regression and Linear Classification**
  - (regression) $y = w1 \cdot x1 + w2 \cdot x2 + b$
  - (classification) $w1 \cdot x1 + w2 \cdot x2 + b = 0$





Linear Regression

- **Gradient Descent Algorithm**
  - **Loss** (or **cost**) function: MSE (mean square error)

$$\mathcal{L}(y, t) = \frac{1}{2}(y - t)^2$$

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j}$$

$$= w_j - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, x_j^{(i)}$$

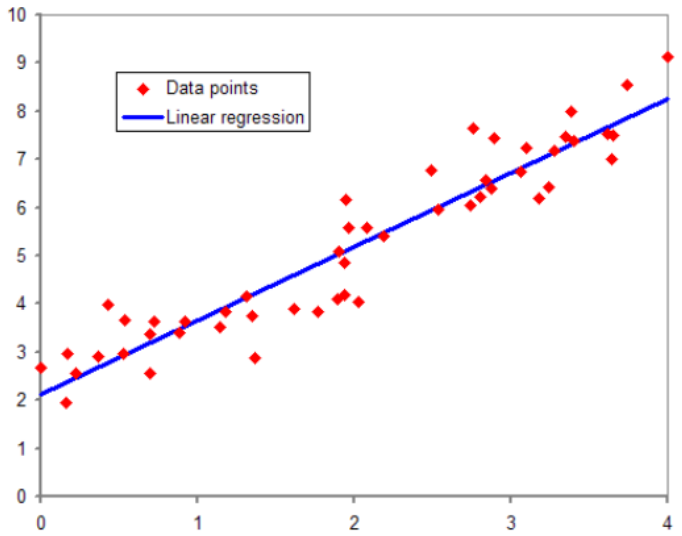
  - In vector form

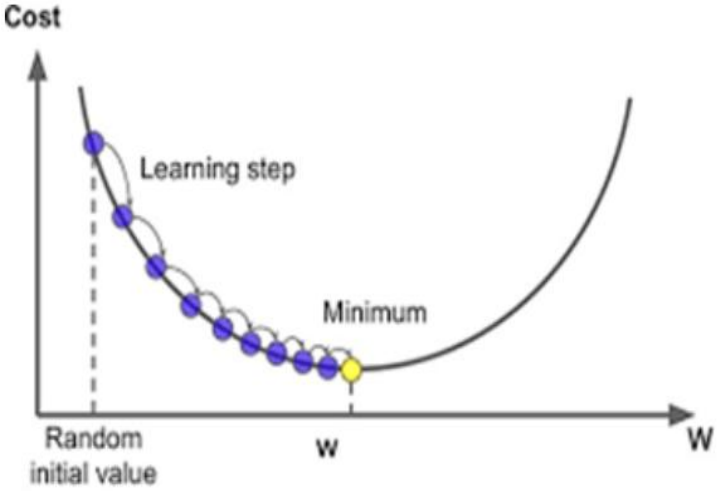
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

$$= \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)}$$

$$\frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial w_D} \end{pmatrix}$$

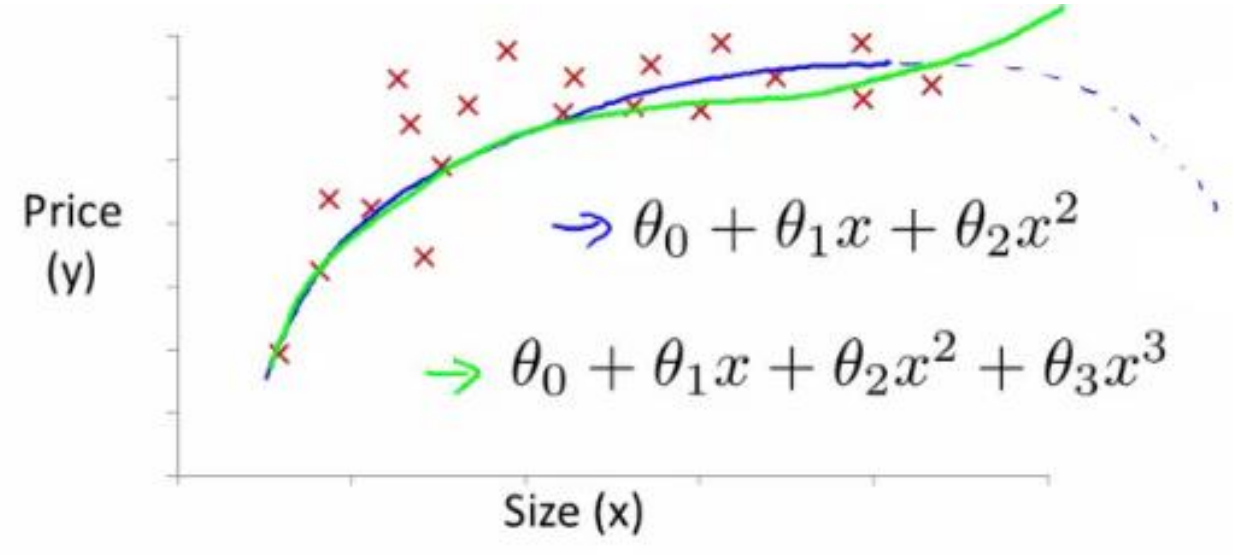
$$y = wx + b$$





Linear Regression

- **Polynomial Regression**

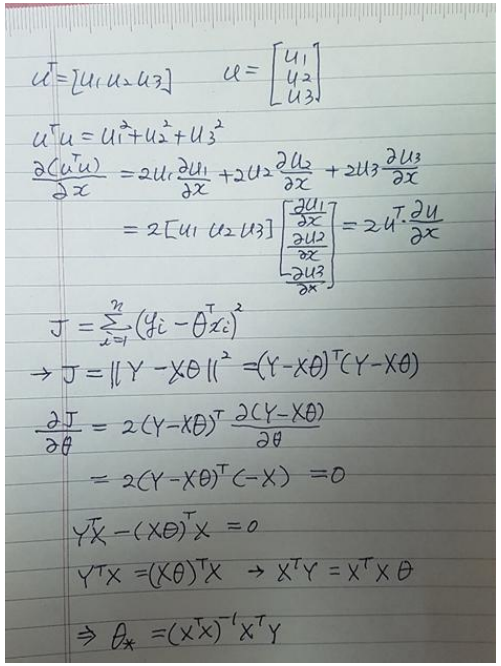


  - To map our old linear hypothesis and cost functions to these polynomial descriptions the easy thing to do is set
    - $x_1 = x$
    - $x_2 = x^2$
    - $x_3 = x^3$
  - By selecting the features like this and applying the linear regression algorithms you can do polynomial linear regression

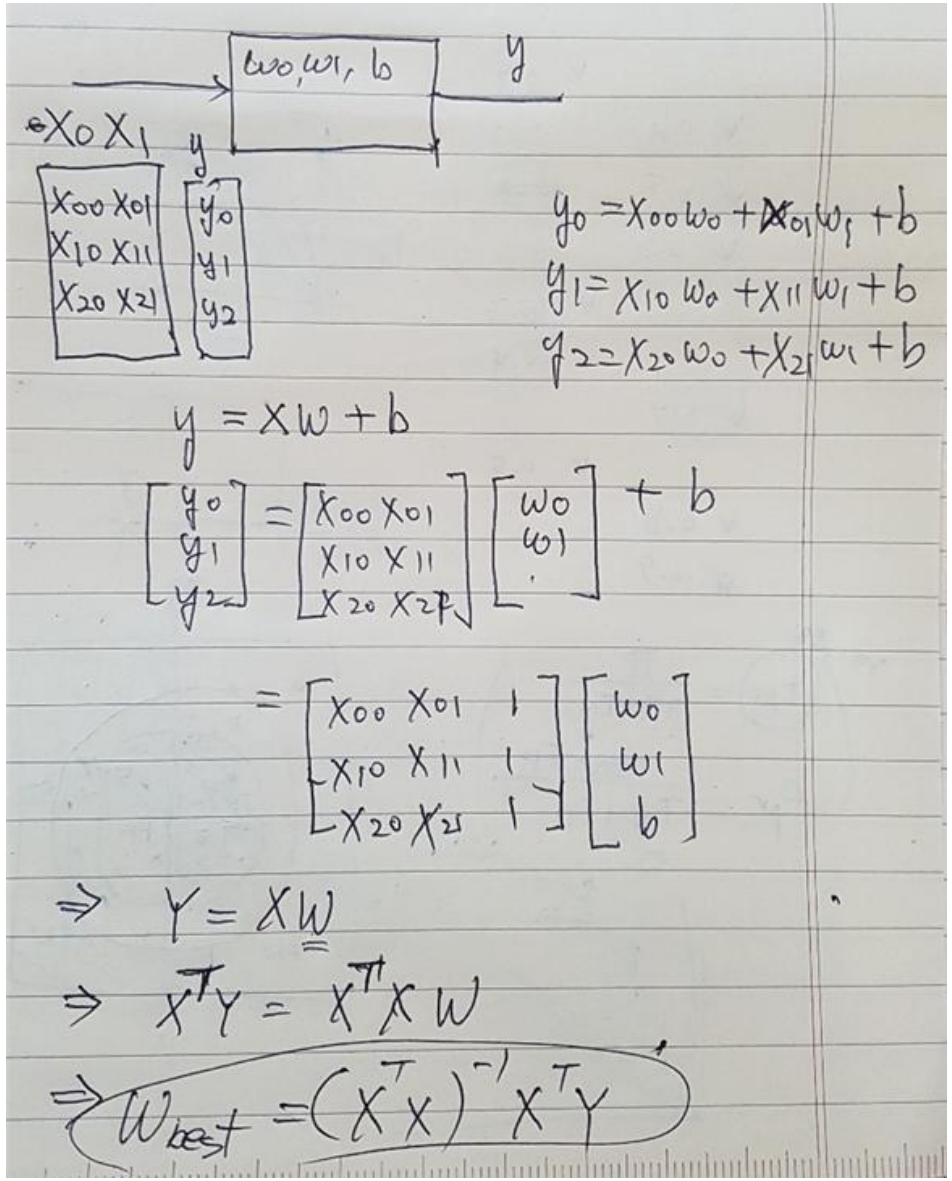
Ref: http://holehouse.org/mlclass/06_Logistic_Regression.html

Linear Regression

- **Normal equation (Ordinary Least Squares)**
  - LinearRegression() in sklearn library
  - Don't require learning rate (no iterative steps)
  - High computational complexity (inverse requires $O(n^3)$ complexity)



$$\hat{\theta} = (X^T \cdot X)^{-1} \cdot X^T \cdot y$$



Linear Regression

- **OLS regression analysis**

```
sm.OLS(y_train, X_train_ols).fit().summary()
```

OLS Regression Results

Dep. Variable:	SystemProduction	R-squared:	0.641
Model:	OLS	Adj. R-squared:	0.641
Method:	Least Squares	F-statistic:	2084.
Date:	Tue, 26 Nov 2024	Prob (F-statistic):	0.00
Time:	09:14:26	Log-Likelihood:	-57635.
No. Observations:	7008	AIC:	1.153e+05
Df Residuals:	7001	BIC:	1.153e+05
Df Model:	6		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	697.0526	10.787	64.618	0.000	675.906	718.199
x1	19.7436	11.578	1.705	0.088	-2.953	42.440
x2	-214.2258	17.908	-11.963	0.000	-249.331	-179.121
x3	-66.7511	10.909	-6.119	0.000	-88.136	-45.366
x4	1196.0869	19.381	61.714	0.000	1158.094	1234.080
x5	86.6055	12.972	6.676	0.000	61.177	112.034
x6	-177.8948	15.225	-11.685	0.000	-207.739	-148.050

Omnibus:	1086.969	Durbin-Watson:	2.017
Prob(Omnibus):	0.000	Jarque-Bera (JB):	19237.530
Skew:	0.040	Prob(JB):	0.00
Kurtosis:	11.116	Cond. No.	3.74

결정계수 R^2 (R-Squared):
모델이 종속 변수의 변동을 얼마나 잘 설명하는지 나타냄.
- R^2 = 0: 모델이 아무것도 설명하지 못함.
- R^2 = 1: 모든 변동을 완벽히 설명.

F-통계량 (F-test)
- 회귀모델 전체의 유의성을 평가
- H0: "모든 회귀 계수가 0이다" (독립 변수들이 종속 변수에 영향을 미치지 않는다)
- P-value < 0.05 (reject H0 -> 모델이 유의미하다)

개별독립 변수의 유의성
- 각 독립 변수가 종속 변수에 유의미한 영향을 미치는지를 평가 (t-검정)
- H0: "해당 독립 변수의 회귀 계수 $\beta i=0$, 즉 종속 변수에 영향을 미치지 않는다"

Omnibus: 잔차(residuals)가 정규성을 따르는지를 검정 (잔차의 왜도와 첨도를 함께 분석)
- H0: "잔차가 정규분포를 따른다"
- prob(omnibus): p-value < 0.05 (reject H0, 정규성을 벗어남)

Linear Regression

- **(결과 해석)** F-test, t-test 는 모두 유의미하지만 잔차는 정규성을 벗어나고 있다.

  (1) **비선형성 존재:**
  - 독립 변수와 종속 변수의 관계가 선형이 아닌 경우, 회귀 모델은 오차를 정규적으로 처리하지 못한다.
  - 하지만, 모델은 여전히 전체 데이터의 일부 패턴을 학습하여 유의미한 결과를 낼 수 있다.

  (2) 이상치(Outliers):
  - 데이터셋에 이상치가 포함되면 잔차의 분포가 왜곡될 수 있다.
  - 이상치는 잔차의 정규성을 심각하게 훼손하지만, t-test나 F-test에는 상대적으로 덜 민감할 수 있다.

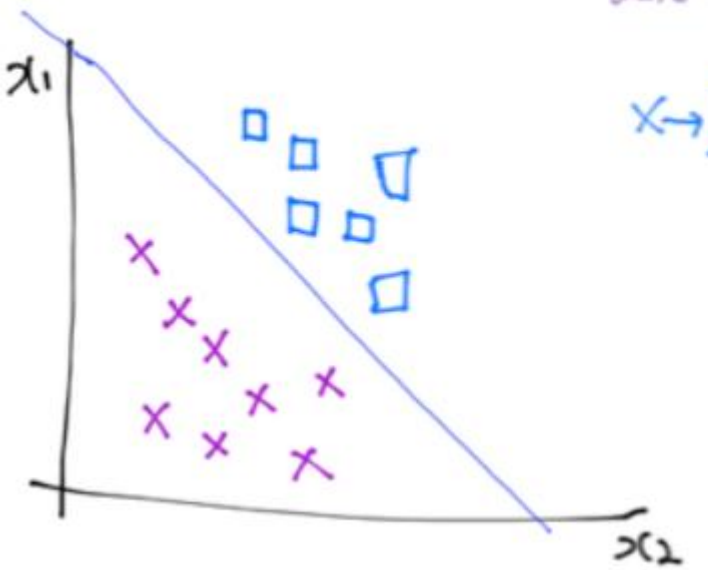
  (3) 데이터 변환의 필요성:
  - 독립 변수나 종속 변수가 특정 분포(예: 비정규 분포)를 가진다면, 데이터 변환(예: 로그 변환, Box-Cox 변환)이 필요할 수 있다.
  - 변환을 하지 않으면 잔차의 정규성이 깨질 가능성이 크다.

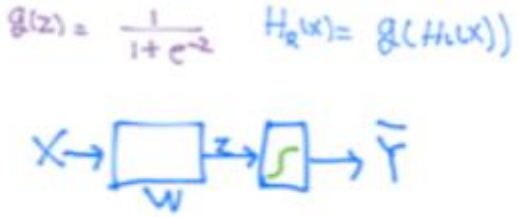
  (4) 다중공선성(Multicollinearity):
  - 독립 변수들 간 강한 상관관계가 있는 경우, 잔차가 정규성을 벗어나면서도 모델 자체는 유의미한 결과를 보여줄 수 있다.

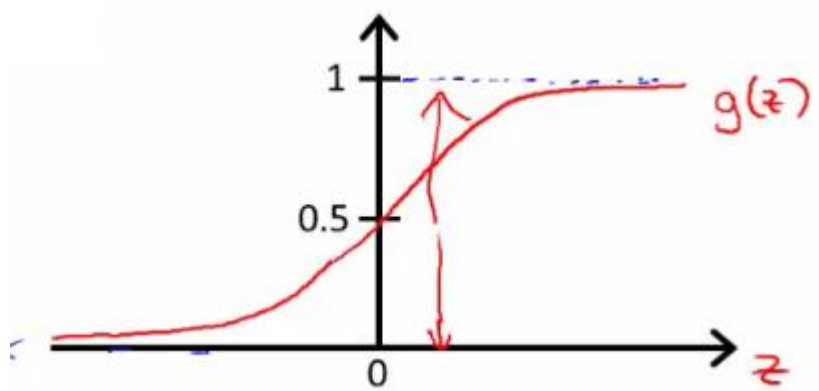
  (5) 해결방안:
  - 비선형 모델 사용, 이상치 제거, 데이터 변환 시도, 높은 상관관계 변수 제거, 등

Linear Classification

- **Logistic Regression Classifier (Binary)**







- Since this is a binary classification task we know y = 0 or 1
  - So the following must be true
    - $P(y=1|x;\theta) + P(y=0|x;\theta) = 1$
    - $P(y=0|x;\theta) = 1 - P(y=1|x;\theta)$

Ref: http://holehouse.org/mlclass/06_Logistic_Regression.html

Linear Classification

- **결정 경계(Decision Boundary)**
  - 2차원: $f = w_1x_1 + w_2x_2 + b = 0$ 은 직선
  - 3차원 데이터라면 평면이 되고, 그 이상의 고차원 데이터에서는 초평면(Hyperplane)
  - 클래스 분류: f>0 은, f<0 이면 0 으로 분류
  - Perceptron: 활성화 함수인 계단 함수(Step-Function)는 뉴런이 활성화되는지 여부만 판단하는 매우 단순한 역할임.
  - SVM(Support Vector Machine): 확률을 위해서는 플랫 스케일링 (SVM 출력 거리값을 별도의 Logistic Regression 에 훈련시켜 얻는다.) (ex) model = SVC(kernel='rbf', probability=True)
- 바로 적용하지 않는 경우가 많을까?
  - 확률적인 의미가 없다. (예: f=0.1 과 f=0.99 모두 클래스 1으로 예측)
  - 모델의 확신도를 해석하기 어렵다. (점수 자체로는 신뢰도 파악 어려움)
- 해결책:
  - 활성화 함수 (Activation Function): logistic Regression(sigmoid): $P(y=1|x) = \sigma(f) = \frac{1}{1+e^{-f}}$

Linear Classification

- **Logistic Regression Classifier (Binary)**

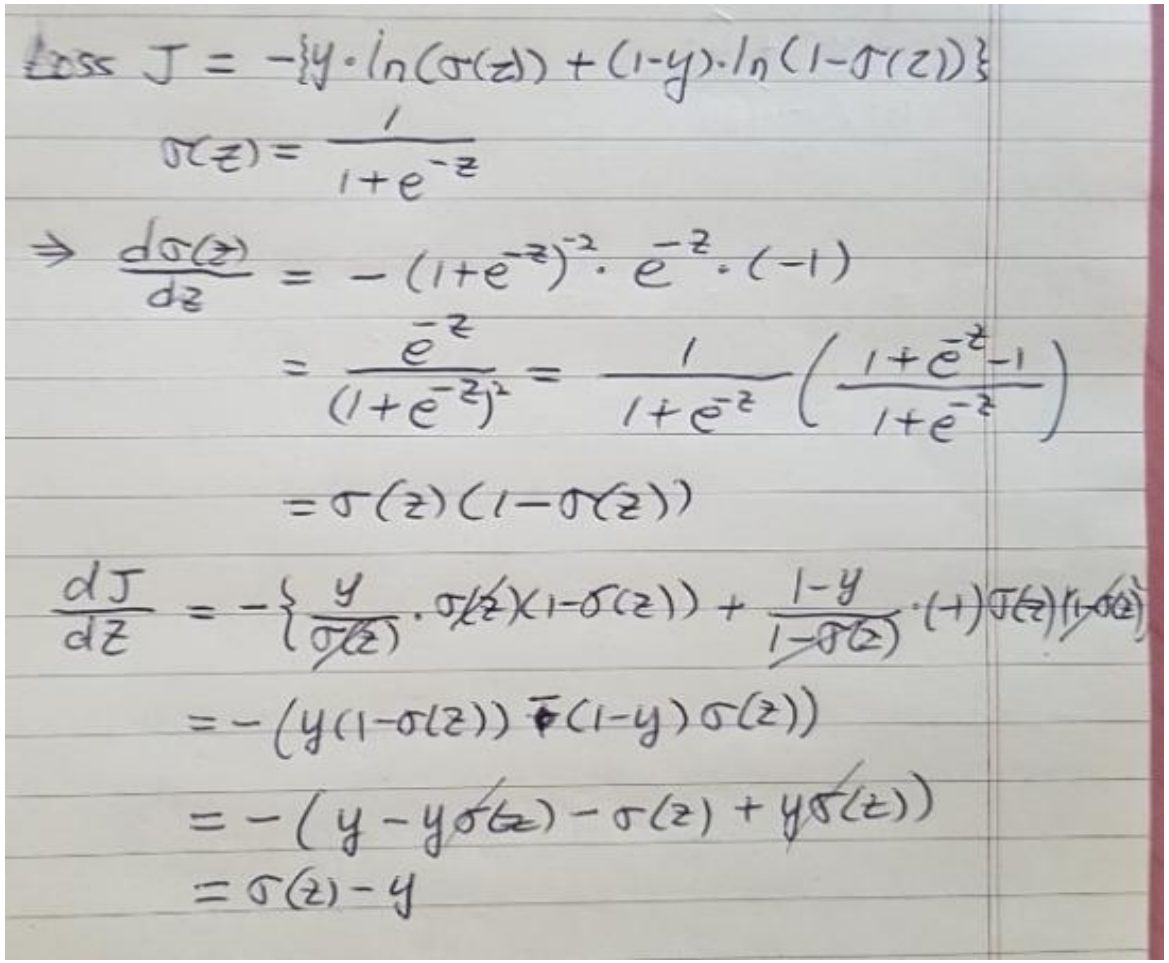
Binary cross entropy loss function:

$$J(\hat{y}) = \frac{-1}{m}\sum_{i=1}^{m} y_i \log(\hat{y}_i) + (1 - y_i)(\log(1 - \hat{y})$$

where

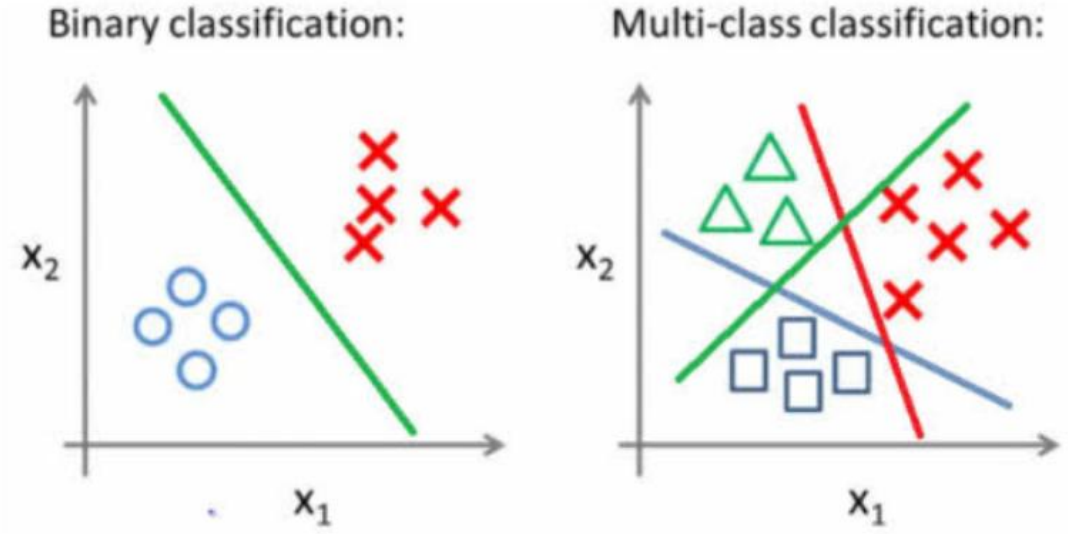
m = number of training examples
y = true y value
$\hat{y}$ = predicted y value

dJ/dw1 = (y_pred – y)*w1
dJ/dw2 = (y_pred – y)*w2
dJ/db = (y_pred – y)*1



Linear Classification

- **Binary classification vs. Multi-class classification**



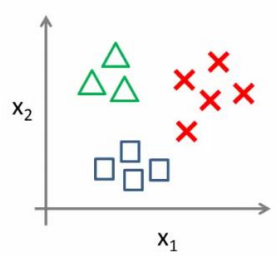
- Multi-class classification (with *n*-classes)
  - One vs. All: *n* binary classifier models (preferred)
    but prone to creating an imbalance
  - One vs. One: ${}_nC_2 = n*(n-1)$ binary classifier models

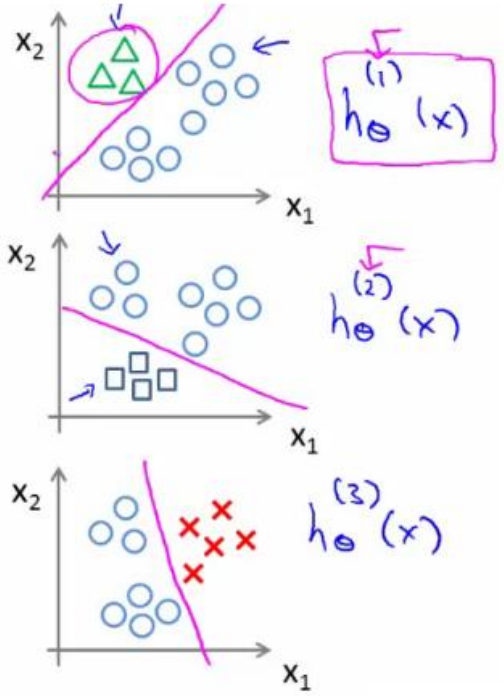
https://towardsdatascience.com/multi-class-classification-one-vs-all-one-vs-one-94daed32a87b

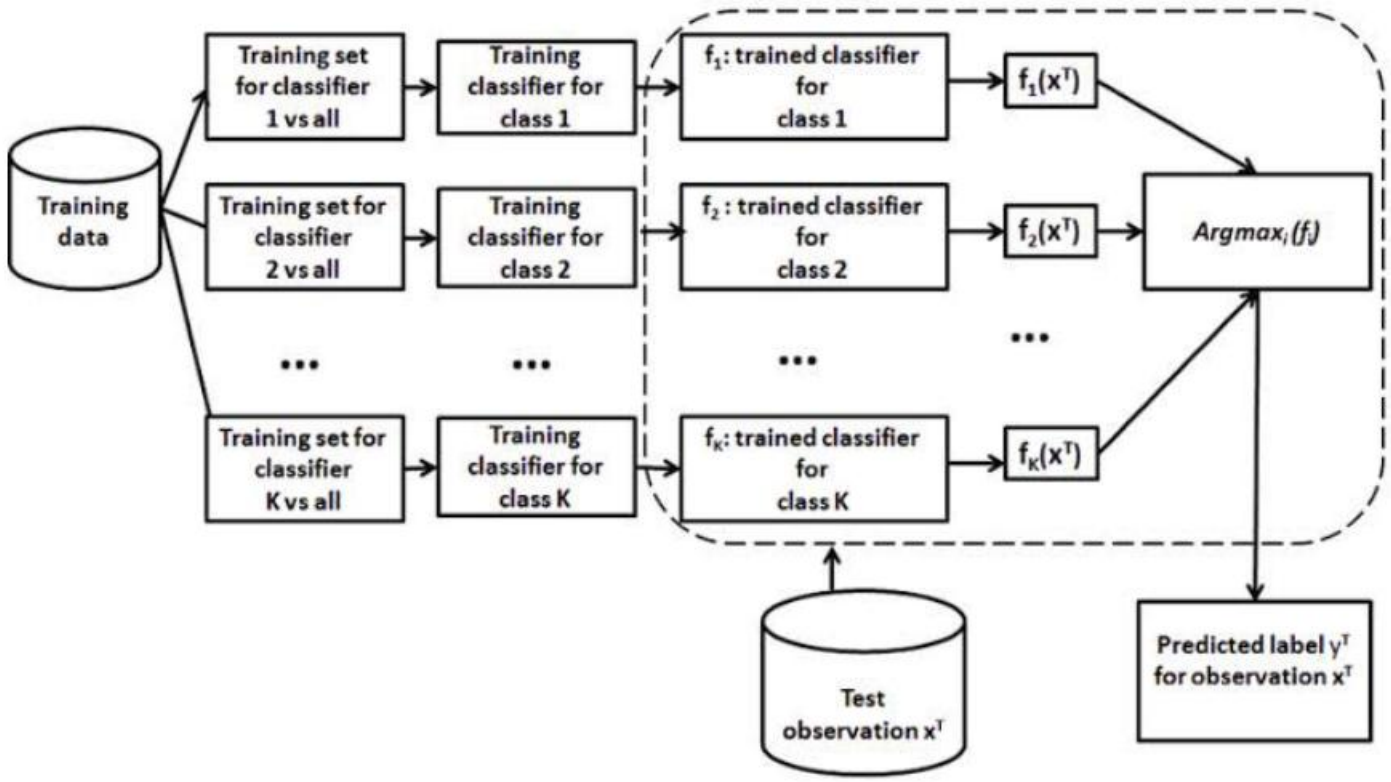
Linear Classification

- **Multinomial (Multi-class) Classifier (One-vs-Rest or One-vs-All)**

  (ex) LogisticRegression(multi_class='ovr')







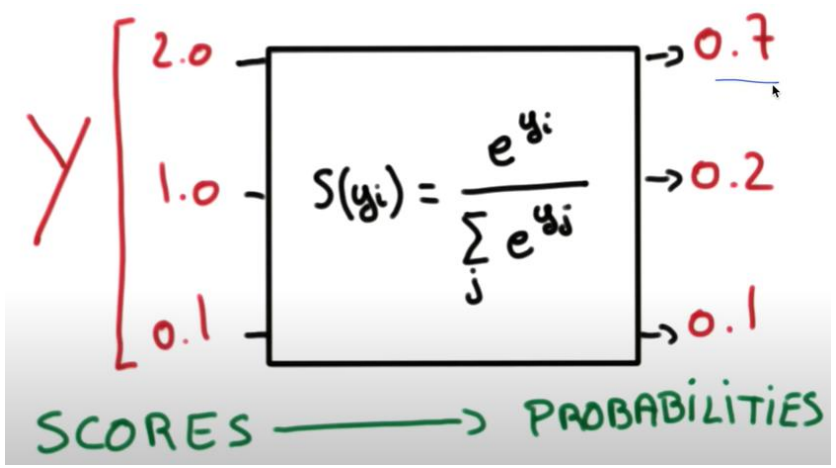
Overall

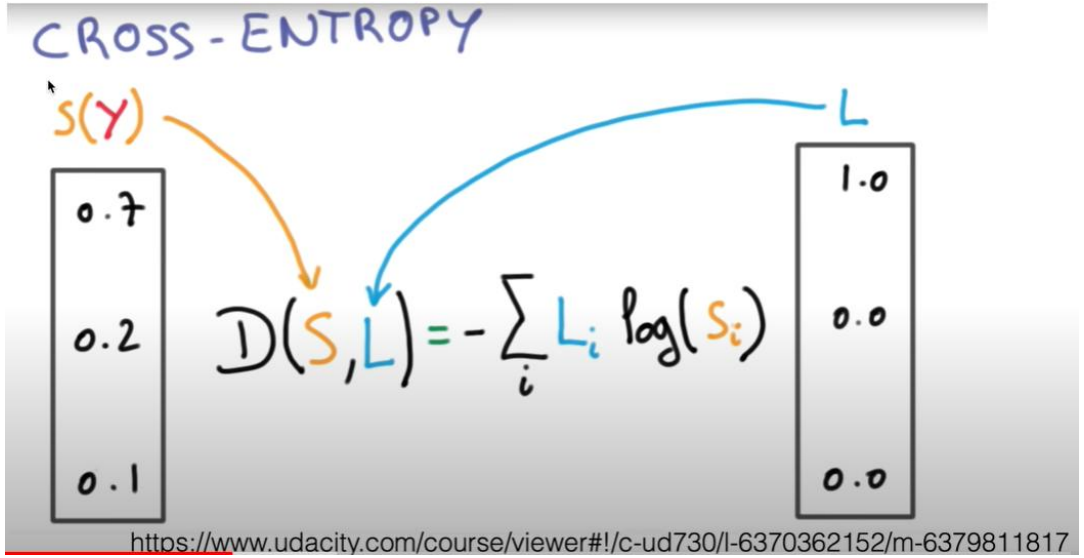
- Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class i to predict the probability that y = i
- On a new input, x to make a prediction, pick the class i that maximizes the probability that $h_\theta^{(i)}(x) = 1$

https://towardsdatascience.com/multi-class-classification-one-vs-all-one-vs-one-94daed32a87b

Logistic Regression and Softmax Regression

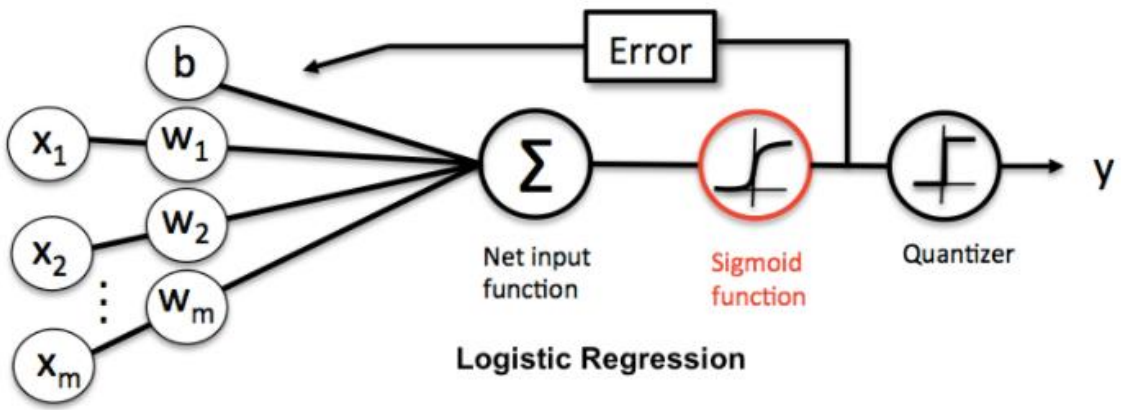
- **Softmax (regression) Classifier**
  - Multi-class version of Logistic Regression
  - Also called: **Multinomial Logistic**, Maximum Entropy Classifier, **Multi-class Logistic Regression**
  - Generalization of logistic regression (assuming that the classes are mutually exclusive)
  - **Uses Categorical cross entropy**



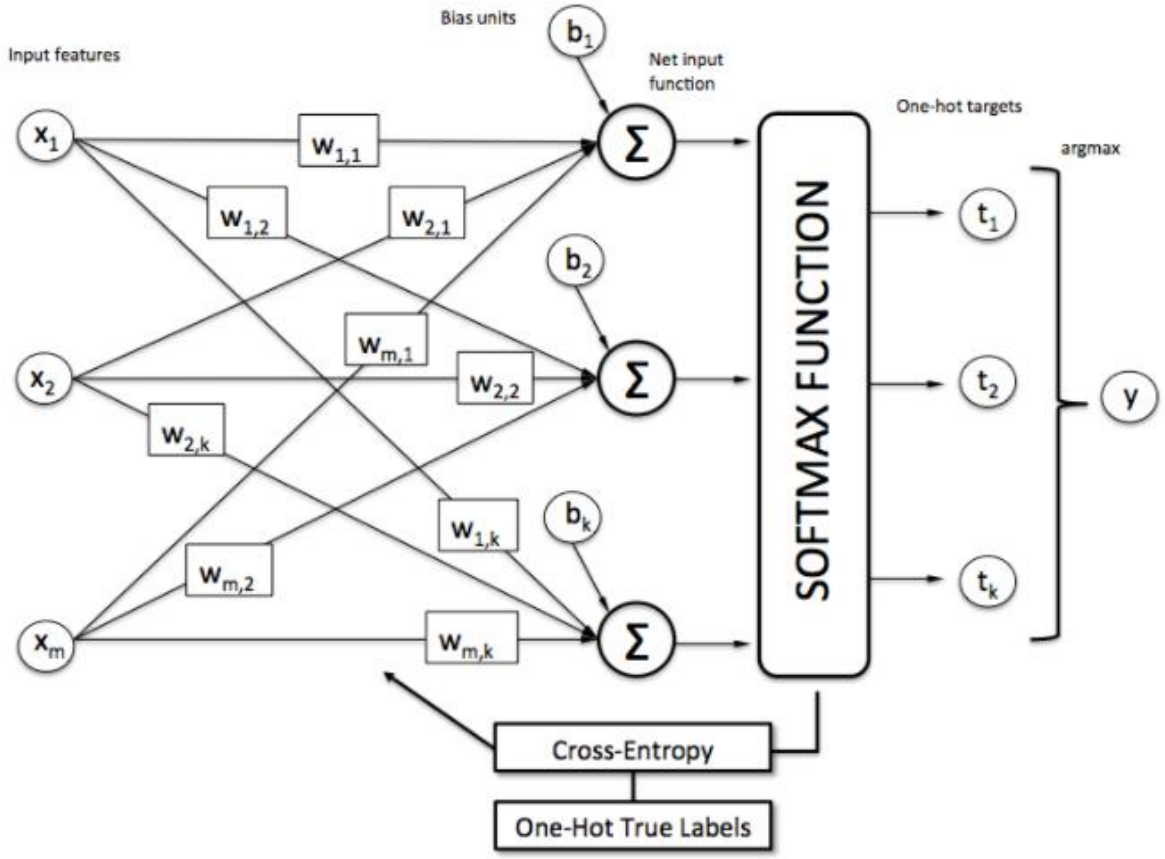


Logistic Regression and Softmax Regression

- Binary
- Multi-class



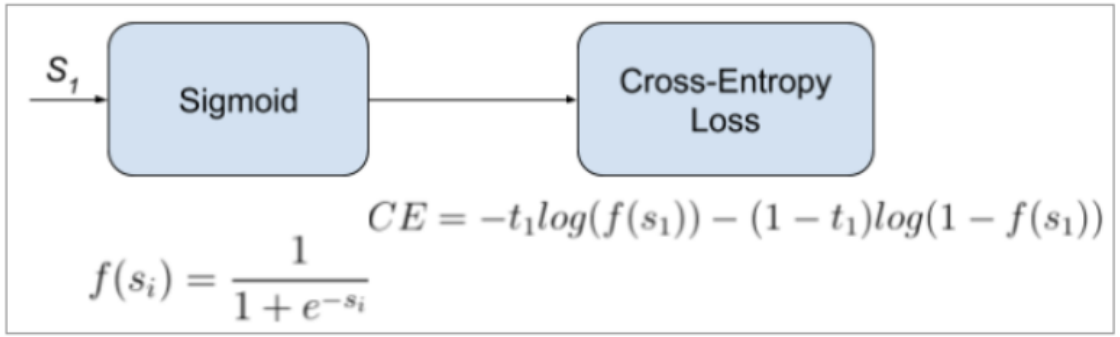
Logistic Regression



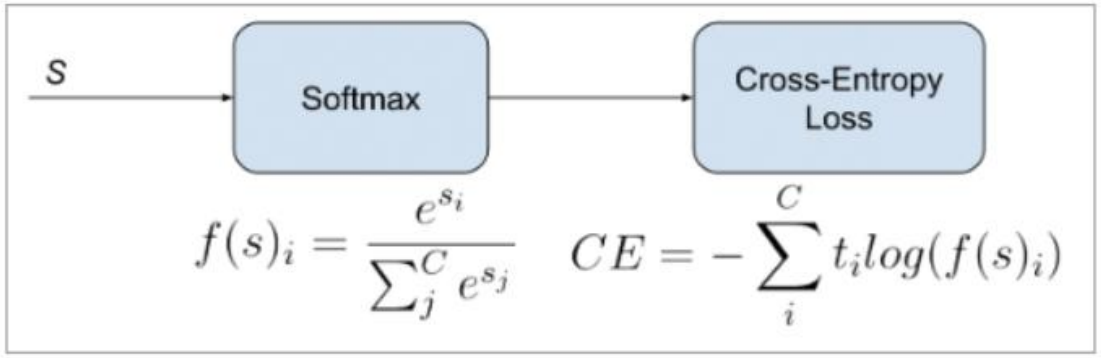
Softmax Regression

Logistic Regression and Softmax Regression

- **Cross Entropy (CE)**
  - Binary CE

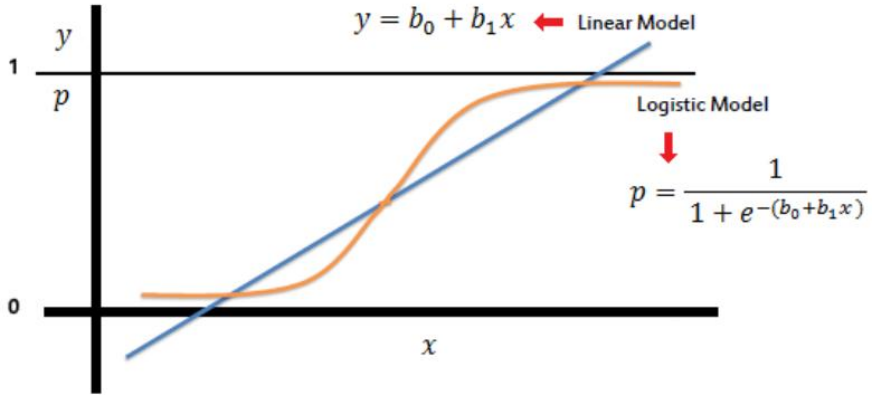


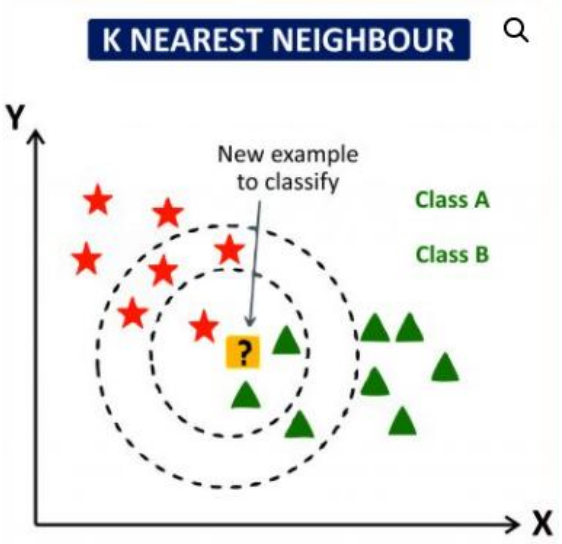
  - Categorical (Multi-class) CE

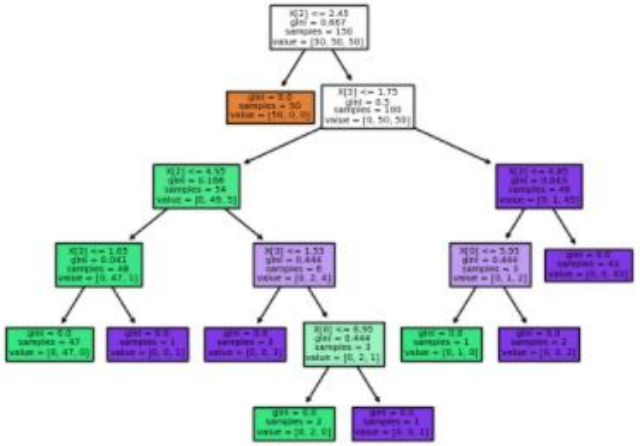


Nonlinear Classification Models

- **Classification algorithms (linear and nonlinear)**
  - Logistic Regression Classifier
  - Knn (k-nearest neighbor)
  - Decision Tree
  - Ensemble
  - SVM

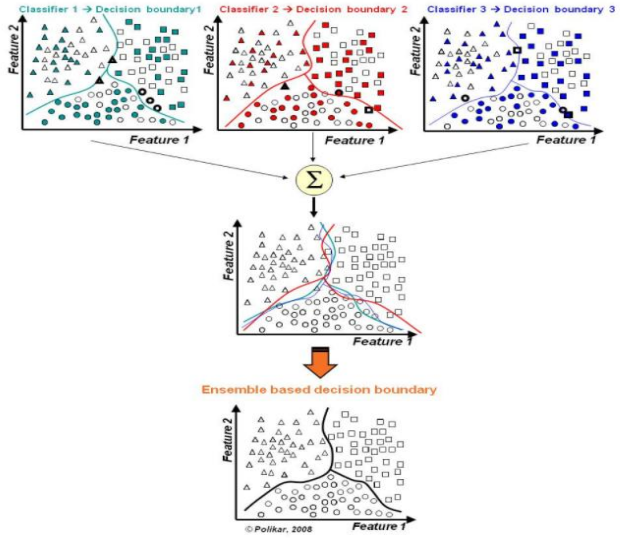




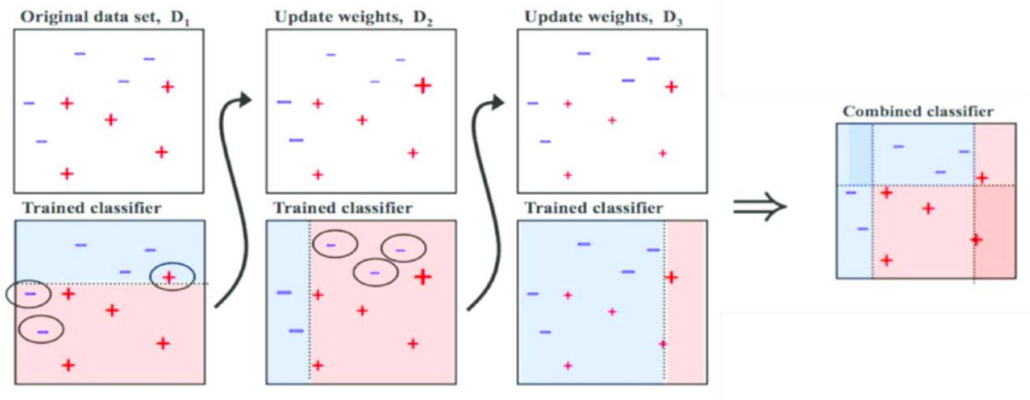


Nonlinear Classification

- **Ensemble method**
  - Combine many weak learners
  - Bagging: learns them independently in parallel and average them (ex: Random Forest)
  - Boosting: learns them sequentially in adaptive way and combines them (ex: Gradient Boost)



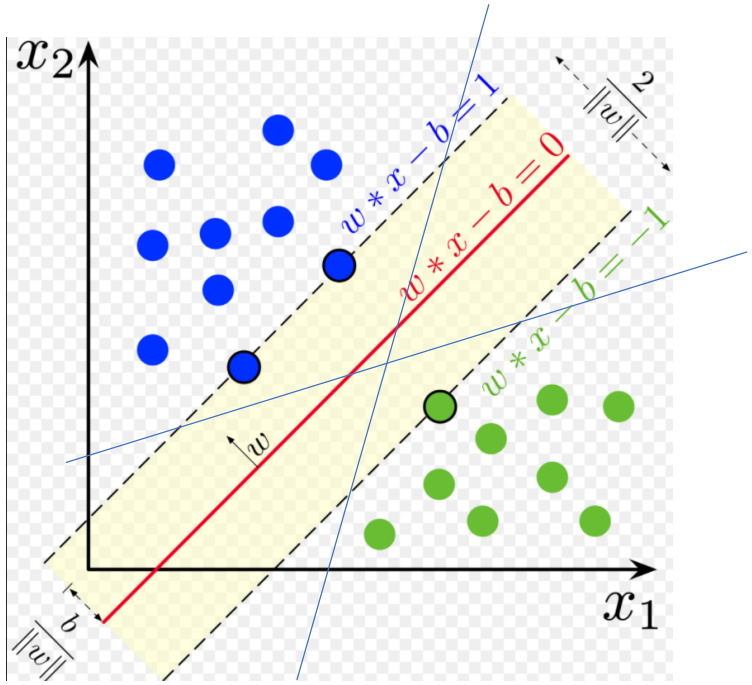
출처: https://swalloow.github.io/bagging-boosting

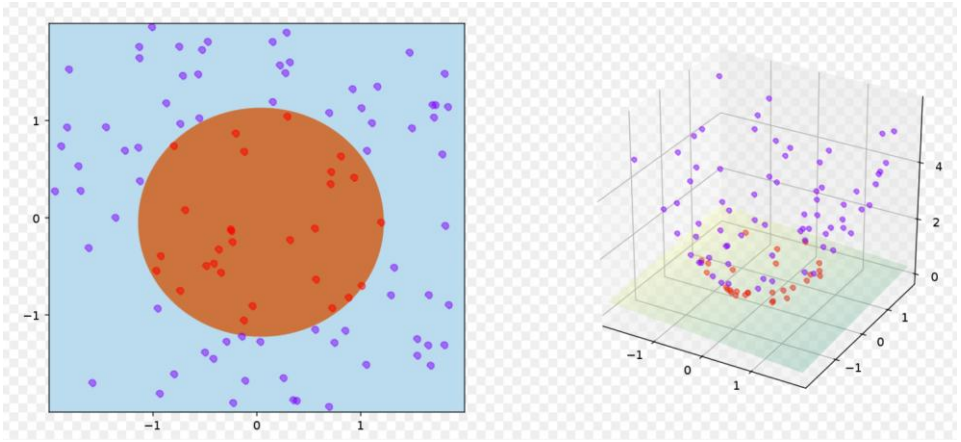


출처: Medium (Boosting and Bagging explained with examples)

Nonlinear Classification

- **SVM (Support Vector Machine)**
  - Finds a maximum-margin hyperplane
  - Linear SVM
  - Nonlinear SVM: use kernel (polynomial, sigmoid, rbf)

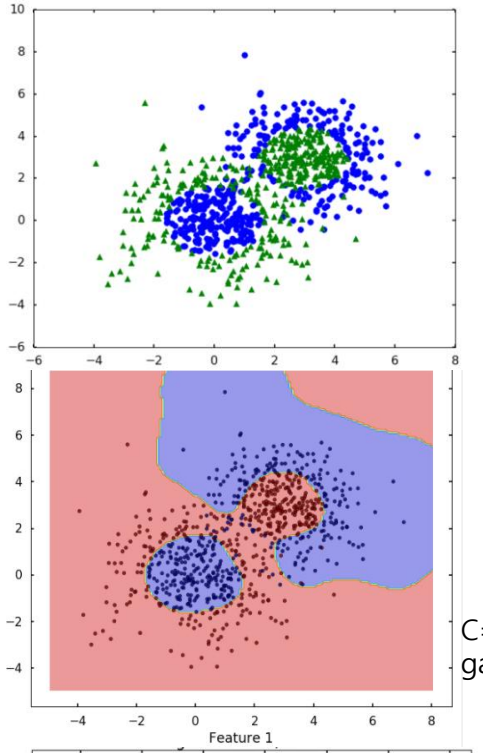


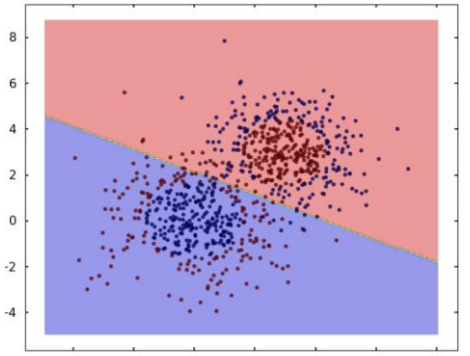


SVM with kernel given by $\varphi((a, b)) = (a, b, a^2 + b^2)$

Nonlinear Classification

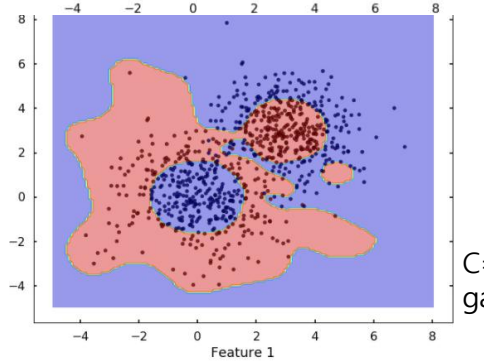
- **SVM (continued)**
  - '**rbf**' kernel (hyperparameters: C and gamma)
  - C: tradeoff between classification error and simplicity of the boundary
  - gamma: defines how far the influence of a single example reaches (high value is 'close')
  - class_weight: imbalance cases



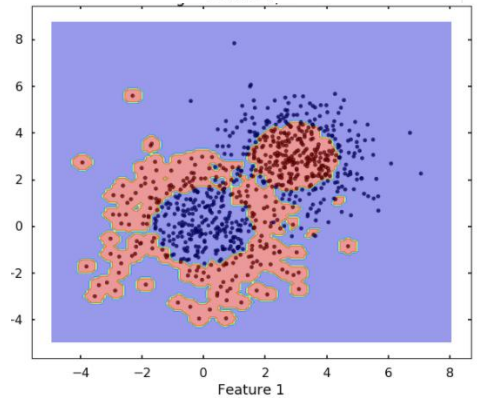


linear

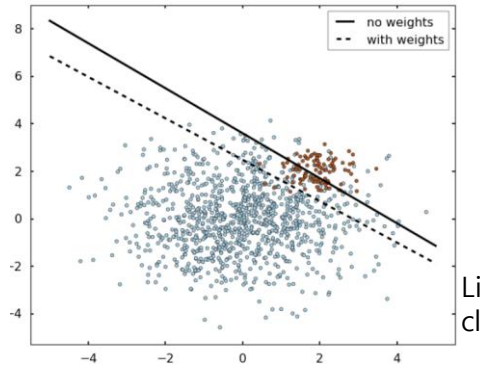
C=1
gamma=0.5



C=10000
gamma=0.5

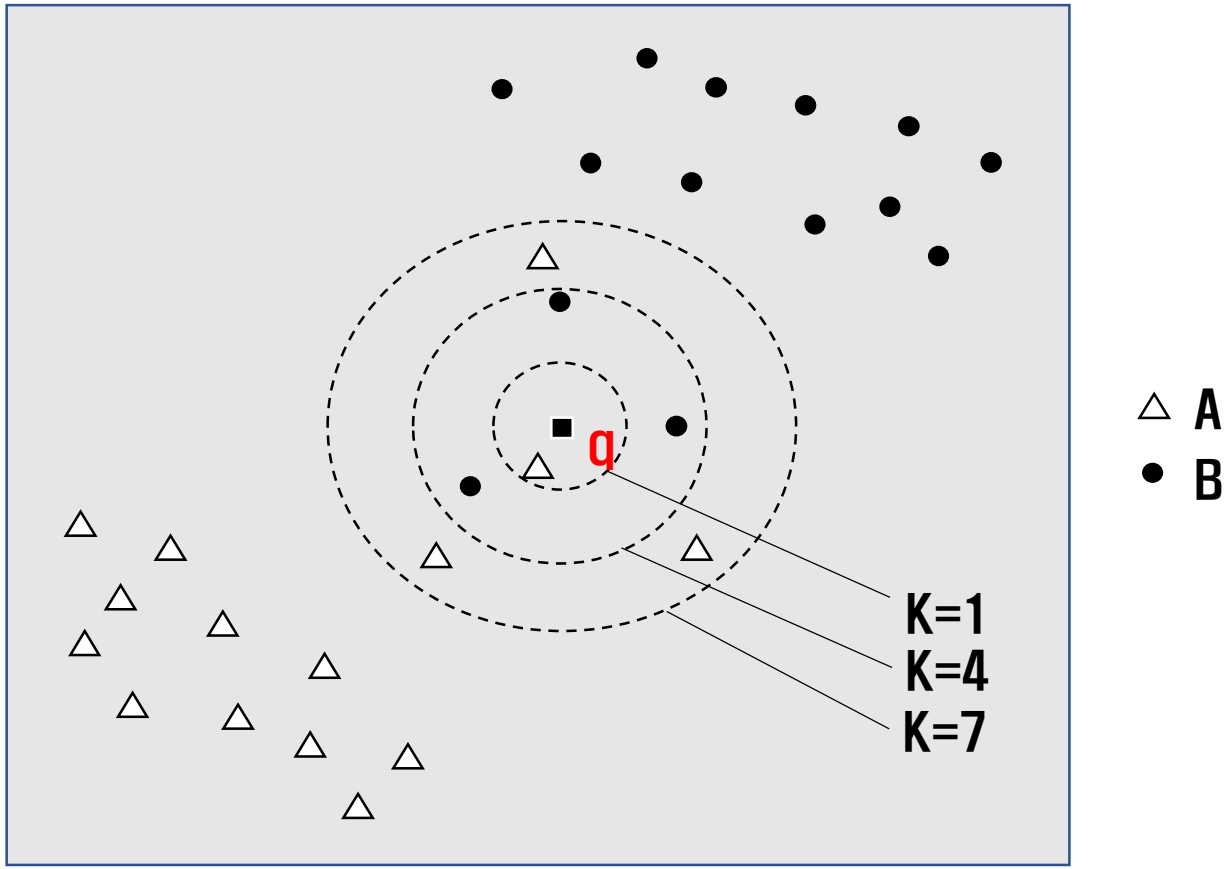


C=1
gamma=50



Linear with
class_weight=1:10

Knn (K-Nearest Neighbor)



Knn (K-Nearest Neighbor)

- kNN의 장점
  - 훈련시간이 거의 없다
  - 알고리즘의 개념이 명확
  - 모델링에 필요한 하이퍼파라미터 : k 값 하나뿐
  - 특성 변수만 잘 선정하면 예측 성능도 좋다.
- kNN의 단점
  - 분류를 처리하는 시간, 즉 알고리즘을 수행하는 시간이 길다.
  - 확보한 샘플들을 모두 비교해서 어떤 그룹에 가까운 지 새로 계산해야 한다.
  - 또한 새로운 샘플이 계속 추가될 때마다 가까운 이웃이 달라진다.
  - Lazy 알고리즘: 나중에 계산량이 많은 알고리즘
- 개선책: 샘플들간의 거리에 대한 가중치를 고려
  - 가까이 있는 이웃에 대해서는 가중치를 크게

Decision Trees

- **Decision Tree**
  - Handles each feature independently
  - Both Regression and Classification
  - Use Classification And Regression Tree (CART) algorithm to train Decision Trees
- **CART algorithm**
  - first splits the training set in two subsets using a single feature k and a threshold t_k
  - How to choose it? It searches for the pair (k, t_k) for purest subsets (greedy)
  - It splits the subsets using the same logic recursively.

Equation 6-2. CART cost function for classification

$$J(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}}$$

where $\begin{cases} G_{\text{left/right}} \text{ measures the impurity of the left/right subset,} \\ m_{\text{left/right}} \text{ is the number of instances in the left/right subset.} \end{cases}$

Decision Trees

- 결정트리는 나누려는 그룹의 순도가 가장 높아지도록 그룹을 나누어야 한다.
- 불순도(Impurity): 해당 범주 안에 서로 다른 데이터가 얼마나 섞여 있는지의 정도
- 그룹의 불순도를 표현
  - 지니(Gini) 계수

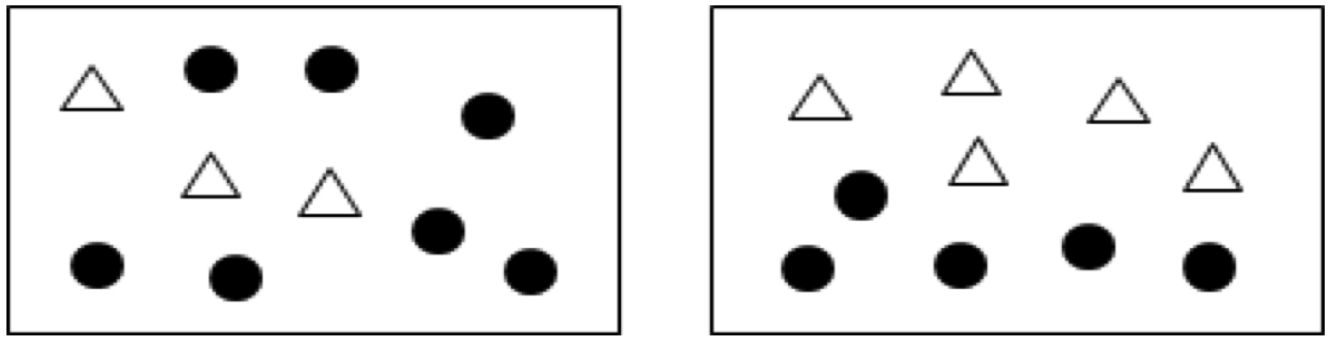
$$Gini = 1 - \sum_{k=1}^{m} p_k^2$$

  - 엔트로피(entrophy)

$$Entropy = -\sum_{k=1}^{m} p_k \log_2(p_k)$$

  - 성능은 비슷하지만 연산 속도는 Gini 가 빠름 (log 연산 없음)

Decision Trees

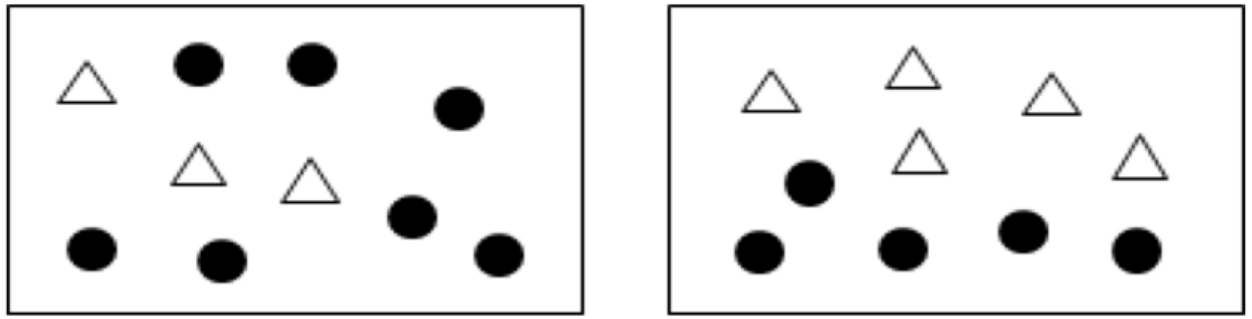


좌측 박스: $\text{지니}(7:3) = 1 - \left[\left(\frac{7}{10}\right)^2 + \left(\frac{3}{10}\right)^2\right] = 1 - (0.49 + 0.09) = 0.42$

우측 박스: $\text{지니}(5:5) = 1 - \left[\left(\frac{5}{10}\right)^2 + \left(\frac{5}{10}\right)^2\right] = 1 - (0.25 + 0.25) = 0.5$

(*) worst: 0.5
Best: gini=0 (all in one class)

Decision Trees

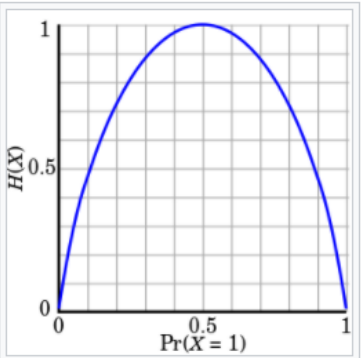


$$Entropy = -\sum_{k=1}^{m} p_k \log_2(p_k)$$

$$\text{좌측}(7:3) = -\left[0.7^*\log_2(0.7) + 0.3^*\log_2(0.3)\right]$$
$$= -\left[(-0.36) + (-0.52)\right] = -(-0.88) = 0.88$$

$$\text{우측}(5:5) = -\left[0.5^*\log_2(0.5) + 0.5^*\log_2(0.5)\right]$$
$$= -\left[(-0.5) + (-0.5)\right] = -(-1) = 1$$

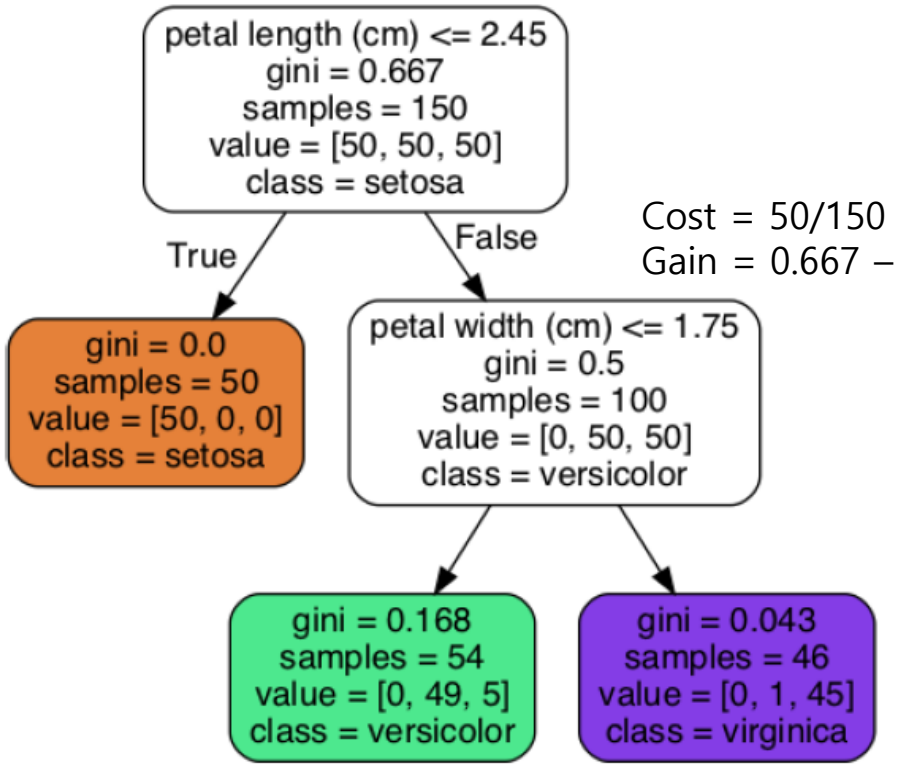
(*) worst: 1



Entropy of a Bernoulli trial as a function of binary outcome probability, called the **binary entropy function**.

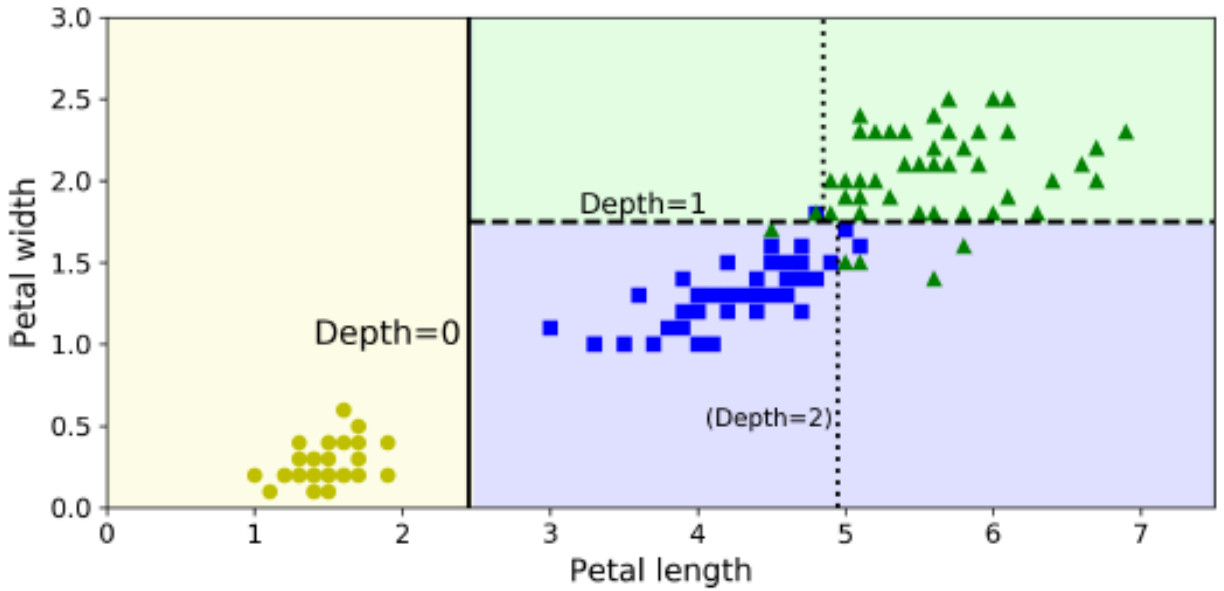
Decision Trees

Gini = 1 – $[(1/3)^2 + (1/3)^2 + (1/3)^2]$
= 0.667



Cost = 50/150 * 0 + **100/150 * 0.5** = 0.333
Gain = 0.667 – 0.333 = 0.334

Cost = 54/100 * 0.168 + 46/100 * 0.043 = 0.11
Gain = 0.5 – 0.11 = 0.39



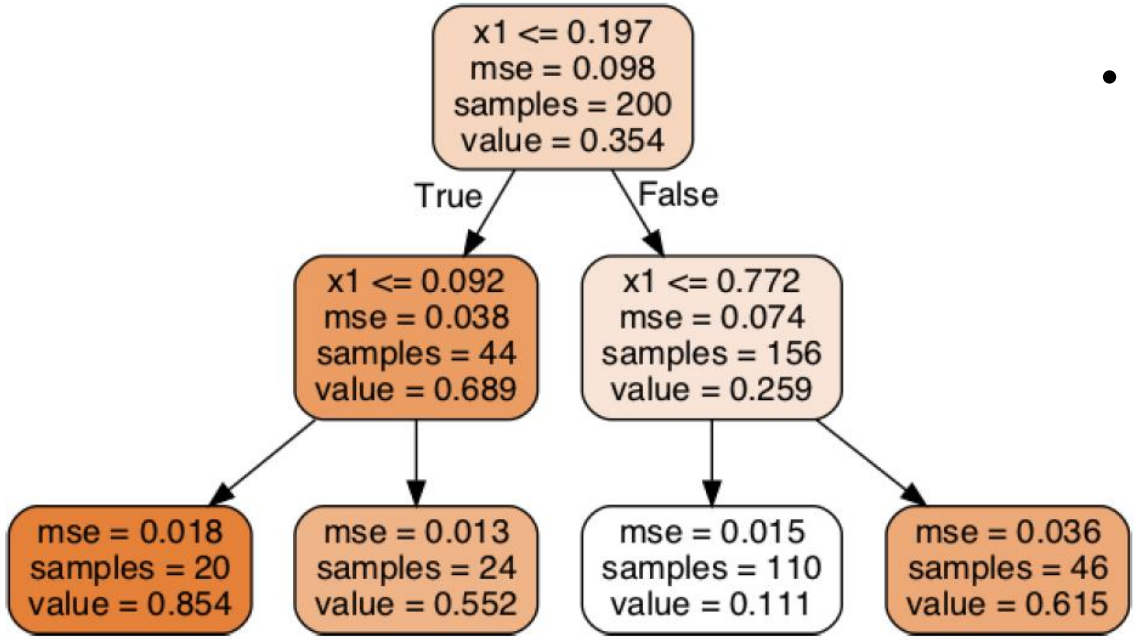
Decision Trees

- **Hyper-Paramters**
  - max_depth: 트리의 최대 깊이 (이보다 깊은 트리를 만들지 않는다)
  - max_leaf_nodes: 리프 노드의 최대 수 (리프 노드를 이보다 많이 만들지 않는다)
  - max_samples_split: 분할하기 위한 최소 샘플수 (이보다 작으면 분할하지 않는다)
  - min_samples_leaf: 리프 노드에 포함될 최소 샘플수 (이보다 작은 노드는 만들지 않는다)
  - max_features: 최대 특성수 (분할할 때 이보다 적은 수의 특성만 사용한다)
- **Internal Parameters**
  - 결정 트리 모델을 만든 후에, 어떤 특성이 결정 트리를 생성할 때 중요한 역할을 했는지 비중을 파악 가능
  - 이 결과를 보고 중요하지 않은 특성은 향후에 제외하기도 함 (Feature Selection)
  - 내부 변수로 확인: feature_importances_

Decision Trees

- **Computational complexity**
  - Prediction: traversing the Decision Tree from the root to a leaf
  - Training: compares all features on all samples at each node
  - Finding the optimal tree is known to be NP-complete (O(exp(m)).
  - Use the Greedy algorithm.

Decision Tree Regression

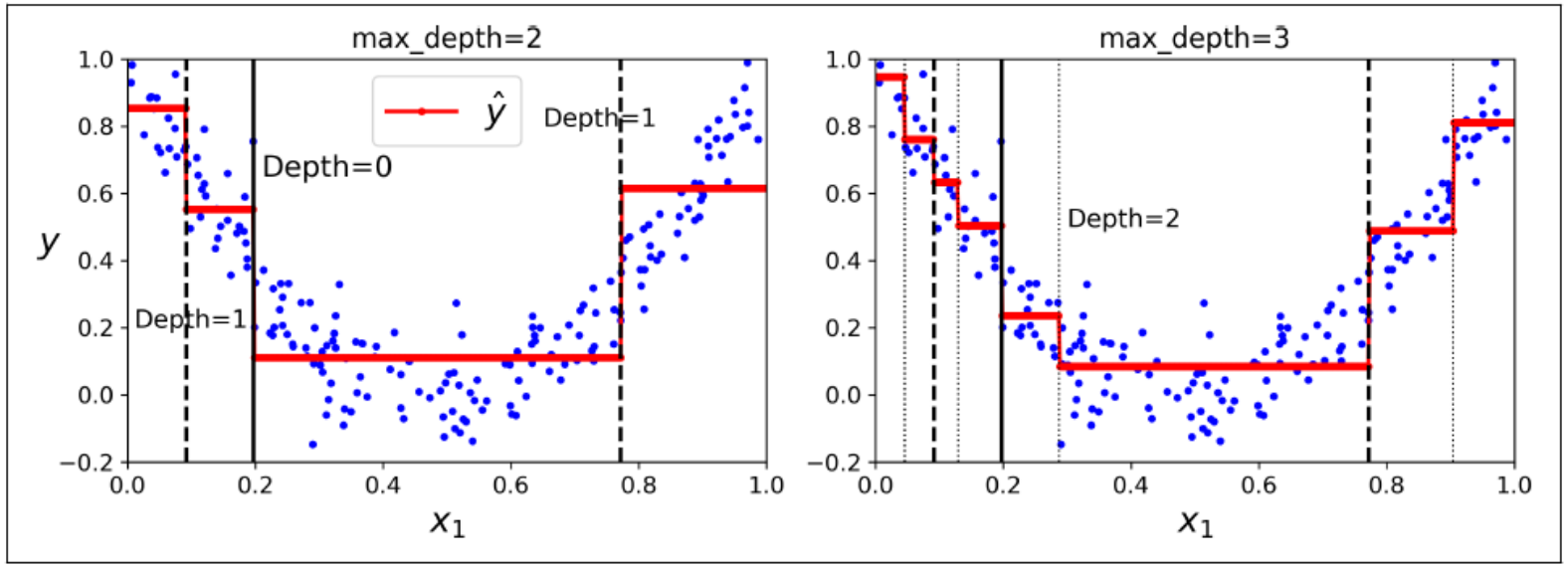


- It now tries to split the training set in a way that **minimizes the MSE**. (instead of minimizing impurity)

Equation 6-4. CART cost function for regression

$$J(k, t_k) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}} \quad \text{where} \begin{cases} \text{MSE}_{\text{node}} = \sum_{i \in \text{node}} \left(\hat{y}_{\text{node}} - y^{(i)}\right)^2 \\ \hat{y}_{\text{node}} = \frac{1}{m_{\text{node}}} \sum_{i \in \text{node}} y^{(i)} \end{cases}$$

Decision Tree Regression

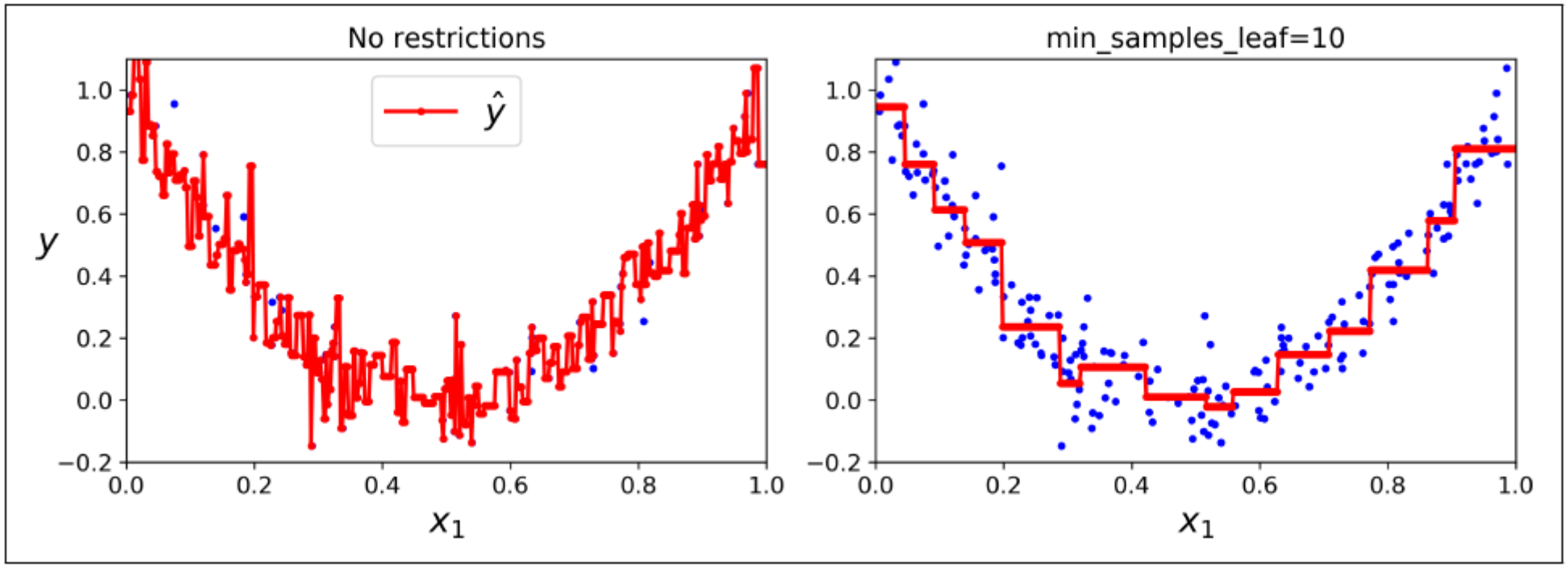


Equation 6-4. CART cost function for regression

$$J(k, t_k) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}} \quad \text{where} \begin{cases} \text{MSE}_{\text{node}} = \sum_{i \in \text{node}} \left(\hat{y}_{\text{node}} - y^{(i)}\right)^2 \\ \hat{y}_{\text{node}} = \frac{1}{m_{\text{node}}} \sum_{i \in \text{node}} y^{(i)} \end{cases}$$

Decision Tree Regression

- **Regularizing the Model**



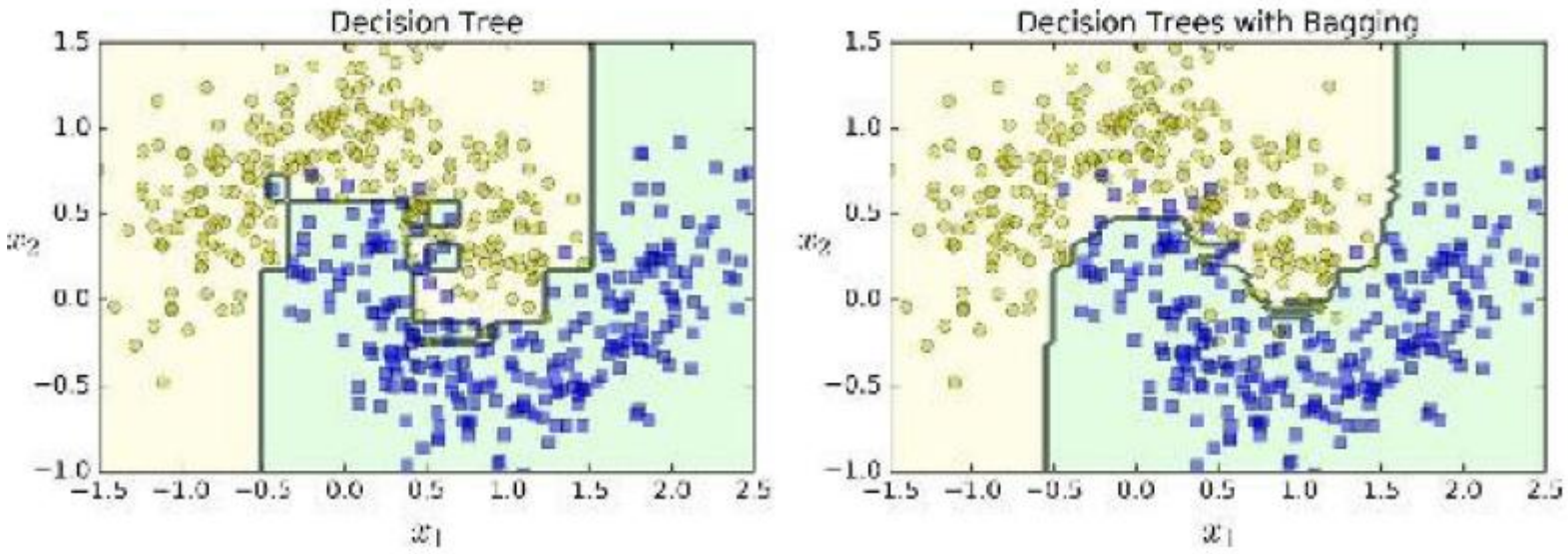
Ensemble Models

- **Ensemble method:**
  - to aggregate the predictions of each classifier and predict the class that gets the most votes (Hard Voting: 직접투표) or Majority Voting
    - May work better in cases where there are some outliers.
  - to predict the class with the highest class probability, averaged over all the individual classifiers (Soft Voting: 간접투표)

	P일 확률	Q일 확률	판정결과 (Hard Voting)
세부 모델 A	0.9	0.1	P
세부 모델 B	0.4	0.6	Q
세부 모델 C	0.3	0.7	Q
확률의 평균 (Soft Voting)	(1.6)/3 = 0.533	(1.4)/3 = 0.456	P or Q

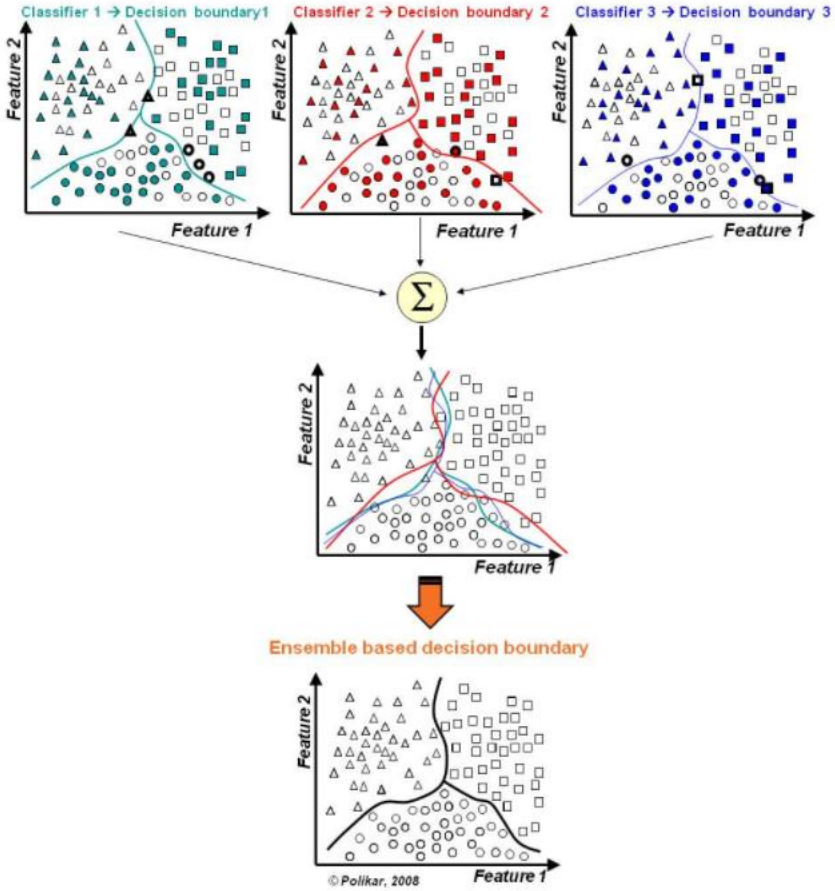
Ensemble Models

- **Decision Tree and Decision Tree with Bagging**
  - Moon dataset with 500 decision trees
  - The ensemble has a comparable bias, but a smaller variance. (roughly the same number of errors on the training set, but the decision boundary is less irregular)



Ensemble Models

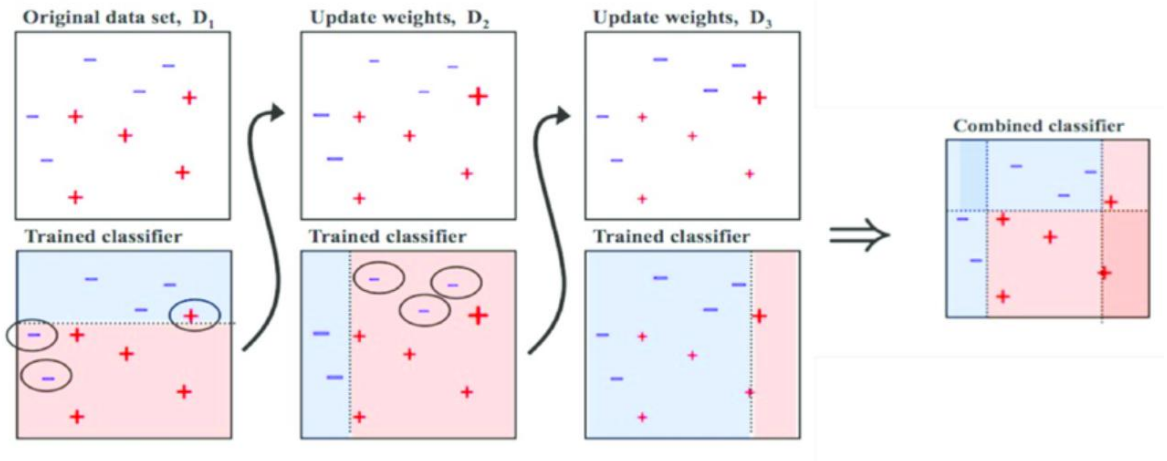
- **Bagging: 중복을 허용**
  - 중복을 허용한 n 개의 샘플을 추출하여 평균을 구하는 작업을 m 번 반복.
  - Overfitting 을 효율적으로 줄이고 일반적인 모델을 만드는데 집중.
  - Parallel fashion
  - (ex) RandomForest (with majoity Voting)



출처: https://swalloow.github.io/bagging-boosting

Ensemble Models

- **Boosting:**
  - Bagging은 독립적인 input data를 가지고(복원 추출) 독립적으로 예측하지만, 부스팅은 **이전 모델이 다음 모델에 영향을 준다. (틀린 부분에 더 큰 가중치)**
  - Serial fashion
  - Bagging과 다르게 일반적인 모델에 집중되어 있지 않고, 맞추기 어려운 문제를 맞추는데 초점
  - (ex) XGBoost, AdaBoost, GradientBoost



출처: Medium (Boosting and Bagging explained with examples)

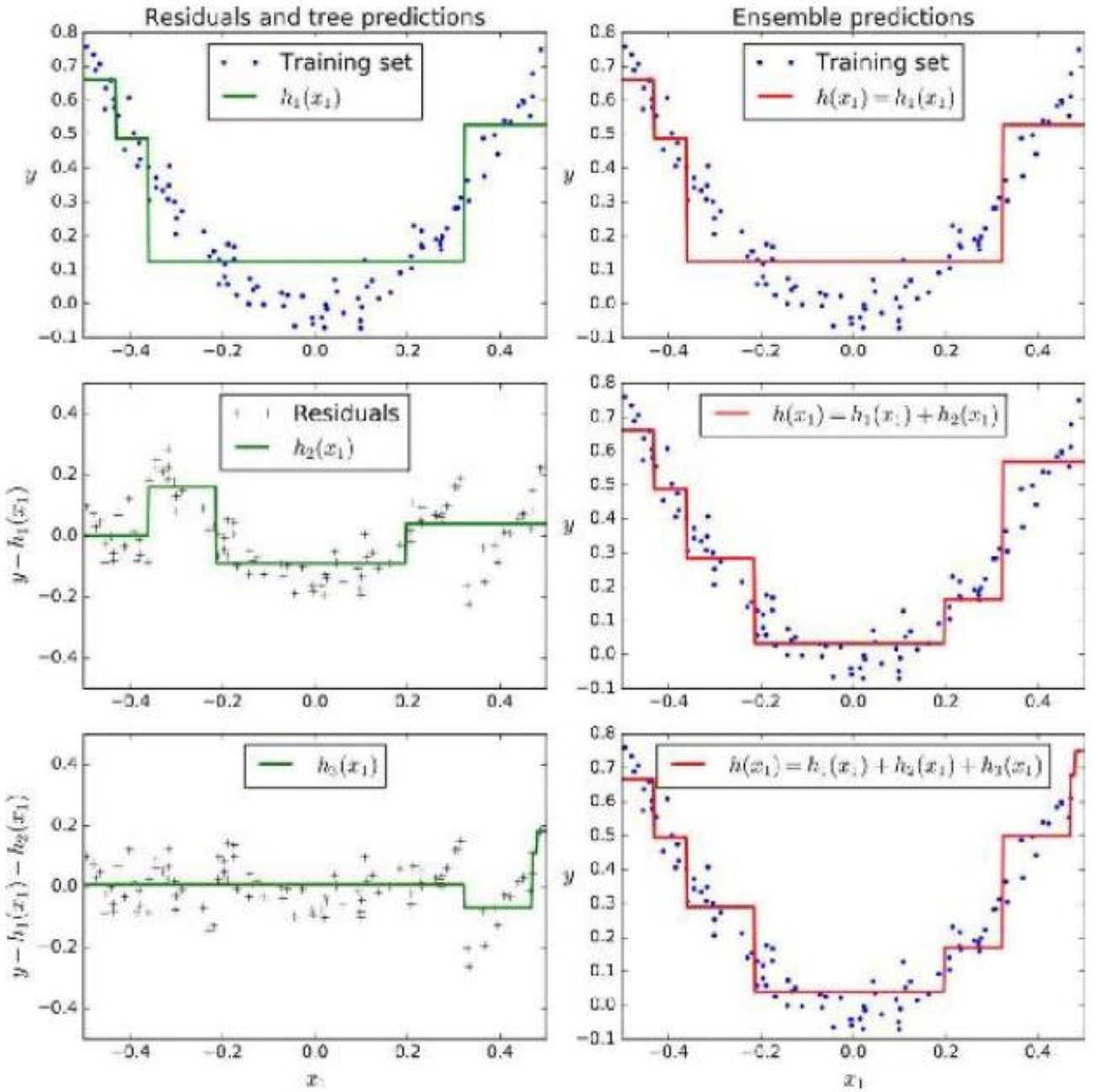
Ensemble Models

- **Adaboost classifier**
  - pays a bit more attention to the training instances that the predecessor underfitted.
  - This results in new predictors focusing more and more on the hard cases.
  - the new predictor's weight is computed, the instance weights are updated, then another predictor is trained, and so on

1. Initialize the obervation weights $w_i = 1/N$
2. For $m = 1, 2, \ldots, M$
   - Train $G_m(x)$
   - Compute the weighted error $Err_m = \frac{\sum_{i=1}^{N} w_i \mathcal{I}(y^{(i)} \neq G_m(x^{(i)}))}{\sum_{i=1}^{N} w_i}$ ← Weights on the error (loss)
   - Compute coefficient $\alpha_m = \log\left(\frac{1-err_m}{err_m}\right)$ ← Contribution (weight) of each G(x) (the more accurate, the higher influence)
   - Set data weights $w_i \leftarrow w_i \exp[\alpha_m \mathcal{I}(y^{(i)} \neq G_m(x^{(i)}))]$ ← Higher weight on misclassified
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$ ← Weighted majority vote

Ensemble Models

- **Gradient Boosting Regression Trees (GBRT)**
  - Just like Adaboost, it sequentially adds predictors to an ensemble, each one correcting its predecessor
  - (instead of tweaking the instance weights) It **tries to fit the new predictor to the *residual errors*** made by the previous predictor.
  - Different residual calculation for classification



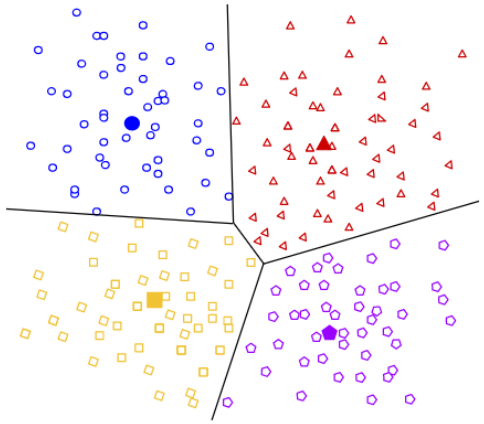
Ensemble Models

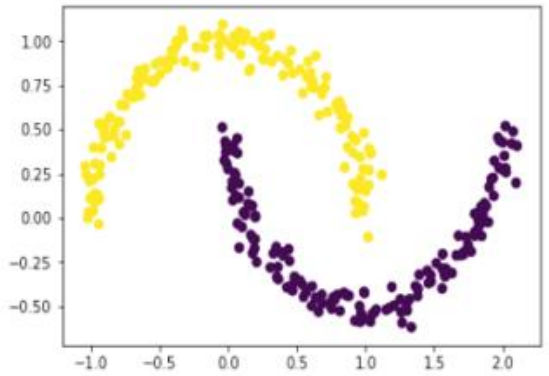
- **배깅(bootstrap aggregation)**
  - 전체 훈련 데이터에서 "중복을 허용"하여 데이터를 샘플링을 하는 방법
  - bootstrap resampling의 줄임말로 부트 스트래핑이라고도 함
  - 목적 : 부족한 훈련 데이터를 효과적으로 늘리기 위함
- **페이스팅(pasting)**
  - 배깅과 달리 주어진 원래 데이터에서 중복을 허용하지 않고, 즉, 한 번 샘플링 된 것은 다음 샘플링에서 제외하는 방식
- 배깅을 수행하면 학습에 선택되지 않는 샘플은 평균 37% 정도
  - 이 샘플을 oob(out of bag) 샘플이라고 함
  - 이 oob 데이터는 훈련에 사용되지 않았으므로 검증에 사용하기에 좋다
- RandomForest:
  - 결정 트리 구조에 배깅을 적용한 방식

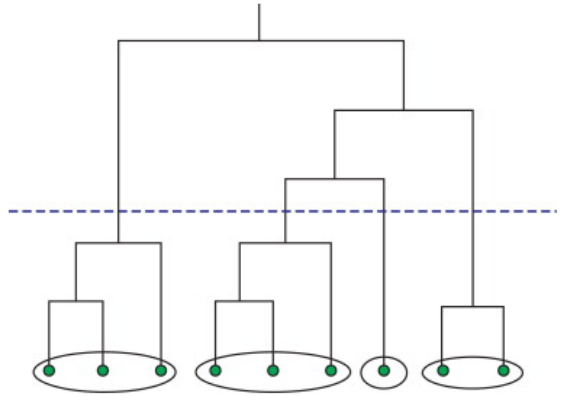
4. Unsupervised Learning

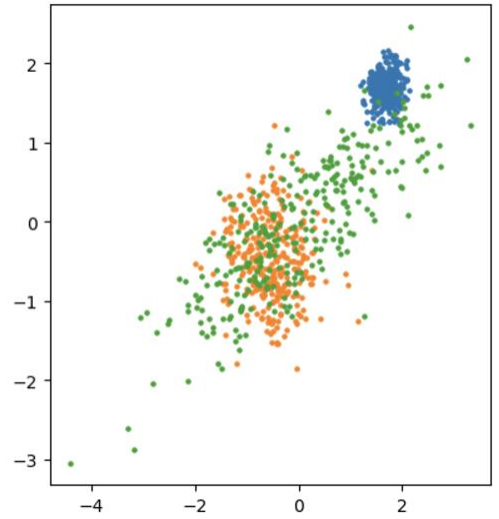
Unsupervised Learning

- **Clustering (or Grouping)**
  - Divide the data points into several clusters based on similarity (유사도)
  - Need scaling as a preprocessing step
  - Applications: detect hackers and criminal activity, identifying fake news, etc.
  - Centroid-based (K-means)
  - Density-based (DBSCAN)
  - Hierarchical (ex: dendrogram)
  - GMM (Gaussian Mixture Model)



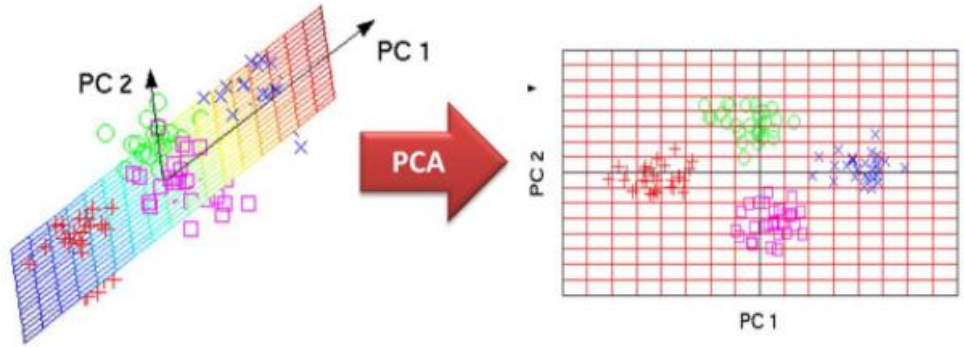






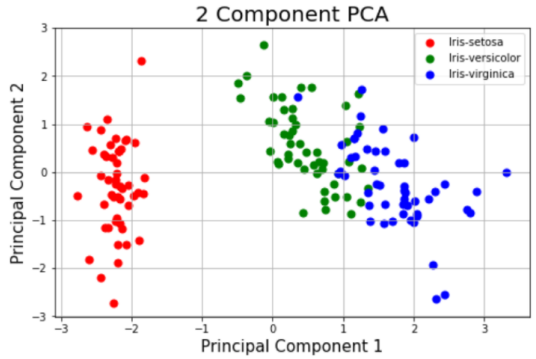
Unsupervised Learning

- **Dimension reduction by PCA**
  - Standard scaling
  - Calculate covariance (or correlation) matrix
  - Eigen-decomposition ($A = P\Lambda P^{-1}$)
  - Select k eigenvectors
  - pca_result = PCA(n_components=2).fit_transform(X_all)
  - Also, tSNE(), Autoencoder
  - SelectPercentile()



	sepal_len	sepal_wid	petal_len	petal_wid	class
145	6.7	3.0	5.2	2.3	Iris-virginica
146	6.3	2.5	5.0	1.9	Iris-virginica
147	6.5	3.0	5.2	2.0	Iris-virginica
148	6.2	3.4	5.4	2.3	Iris-virginica
149	5.9	3.0	5.1	1.8	Iris-virginica

	principal component 1	principal component 2	species
0	-2.264542	-0.505704	Iris-setosa
1	-2.086426	0.655405	Iris-setosa
2	-2.367950	0.318477	Iris-setosa
3	-2.304197	0.575368	Iris-setosa
4	-2.388777	-0.674767	Iris-setosa



Clustering

- 유사도가 큰 항목끼리 묶음
  - 비정상 패턴 (Outlier) 식별에도 사용 (컴퓨터시스템 해커 등)
- Similarity (유사도)
- Need Scaling as a preprocessing step
- K-Means()
- Agglomerative Clustering
- DBSCAN
- Many more …

Clustering

- **Similarity** (유사도) and **Distance** (거리)
  - 항목 간의 유사한 정도를 수치로 표현
  - 유사도 결과에 따라 데이터 분석 결과가 달라짐
  - 분석 경험과 도메인에 대한 이해 필요함
  - 최적의 분석 결과가 나오도록 유사도를 변경해 가면서 반복 수행 필요함
  - 유사도 s(similarity)는 $0 \leq s \leq 1$ (1에 가까울수록 유사도 높음)
  - 유사도의 상대 개념으로 거리(distance) 사용
    - 유사도와 거리의 관계: $d = 1 - s$
  - (ex) A,B,C 중 누가 서로 가까운지?
    - 보통 상대적인 차이 사용 (Z-변환 or standard Scaling)

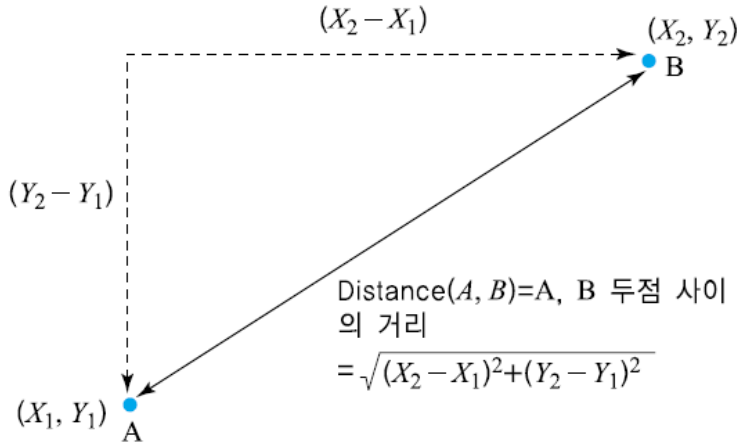
구분	키	몸무게	나이
A	174cm	70kg	21세
B	170cm	61kg	27세
C	162cm	73kg	29세

Clustering

- **Similarity (유사도) and Distance (거리)**
  - **Euclidian distance**

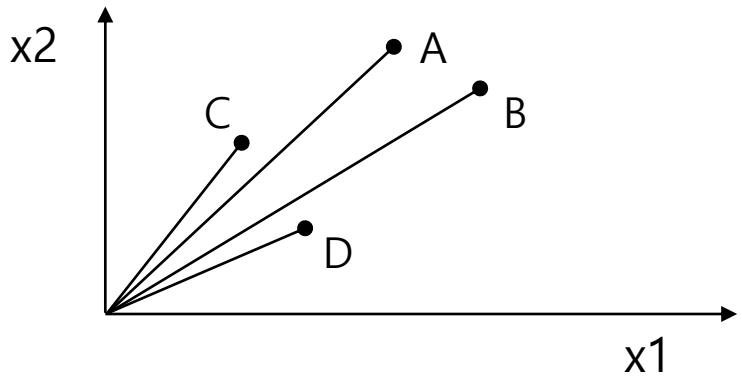
N-차원

$$\sqrt{(p_1-q_1)^2+(p_2-q_2)^2+\ldots+(p_n-q_n)^2}=\sqrt{\sum_{i=1}^{n}(p_i-q_i)^2}$$



  - **Cosine distance – 방향성, 취향**

$$s_{\cos}(x,y)=\frac{X \bullet Y}{|X||Y|}$$



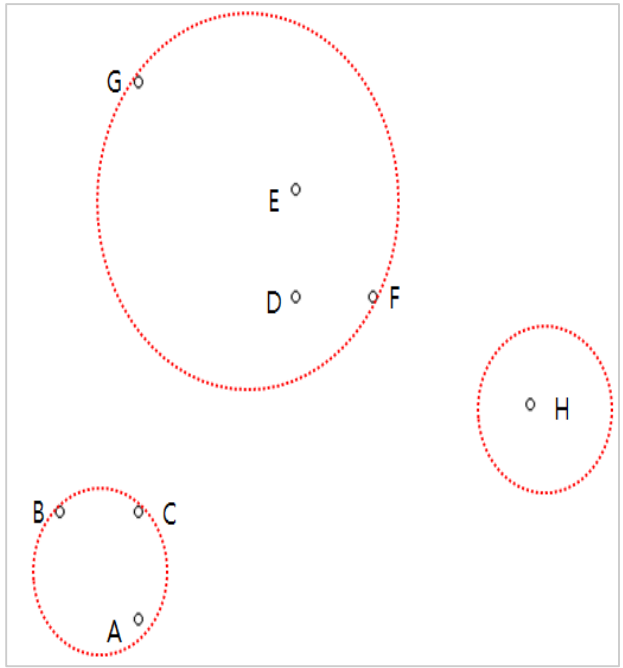
Clustering

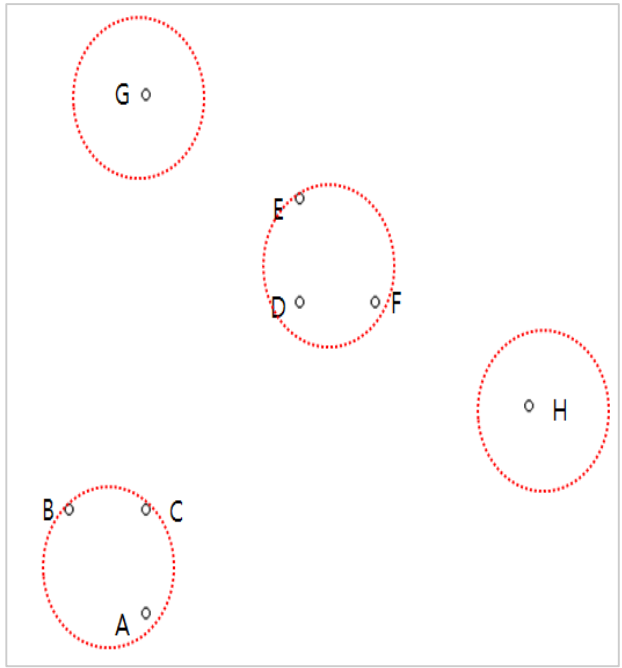
- **Jaccard similarity (자카드 유사도)**
  - **비슷한 취향**의 사람을 찾을 때 사용 - 영화, 도서, 음악 추천 등
  - 영화 보는 취향에 따른 유사도 측정
  - (ex) 지난 1년 동안 국내에 개봉된 영화가 500편
    - A와 B가 본 영화 중 겹치는 영화가 5편, 5/500 = 0.01
    - A와 C가 본 영화 중 겹치는 영화가 10편, 10/500 = 0.02
    - 즉, 0.01 < 0.02이므로 A와 C가 더 가깝다고 할 수 있음
    - 위와 같은 계산 방법이 적절한가?
  - A, B, C가 각각 지난해 본 영화의 총 개수가 20편, 50편, 200편이라면?
    - J(A,B) = 5 / (20+50-5) = 0.076
    - J(A,C) = 10 / (20+200-10) = 0.047
    - 즉, 0.076 > 0.047이므로 A와 B가 더 가깝다고 할 수 있음

$$S_{Jaccard}(X, Y) = \frac{|X \cap Y|}{|X \cup Y|}$$

Clustering (군집화)

- **Number of clusters, *k* (important hyper-parameter)**
  - 적당한 군집의 수 (k) 를 먼저 찾아야 함

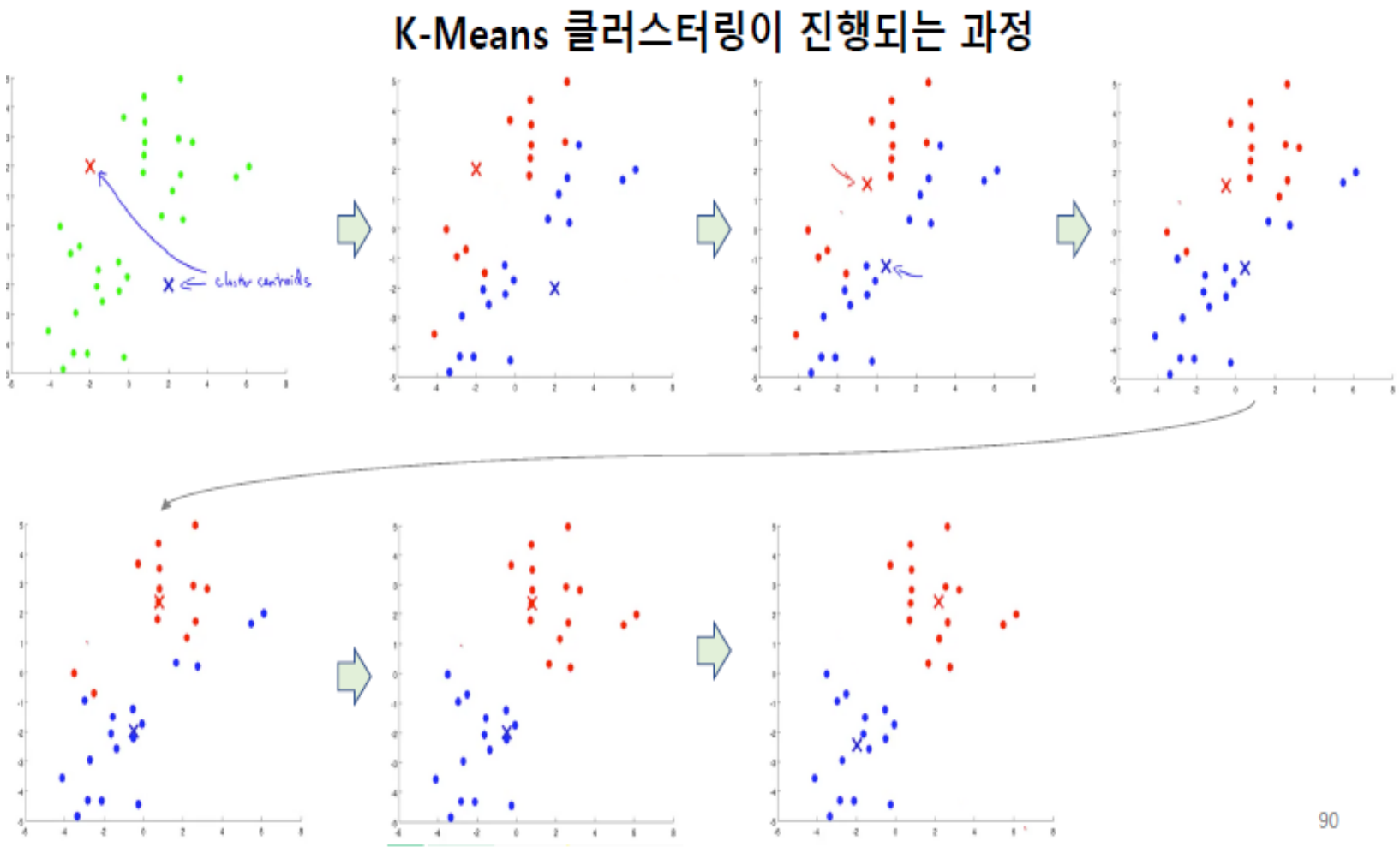




Clustering (군집화)

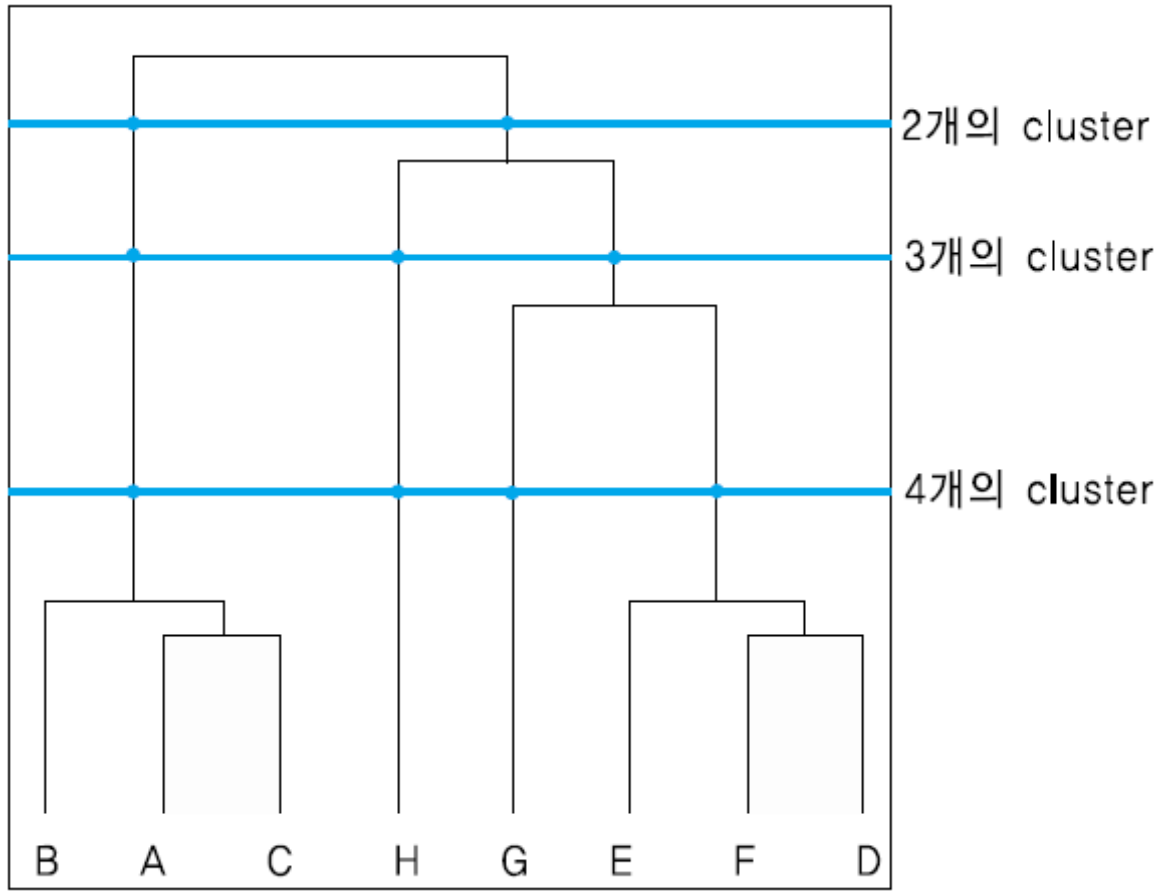
- **K-means()**
  - 공간상에 임의의 k 개의 임의의 초기 지점을 클러스터 중점으로(cluster center) 정함
  - 클러스터 중점을 중심으로 거리가 가까운 항목을 선택하여 클러스터 공간을 나눔
  - 각 클러스터에 포함된 항목들의 평균 위치를 구해 이를 새로운 클러스터 중점(centroid)으로 변경
  - 새로 설정된 **센트로이드**를 중심으로 경계를 다시 그림 (각 항목들이 소속된 클러스터가 바뀔 수 있음)
  - 변경된 항목들을 가지고 클러스터 중심을 다시 계산
  - 더 이상 클러스터의 모양이 바뀌지 않을 때까지 반복 수행
    - **KMeans()** 사용

Clustering (군집화)



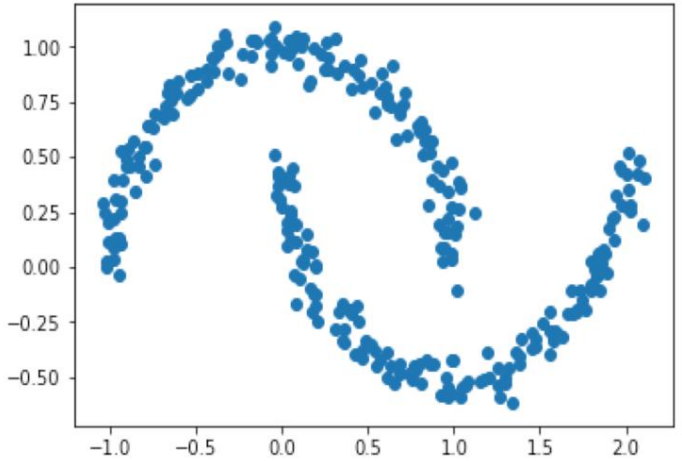
Clustering (군집화)

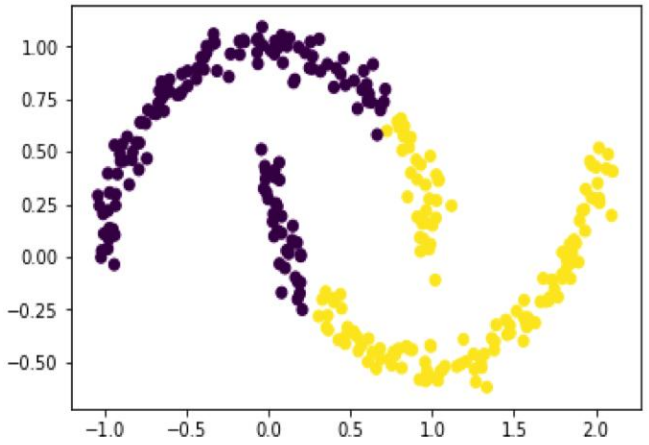
- **Agglomerative hierarchical clustering (Dendrogram)**
  (계층적 병합 군집화)

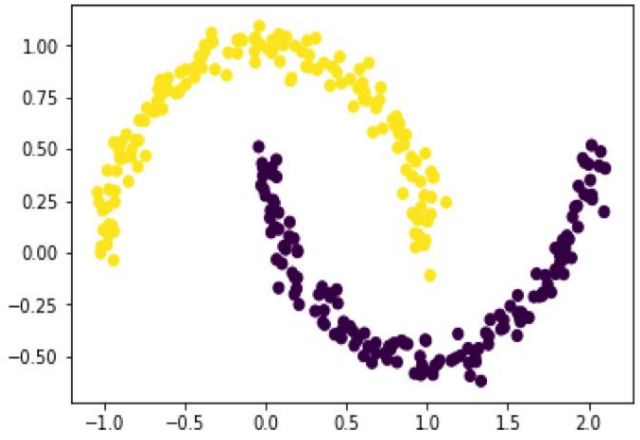


Clustering (군집화)

- **Two Moon dataset**

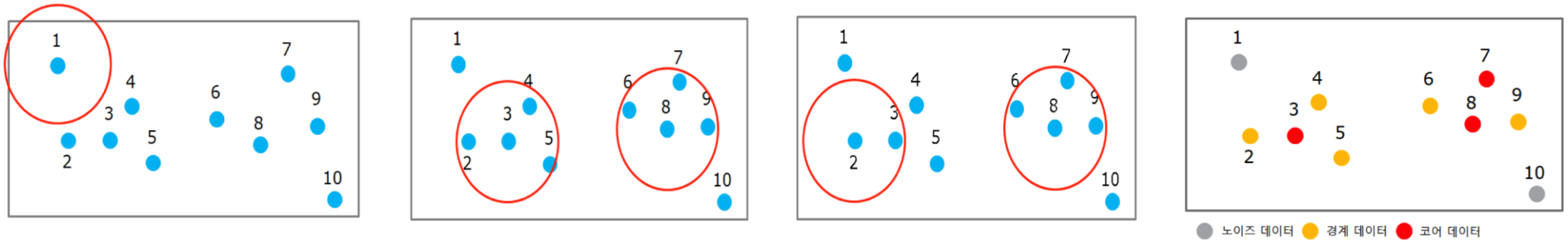






Clustering (군집화)

- **DBSCAN(**Density Based Spatial Clustering of Applications with Noise)
  - One of the most common clustering algorithm
  - Density-based (밀도기반): "가까이 있는 샘플들은 같은 군집에 속한다" 는 원칙
    - **Core point**:거리 e (epsilon) 내에 m (minPts) 개의 점이 있을 때 – 스스로 Cluster 형성
    - **Border point**: Core point 는 아니지만 Core point 의 군집에 속할 때
    - **Noise point**: 어느 군집에도 포함되지 않은 점
    - **Core Point 가 다른 Core 의 군집 일부가 되면 하나의 군집으로 연결**
    - (ex) m = 4

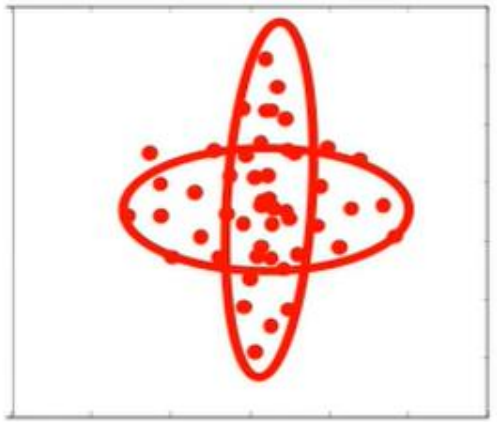


GMM (Gaussian Mixture Model)

Mixtures of Gaussians

- K-means algorithm
  - Assigned each example to exactly one cluster
  - What if clusters are overlapping?
    - Hard to tell which cluster is right
    - Maybe we should try to remain uncertain
  - Used Euclidean distance
  - What if cluster has a non-circular shape?

- Gaussian mixture models
  - Clusters modeled as Gaussians
    - Not just by their mean
  - EM algorithm: assign data to cluster with some *probability*
  - Gives probability model of x! ("generative")



https://www.youtube.com/watch?v=qMTuMa86NzU

GMM (Gaussian Mixture Model)

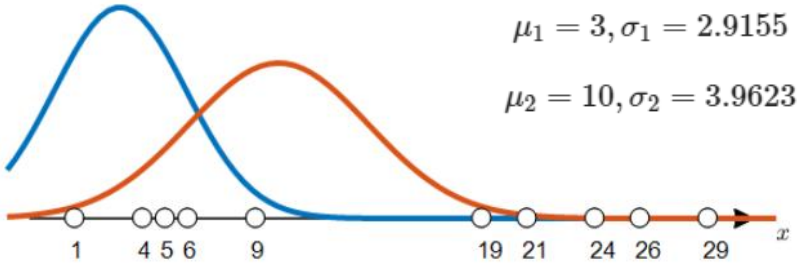
- **Example: the number of components=2**

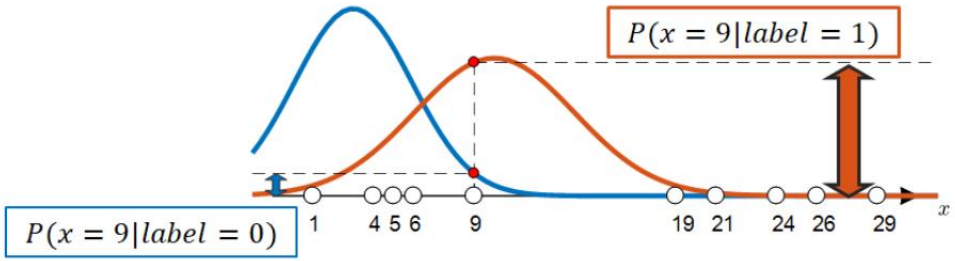
data given without labels

randomly select parameters

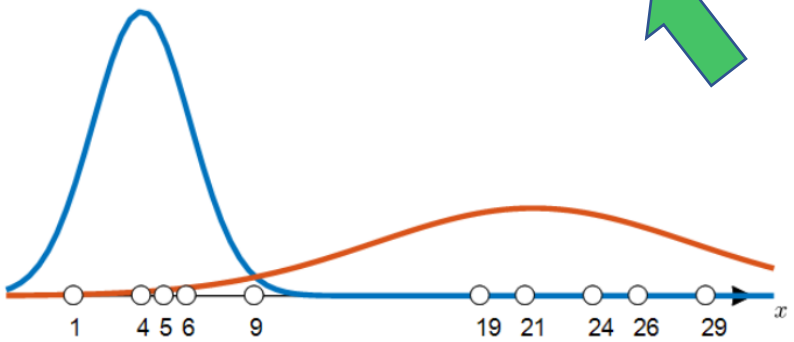
$\mu_1 = 3, \sigma_1 = 2.9155$

$\mu_2 = 10, \sigma_2 = 3.9623$





determine the labels for all the sample data
(e.g. x=9)



predict the parameters based on determined labels (MLE)

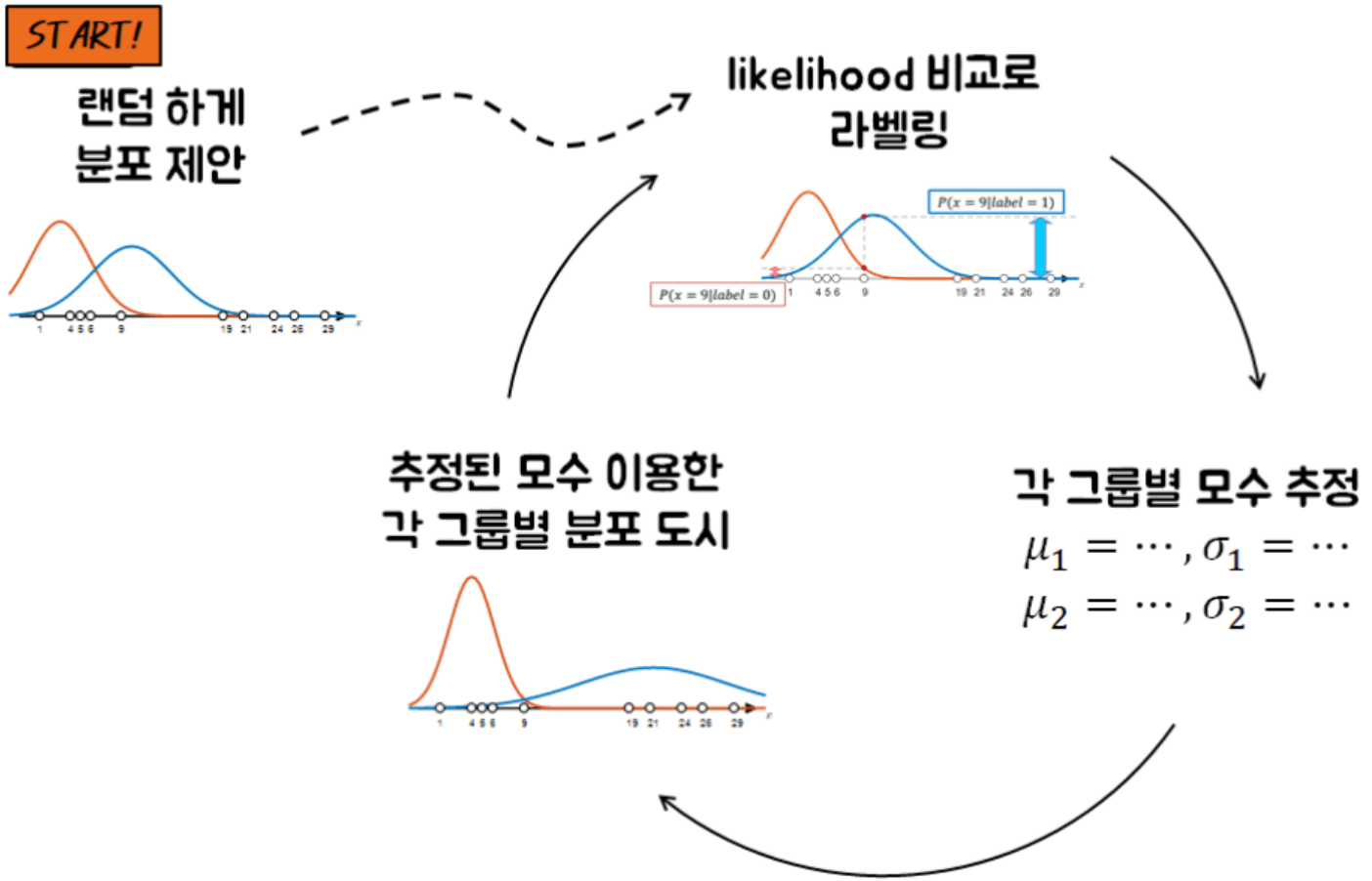
$\mu_1 = 4, \sigma_1 = 2.1602$

$\mu_2 = 21.33, \sigma_2 = 7.0048$

https://angeloyeo.github.io/2021/02/08/GMM_and_EM.html

GMM (Gaussian Mixture Model)

- Good reference: https://angeloyeo.github.io/2021/02/08/GMM_and_EM.html
- Good You-Tube: https://www.youtube.com/watch?v=qMTuMa86NzU



GMM (Gaussian Mixture Model)

- **EM(Expectation-Maximization) algorithm**
  - Expectation: determines a label for each data
  - Maximization: recalculate parameters for each cluster based on MLE(Maximum Likelihood Estimation)

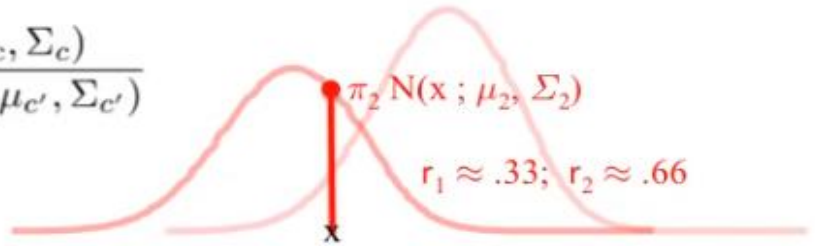
EM Algorithm: E-step

- Start with clusters: Mean μ_c, Covariance Σ_c, "size" π_c

- E-step ("Expectation")
  - For each datum (example) x_i,
  - Compute "r_{ic}", the probability that it belongs to cluster c
    - Compute its probability under model c
    - Normalize to sum to one (over clusters c)

responsibility (or soft assignment)

$$r_{ic} = \frac{\pi_c \mathcal{N}(x_i \; ; \; \mu_c, \Sigma_c)}{\sum_{c'} \pi_{c'} \mathcal{N}(x_i \; ; \; \mu_{c'}, \Sigma_{c'})}$$



  - If x_i is very likely under the c^{th} Gaussian, it gets high weight
  - Denominator just makes r's sum to one

https://www.youtube.com/watch?v=qMTuMa86NzU

GMM (Gaussian Mixture Model)

EM Algorithm: M-step

- Start with assignment probabilities r_{ic}
- Update parameters: mean μ_c, Covariance Σ_c, "size" π_c

- M-step ("Maximization")
  - For each cluster (Gaussian) z = c,
  - Update its parameters using the (weighted) data points

$$m_c = \sum_i r_{ic}$$ Total responsibility allocated to cluster c

$$\pi_c = \frac{m_c}{m}$$ Fraction of total assigned to cluster c

$$\mu_c = \frac{1}{m_c} \sum_i r_{ic} x^{(i)}$$ Weighted mean of assigned data

$$\Sigma_c = \frac{1}{m_c} \sum_i r_{ic} (x^{(i)} - \mu_c)^T (x^{(i)} - \mu_c)$$ Weighted covariance of assigned data (use new weighted means here)

https://www.youtube.com/watch?v=qMTuMa86NzU

EM Algorithm

The **EM algorithm** is the iterative process used to find the maximum likelihood estimates of these parameters, starting from random initial guesses. It alternates between assigning data to Gaussian components (E-step) and re-estimating the parameters based on those assignments (M-step).

EM Algorithm for GMM: Detailed Steps

1. **Initialization**:
    - **Randomly initialize** the parameters of each Gaussian: means ($\mu_1, \mu_2, ..., \mu_k$) and covariances ($\Sigma_1, \Sigma_2, ..., \Sigma_k$).
    - **Assign equal weights** (mixing coefficients π_k) to each Gaussian component initially.

2. **Expectation Step (E-step)**:
    - For each data point x_i, calculate the **responsibility** (or **soft assignment**) that each Gaussian k has for generating x_i.
    - These responsibilities are probabilities, calculated using the **likelihood** of each data point under each Gaussian, normalized across all components.

Mathematically, for each data point x_i and Gaussian k, the responsibility $\gamma(z_{ik})$ is:

$$\gamma(z_{ik}) = \frac{\pi_k \cdot \mathcal{N}(x_i|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \cdot \mathcal{N}(x_i|\mu_j, \Sigma_j)}$$

where:

- π_k is the mixing coefficient for Gaussian k,
- $\mathcal{N}(x_i|\mu_k, \Sigma_k)$ is the Gaussian probability density function for component k,
- $\gamma(z_{ik})$ is the soft assignment of point x_i to component k.

$$\sum_{k=1}^{K} \pi_k = 1$$

3. **Maximization Step (M-step)**:
    - Update the parameters μ_k, Σ_k, π_k based on the **current responsibilities**. This is done by calculating the weighted averages for the means and covariances using the responsibilities.

    The new parameter estimates are:

    - **New means**:

$$\mu_k^{new} = \frac{\sum_{i=1}^{N} \gamma(z_{ik}) x_i}{\sum_{i=1}^{N} \gamma(z_{ik})}$$

    - **New covariances**:

$$\Sigma_k^{new} = \frac{\sum_{i=1}^{N} \gamma(z_{ik})(x_i - \mu_k)(x_i - \mu_k)^T}{\sum_{i=1}^{N} \gamma(z_{ik})}$$

    - **New mixing coefficients**:

$$\pi_k^{new} = \frac{1}{N} \sum_{i=1}^{N} \gamma(z_{ik})$$

    where N is the total number of data points.

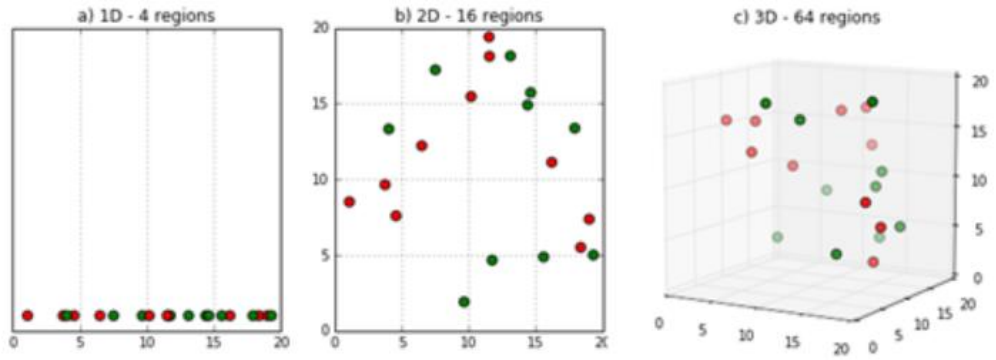
4. **Repeat the Process**:
    - The E-step and M-step are repeated until the parameters converge, meaning that the change in the parameters or the log-likelihood of the model does not change significantly between iterations.

Intuition:

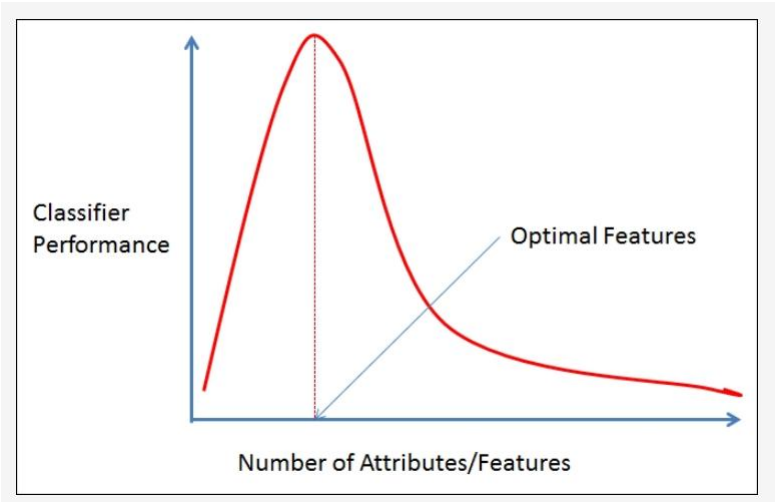
- **E-step**: Softly assigns each data point to one of the Gaussian components based on the current parameters.
- **M-step**: Updates the parameters to maximize the likelihood, given the current soft assignments.

Curse of Dimensionality

- **Curse of dimensionality**
  - **Sparsity** of data occurs when moving to higher dimensions. (risk of massively overfitting)
  - **Distance concentration**: as dimensionality increases, distance may converge to the same value between different samples (critical in distance-based model like knn, clustering, etc.)
- Each features increases the data set requirement **exponentially**.
- **How to mitigate it**
  - **Dimensionality reduction techniques** (feature selection or feature extraction)



sparsity



Curse of dimensionality illustrated in classification

Feature Selection – Statistical Methods

T-Test	두 개의 독립된 표본 간의 평균 차이가 통계적으로 유의한 지를 검정	- 두 그룹의 평균 차이를 계산하고 T-통계량을 이용하여 유의성을 검정함. - T-test수식을 사용하여 두 그룹간의 평균 차이의 유의성을 검정함
Anova Test	세 개 이상의 독립된 그룹 간의 평균 차이가 통계적으로 유의한 지를 검정	- 세 그룹 간의 평균 차이를 계산하고 F-통계량을 이용하여 유의성 을 검정함. - ANOVA 수식을 사용하여 그룹 간의 평균 차이의 유의성을 검정함
Chi-2 Test	두 범주형 변수간의 관계를 분석	
Correlation	두 변수 간의 관계를 분석	- 두 변수 간의 상관계수를 계산하여 관계의 강도와 방향을 파악함. - 이후, 피어슨 상관계수 또는 스피어만 상관계수를 사용하여 변수 간의 관계를 분석 진행함.

Statistical Methods (p-values)

- **p-value:** 귀무가설 하에서 관찰된 값(또는 그보다 극단적인 값)이 나올 확률의 합
- **p-value 예제: 동전 던지기**
  - 상황설정: 동전이 공정하다고 주장하는 사람과 논쟁 (H0: 귀무가설: 동전은 공정하다)
  - 공정하다면? 앞뒷면이 나올 확률은 50% 일 것임
  - 동전을 10번 던져서 앞면이 몇 번 나오는지 실험
- **실험결과**
  - 동전을 10 번 던져 앞면이 8번 나왔다.
- **p-value 계산**
  - 귀무가설 하에서, 동전이 공정하다는 가정에 따라, 앞면이 나올 확률은 p=0.5
  - 이때, 동전을 10번 던졌을 때 앞면이 8번 이상 나올 확률을 계산 (앞면이 2번 이하로 나올 확률도 포함한다)
  - 만약 계산된 p-value가 0.05보다 작다면, 관찰된 결과(8번의 앞면)가 매우 드문 일이므로 귀무가설은 기각 (reject H0)
  - 반대로 p-value가 0.05보다 크다면, 관찰된 결과는 귀무가설 하에서 충분히 발생할 수 있는 일이므로, "이 동전이 공정하지 않다고 결론 내릴 증거가 부족하다"고 해석

Statistical Methods (p-values)

이항분포 확률 계산 $P(X = k) = \binom{n}{k} p^k (1-p)^{n-k}$

- $n = 10$ (시행 횟수)
- $k = 8, 9, 10$ (앞면이 나온 횟수)
- $p = 0.5$ (앞면이 나올 확률)

$$P(X = 8) = \binom{10}{8} \cdot (0.5)^8 \cdot (0.5)^2 = \frac{10!}{8! \cdot 2!} \cdot (0.5)^{10} \quad = 0.0439453$$

$$P(X = 9) = \binom{10}{9} \cdot (0.5)^9 \cdot (0.5)^1 = \frac{10!}{9! \cdot 1!} \cdot (0.5)^{10} \quad = 0.0097656$$

$$P(X = 10) = \binom{10}{10} \cdot (0.5)^{10} = 1 \cdot (0.5)^{10} \quad = 0.0009765$$

- 단측검정: 앞면이 너무 많이 나오는 경우만 관심 있는 경우
- 양측검정: 앞면이 너무 많이 나오거나 너무 적게 나오는 경우 모두 관심 있는 경우 ($P(X \geq 8) + P(X \leq 2)$)

$$P(X \geq 8) = 0.0439453125 + 0.009765625 + 0.0009765625 = 0.0546875 \quad > 0.05$$

결론: 귀무가설(H0: Null Hypothesis)을 기각할 충분한 증거가 없다.

Statistical Methods (p-values)

- ANOVA (Analysis of Variance): 각 그룹간의 분산을 비교해서 서로 다른 그룹의 평균이 통계적으로 유의미한지 판단
- ANOVA의 핵심 아이디어
  - 그룹 간 변동 (Between-group variability)
    - 그룹 평균 간의 차이에 의해 발생하는 변동을 측정
    - 예를 들어, 여러 그룹의 평균이 크게 다를수록 그룹 간 변동이 크다
  - 그룹 내 변동 (Within-group variability)
    - 각 그룹 내부에서 데이터의 분산을 측정
    - 즉, 동일한 그룹 내에서 개별 데이터가 얼마나 퍼져 있는지를 나타냄
  - F-통계량

$$F = \frac{\text{그룹 간 평균 제곱 (MSB)}}{\text{그룹 내 평균 제곱 (MSW)}}$$

    - F-값이 클수록 그룹 간 변동이 그룹 내 변동보다 크다는 것을 의미하며, 이는 그룹 평균 간 차이가 있다는 증거가 될 수 있다.

귀무가설 H_0: 모든 그룹의 평균이 동일하다.

$(\mu_1 = \mu_2 = \mu_3 = \ldots)$

총변동(toal variance):

$$SST = \sum_{i=1}^{N}(x_i - \bar{x})^2$$

$$SSB = \sum_{j=1}^{k} n_j(\bar{x}_j - \bar{x})^2$$

$$SSW = \sum_{j=1}^{k}\sum_{i=1}^{n_j}(x_{ij} - \bar{x}_j)^2$$

$$MSB = \frac{SSB}{k-1}$$

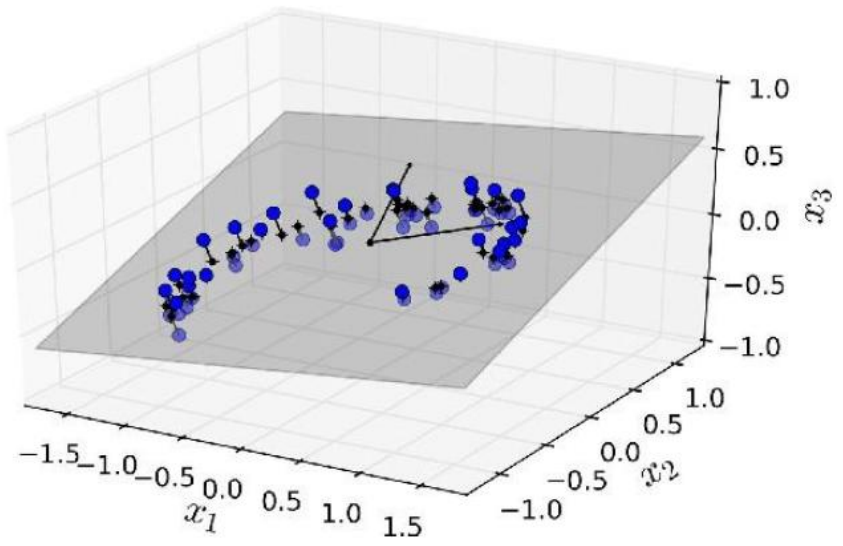
평균

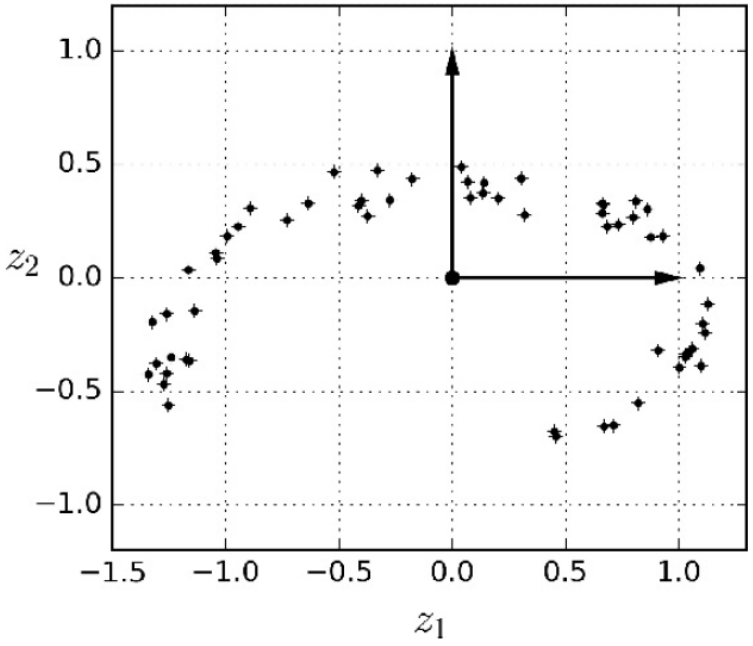
$$MSW = \frac{SSW}{N-k}$$

$$F = \frac{MSB}{MSW}$$

Dimension Reduction

- **Dimension Reduction approach**
  - Projection
  - Manifold Learning

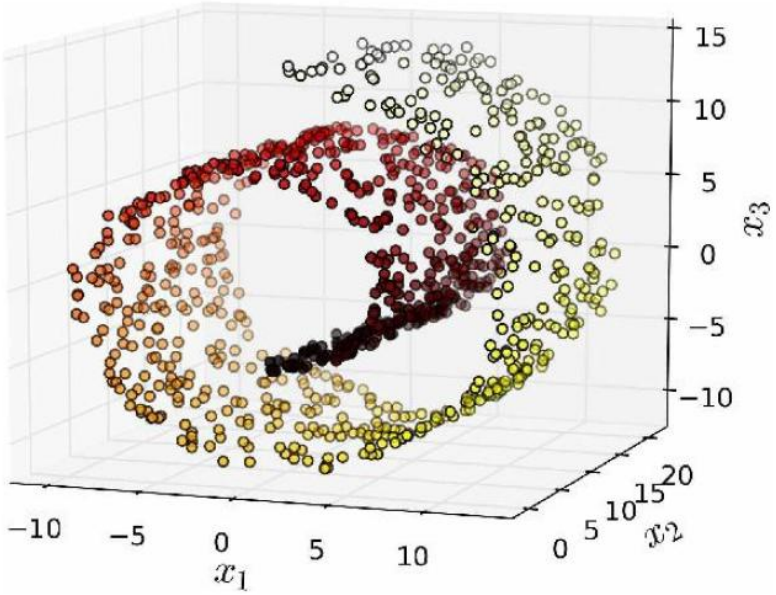


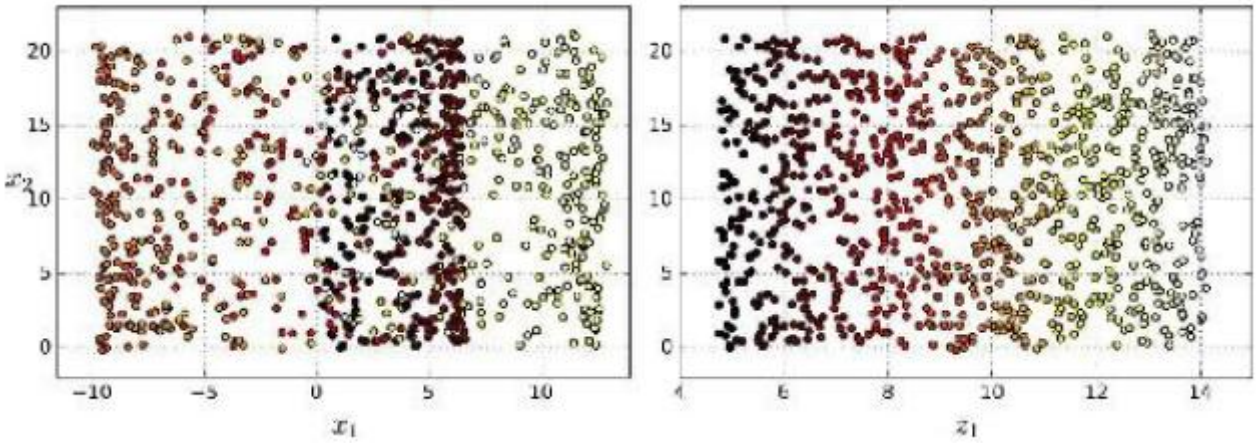


A 3D dataset lying close to a 2D subspace

Dimension Reduction

- **Dimension Reduction approach**
  - Projection
  - Manifold Learning

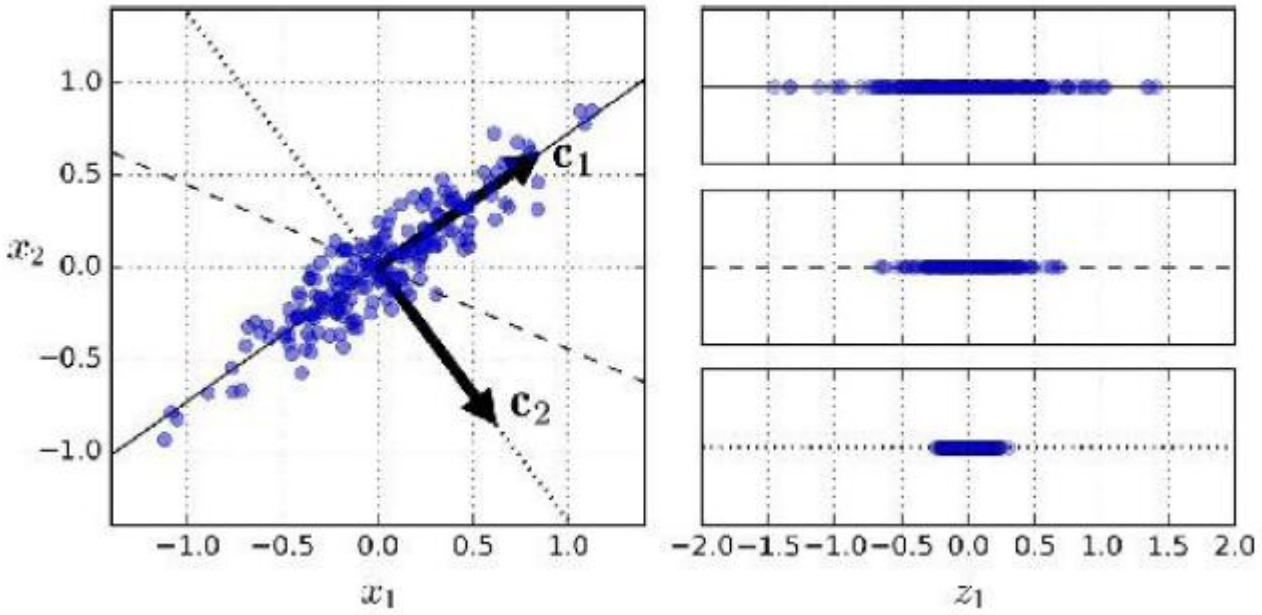




Swiss roll: Projection is not always Good. – Projection and Unrolling.

Dimension Reduction

- **Preserving the Variance**
  - Select the axis that preserves the **maximum amount of Variance** (lose less information)
  - It minimizes the mean squared distance between the original dataset and projected ones.



- PCA에서 projection은 eigenvector와 직각이 되는 것이 아니라, eigenvector 방향으로 데이터를 평행하게 투영한다. (그림자를 드리우듯이 투영)
- PCA의 eigenvector 들은 서로 직교 관계를 이룬다. 따라서, 투영된 값들은 서로 독립적인 새로운 좌표계를 형성한다.

Dimension Reduction

- **Principal Component Analysis – linear**
  - Summarize the data consisting of *p* features into *k* new (uncorrelated) features
  - New *k* features are linear combination of original *p* features
  - project original data on the new axes in a way that preserves the variance of the original data as much as possible.
  - Main purposes:
    - Data Dimension Reduction (n x p -> n x k, where k << p)
    - Data analysis and visualization
  - Can be implemented using **SVD** or **Eigenvalue Decomposition**

Dimension Reduction

- **Eigen-decomposition for PCA**
  - Finds linearly uncorrelated orthogonal axes (called Principal Components (PC)) to project the data points onto those PCs.
  - The PCs can be determined via eigen-decomposition of the covariance matrix ***C***.

$$\mathbf{C} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^{-1}$$

(covariance matrix ***C*** ($m \times m$), eigenvector matrix ***W*** ($m \times m$), diagonal matrix $\boldsymbol{\Lambda}$)

  - The eigenvectors, which are the column vectors in ***W***, are in fact the PCs. We can then use matrix multiplication to project the data onto the PC space (*k* PCS for *k*-dimension).

$$\mathbf{X}_k = \mathbf{X}\mathbf{W}_k$$

Dimension Reduction

- **SVD**
  - Any $n \times m$ matrix can be decomposed as follows:

$$\underset{n\times m}{\mathbf{X}} = \underset{n\times n}{\mathbf{U}} \quad \underset{n\times m}{\mathbf{\Sigma}} \quad \underset{m\times m}{\mathbf{V}^*}$$

$$\mathbf{A}^* \equiv (\overline{\mathbf{A}})^\top = \overline{\mathbf{A}^\top}$$

(conjugate transpose)

In real numbers, orthogonal matrices ($UU^T = I$)

  - Where, **U** and **V** are unitary matrices ($UU^*=VV^*=I$), and $\boldsymbol{\Sigma}$ is a rectangular diagonal matrix.
- **Relationship between PCA and SVD**
  - PCA and SVD are closely related and can be both applied to decompose any matrices.
  - For covariance matrix C,

$$\begin{aligned}
\mathbf{C} &= \frac{\mathbf{X}^\top \mathbf{X}}{n-1} \\
&= \frac{\mathbf{V}\mathbf{\Sigma}\mathbf{U}^\top \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top}{n-1} \\
&= \mathbf{V}\frac{\mathbf{\Sigma}^2}{n-1}\mathbf{V}^\top \\
&= \mathbf{V}\frac{\mathbf{\Sigma}^2}{n-1}\mathbf{V}^{-1} \text{ (because } \mathbf{V} \text{ is unitary)}
\end{aligned}$$

$$\mathbf{\Lambda} = \frac{\mathbf{\Sigma}^2}{n-1}$$

relationship between singular values ($\boldsymbol{\Sigma}$) and eigenvalues ($\boldsymbol{\Lambda}$)

Dimension Reduction

- **Relation between SVD and PCA**

Since any matrix has a singular value decomposition, let's take $A = X$ and write

$$X = U\Sigma V^T .$$

We have so far thought of A as a linear transformation, but there's nothing preventing us from using SVD on a data matrix. In fact, note that from the decomposition we have

$$X^T X = (U\Sigma V^T)^T (U\Sigma V^T) = V\Sigma^T U^T U\Sigma V^T = V(\Sigma^T \Sigma)V^T ,$$

which means that $X^T X$ and $\Sigma^T \Sigma$ are similar. Similar matrices have the same eigenvalues, so the eigenvalues λ_i of the covariance matrix $S = \frac{1}{n-1} X^T X$ are related to the singular values σ_i of the matrix X via

$$\sigma_i^2 = (n-1)\lambda_i ,$$

for $i \in \{1, \ldots, r\}$, where as usual $r = \mathbf{rank}(A)$.

$$\mathrm{Cov}(X_i, X_j) = \frac{1}{n-1} \sum_{k=1}^{n} (X_{ik} - \bar{X}_i)(X_{jk} - \bar{X}_j)$$

$$C = \frac{1}{n-1} X_{\text{centered}}^{\top} X_{\text{centered}}$$

$$X_{\text{centered}} = X - \mu$$

(*) For further details, please refer to the following site: https://intoli.com/blog/pca-and-svd/

Dimension Reduction

- **Summary for SVD and PCA**

Objective: project an $N \times d$ data matrix X using the largest m principal components $V = [v_1, \ldots v_m]$.

1. zero mean the columns of X.
2. Apply PCA or SVD to find the principle components of X.

PCA:

I. Calculate the covariance matrix $C = \frac{1}{N-1} X^T X$.

II. V corresponds to the eigenvectors of C.

SVD:

I. Calculate the SVD of $X = U \Sigma V^T$.

II. V corresponds to the right singular vectors.

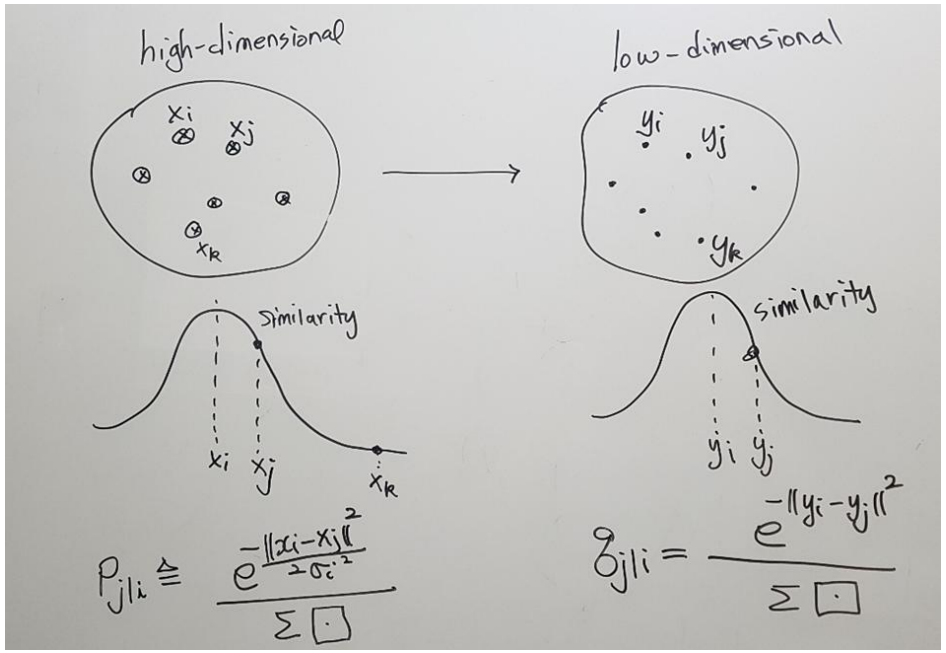
3. Project the data in an m dimensional space: $Y = X V$

Eigenvalues need to be sorted to take the *m* largest values.

https://people.cs.pitt.edu/~milos/courses/cs3750-Fall2014/lectures/class9.pdf

Dimension Reduction

- **t-SNE (T-distributed Stochastic Neighbor Embedding) - nonlinear**
  - Converts similarities between data points to joint probabilities (normalized)
  - Tries to minimize the KL-divergence between the joint probabilities of the low-dimensional embedding and the high-dimensional data
  - Very high time-complexity (recommended to use PCA (dense matrix) or TruncatedSVD (sparse matrix) for high dimensional features)



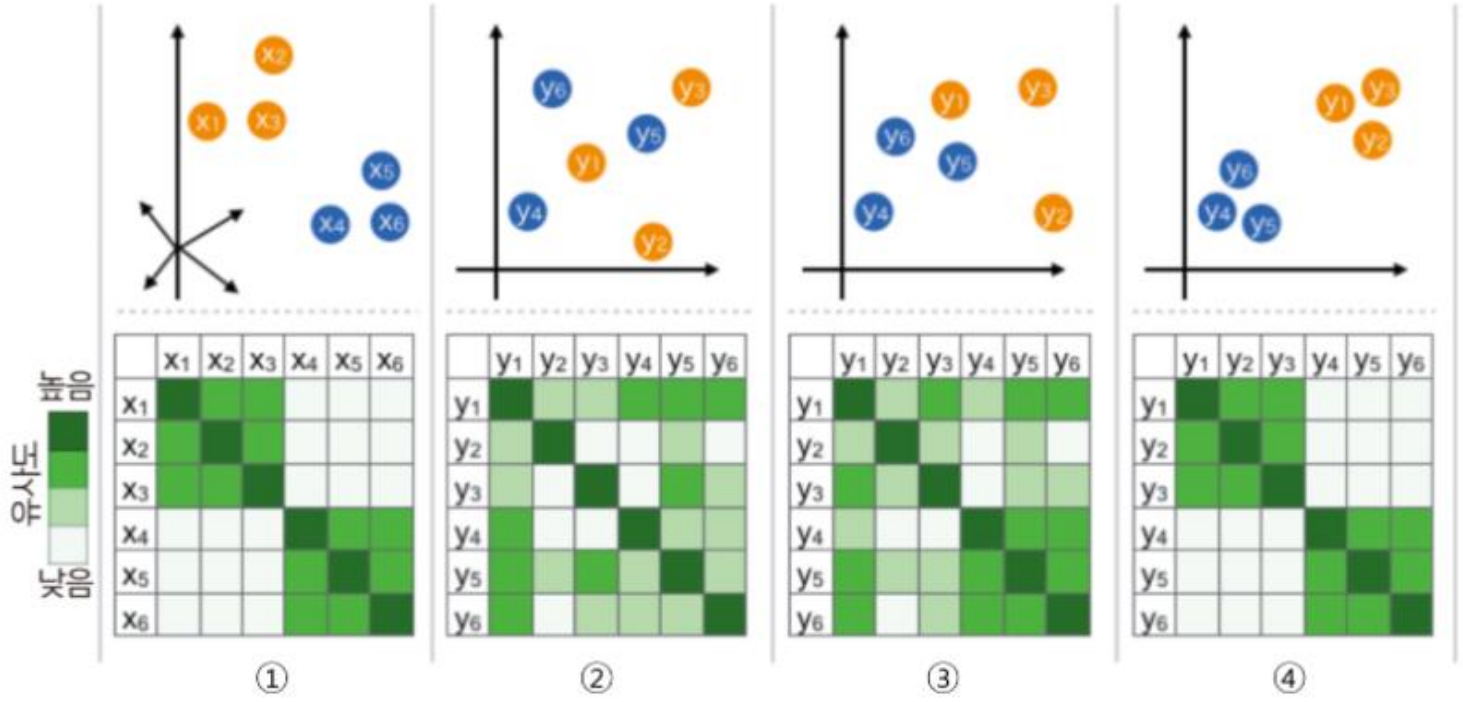
- Hyper–parameter '**perplexity**' controls σ_i, normally 5 ~ 50
- We want to make $q_{j|i}$ -> $p_{j|i}$, the cost function C is

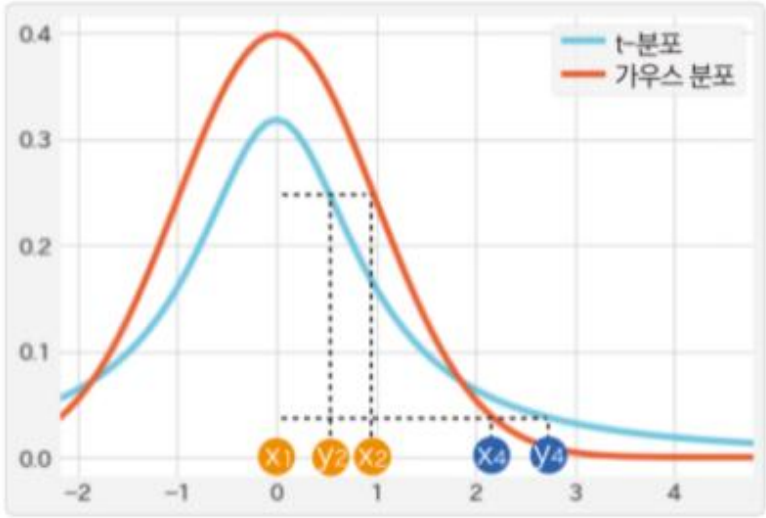
$$C = \sum_i KL(P_i||Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

$$\frac{\delta C}{\delta y_i} = 2 \sum_j (p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j})(y_i - y_j)$$

Dimension Reduction

- **t-SNE (T-distributed Stochastic Neighbor Embedding) - nonlinear**
  - Example showing the t-SNE operation





(low dimensional space상에서)
high similarity 는 더 가깝게, low similarity 는 더 멀게 배치

Dimension Reduction

- **Information t-SNE wants to keep**
  - **Local pair-wise distance** (즉, 두 점 사이의 거리 정보를 이용해 어던 pair-wise distance 가 local 한지 평가를 위해 probabilistic approach 를 사용함)
  - 각각 분포에서 sigma 값에 따라 일정 범위 안의 neighbor 개수가 조정되고 이를 효과적으로 정하기 위해 perplexity 사용
  - "The perplexity can be interpreted as a smooth measure of the effective number of neighbors."

- Probability of picking j given in high D
- Probability of picking j given in low D

$$p_{j|i} = \frac{e^{-\frac{||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma_i^2}}}{\sum_{k \neq i} e^{-\frac{||\mathbf{x}_i - \mathbf{x}_k||^2}{2\sigma_i^2}}} \qquad q_{j|i} = \frac{e^{-||\mathbf{y}_i - \mathbf{y}_j||^2}}{\sum_{k \neq i} e^{-||\mathbf{y}_i - \mathbf{y}_k||^2}}$$

σ ↑ -> H(Pi) ↑ -> more neighbors

$$H(P_i) = -\sum_j p_{j|i} \log_2 p_{j|i} \quad \text{(entropy)}$$

$$Perplexity(P_i) = 2^{H(P_i)}$$

- For detailed information and Python implementation, refer to https://bonzo-here.tistory.com/2

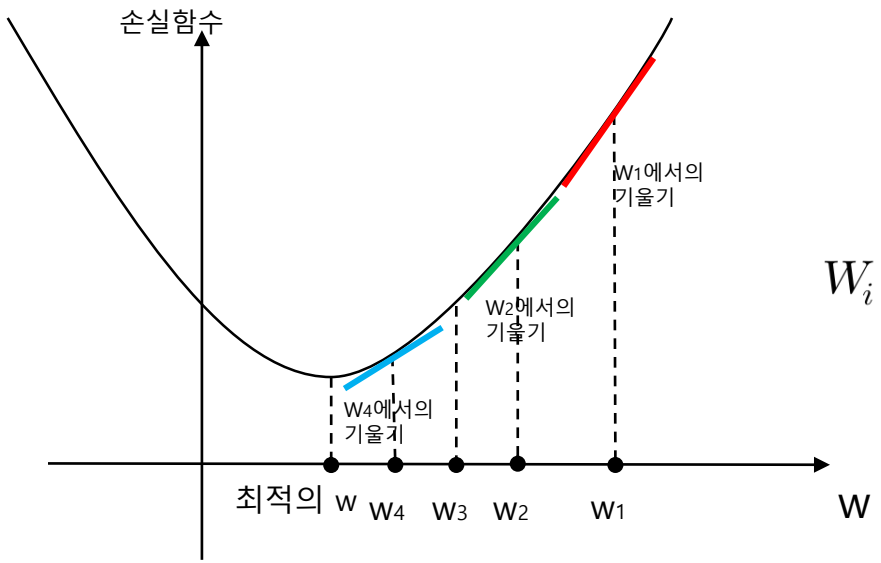
Dimension Reduction

- t-SNE is primarily used for visualization and not as a practical dimension reduction technique.
  - Computational Cost: t-SNE is computationally expensive, especially for large datasets. This makes it impractical for real-world applications where performance is critical. Training an autoencoder or PCA is significantly faster and more efficient.
  - Non-deterministic Results: t-SNE utilizes a stochastic algorithm, meaning that the results can vary slightly with each run. This makes it difficult to rely on the results for practical tasks like prediction or recommendation. Other techniques like PCA and autoencoders provide more consistent and deterministic outputs.
  - Limited Interpretability: The features extracted by t-SNE are difficult to interpret as they are not explicitly related to the original features. This makes them less useful for tasks like feature engineering or anomaly detection, where understanding the underlying features is crucial.
  - Focus on Local Structure: While t-SNE excels at preserving local data structure, it may not capture global relationships well. This can be detrimental for tasks that require understanding the overall distribution and patterns in the data.
  - Difficulty in Reusing: Once trained, t-SNE models are not directly applicable to unseen data. This means you need to retrain the model for any new data point, making it impractical for real-time applications.
- Therefore, while t-SNE offers valuable insights for visualizing high-dimensional data, its limitations render it less suitable for practical dimension reduction tasks compared to techniques like PCA and autoencoders.

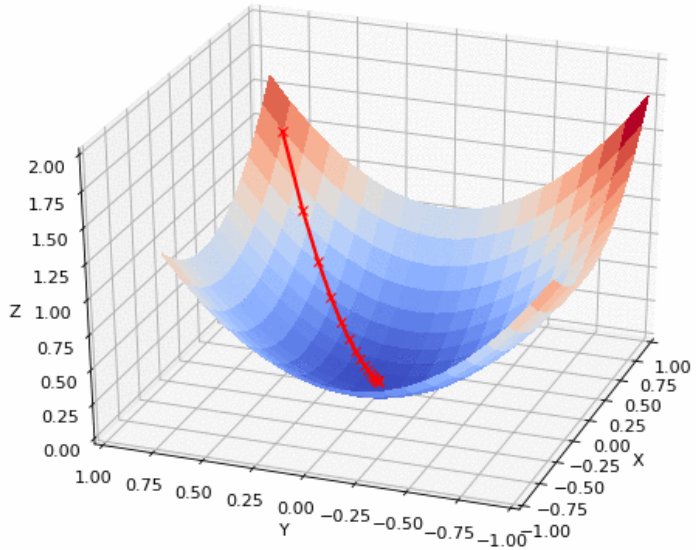
5. Model Evaluation and Optimization

Gradient Descent (GD) algorithm

- **Gradient Descent (경사하강법)**
  - General optimization algorithm
  - take repeated steps in the opposite direction of the **gradient** (or approximate **gradient**) of the function at the current point

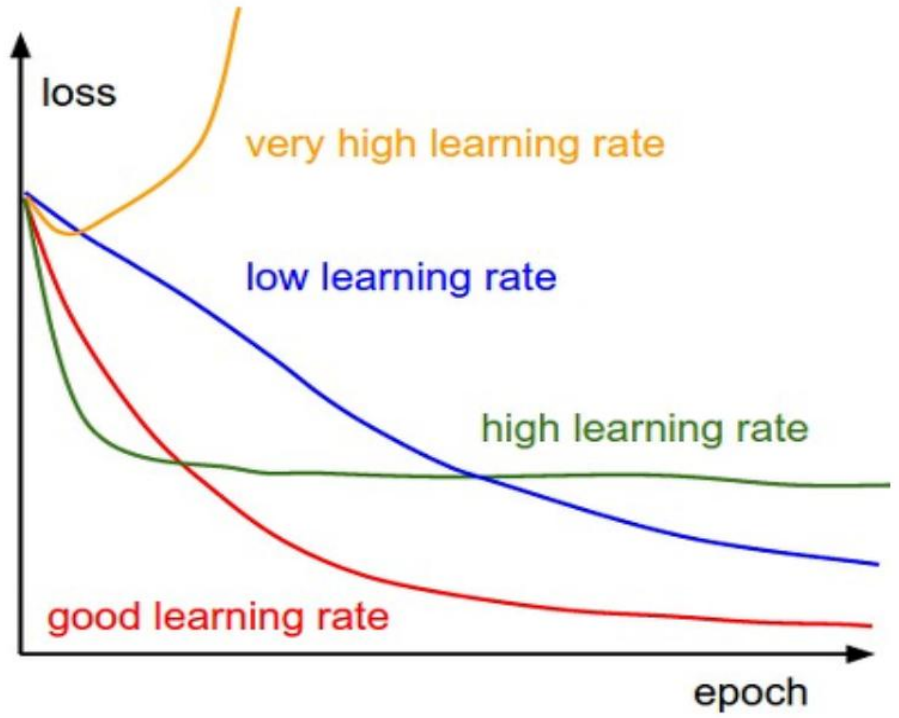


$$W_i = W_{i-1} - \eta Grad(i)$$



Gradient Descent (GD) algorithm

- **Learning rate: η (eta)**
  - low: takes time to converge, and may get stuck in an undesirable local minimum
  - high: may jump over minima
  - too high: may diverge
  - Need adaptive adjustment



Loss Function

- **What to reduce? (Loss or Error or Cost: 손실함수)**
  - Regression (회귀): MSE (Mean Square Error)

$$MSE = \sum_{k=1}^{N} (y - \hat{y})^2$$

  - Classification (분류): Cross Entropy (CE), Gini Coefficient

$$CE = \sum_{i} p_i \log(\frac{1}{p_i}) \qquad Gini = 1 - \sum_{k=1}^{m} p_k^2$$

  - Binary case:

$$H_p(q) = -\frac{1}{N} \sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

Loss Function

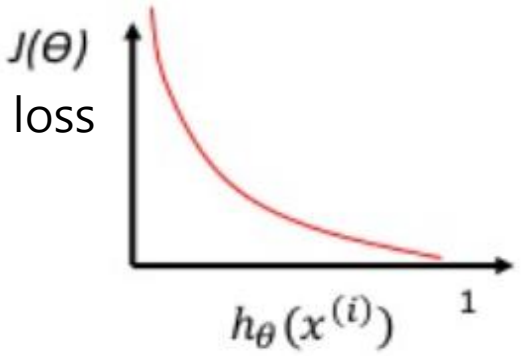
- **Binary Cross Entropy**

$$J(\theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))\right]$$

Sigmoid ft'n

For $y^{(i)} = 1$ *case*

$J(\Theta) = -\log h_\theta(x^{(i)})$



For $y^{(i)} = 0$ *case*

$J(\Theta) = -\log(1 - h_\theta(x^{(i)}))$

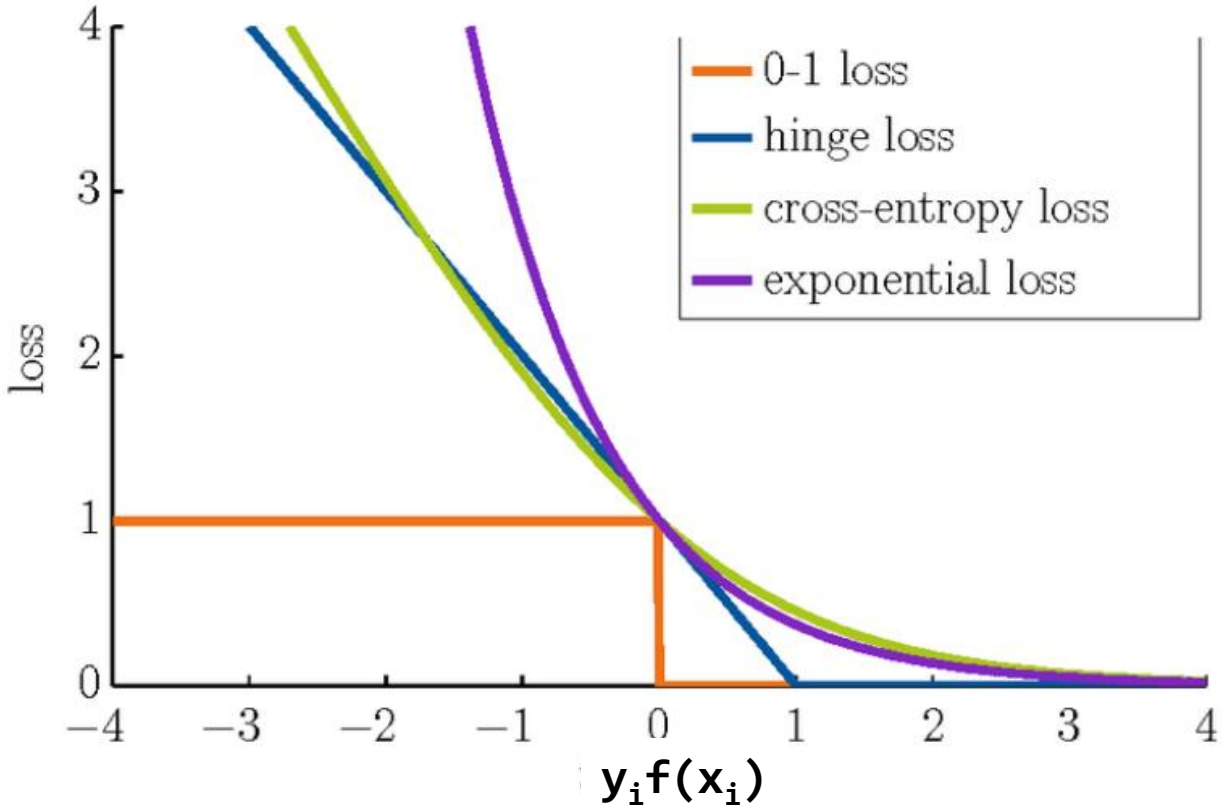
Classification Loss Functions

- Truth value, y_i: [1, -1, 1, -1, 1]
- Output score: $f(x_i)$-> + (likely +1)

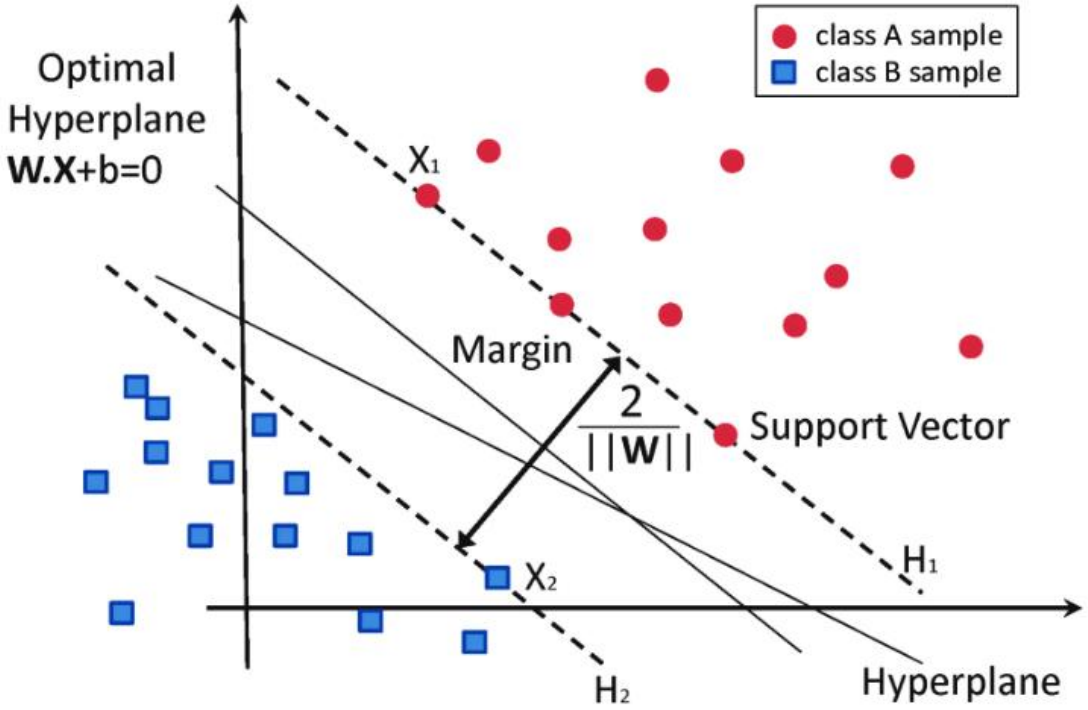
  -> - (likely -1)
- $y_i f(x_i)$ 가 negative 일 때 얼마나 penalty 를 줄 것인지.
- **0/1 Loss**

$$Li = \begin{cases} 0, & \text{if } y_i f(x_i) \geq 0 \\ 1, & \text{if } y_i f(x_i) < 0 \end{cases}$$

- **Exponential loss (Adaboost)**
  - $\exp(-y_i f(x_i))$
- **Hinge Loss (SVM Loss)**
  - Max $[0, 1 - y_i f(x_i)]$
- **Cross Entropy (Log loss) – rescaled**



Classification Loss – Hinge Loss



$$SVMLoss = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$$

true value

predicted value

https://www.section.io/engineering-education/understanding-loss-functions-in-machine-learning/

Log Loss and Cross Entropy

- Log loss:

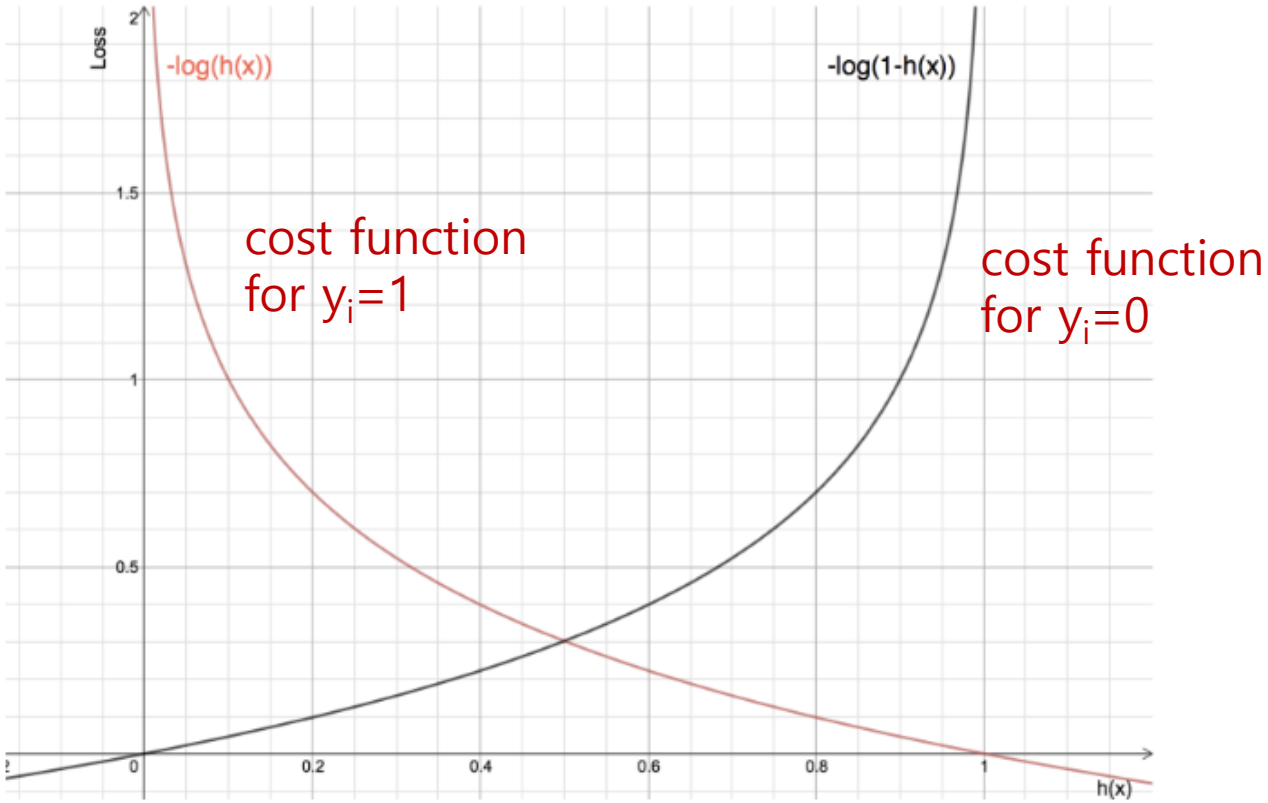
$$Logloss = \frac{1}{N}\sum_{i=1}^{N} logloss_i$$

$$= -\frac{1}{N}\sum_{i=1}^{N}[y_i \, ln \, p_i + (1 - y_i) \, ln(1 - p_i)]$$

- Why not MSE (men square error)?
  - MSE for logistic regression is not convex.
  - But, Log-loss is convex. (we can prove it by showing f’’(x) $\geq$ 0 for all x.)

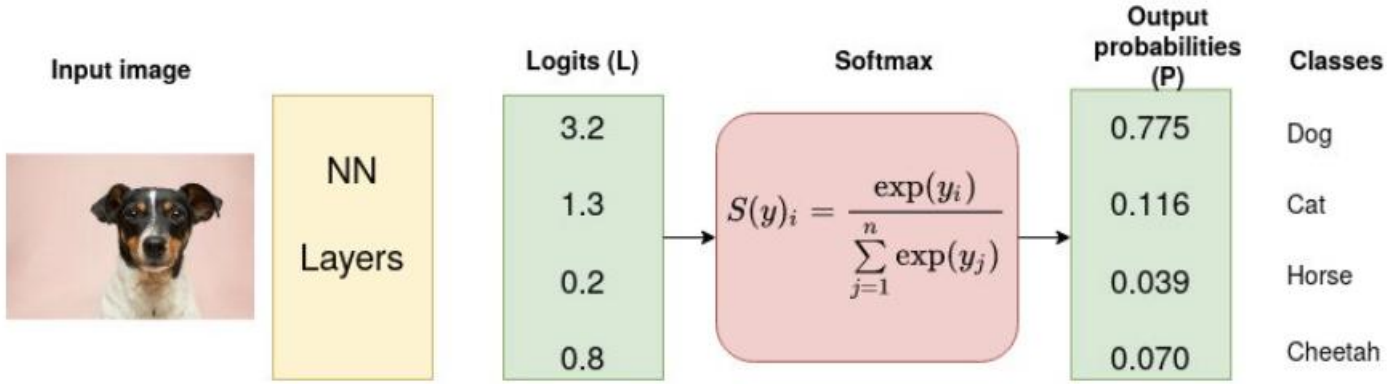
Log Loss and Cross Entropy

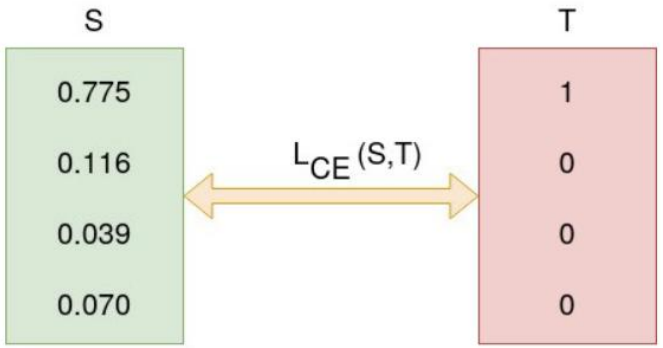
- The benefits of taking logarithm reveal themselves when you look at the cost function graphs for actual classes 1 and 0 :



Log Loss and Cross Entropy Loss

- Cross entropy loss:





$$L_{\text{CE}} = -\sum_{i=1}^{n} t_i \log(p_i), \quad \text{for n classes}$$

$$\begin{aligned} L_{CE} &= -\sum_{i=1} T_i \log(S_i) \\ &= -\left[1 \log_2(0.775) + 0 \log_2(0.126) + 0 \log_2(0.039) + 0 \log_2(0.070)\right] \\ &= -\log_2(0.775) \\ &= 0.3677 \end{aligned}$$

https://towardsdatascience.com/cross-entropy-loss-function-f38c4ec8643e

Entropy and Cross Entropy

- Entropy
  - Entropy of a random variable X: the average level of “information”, “surprise”, or “uncertainty” inherent to the variable’s possible outcome (wikipedia)
  - For a discrete random variable X, which takes values in χ and is distributed according to p: $\chi \rightarrow \{0.1\}$:

$$\mathrm{H}(X) = -\sum_{i=1}^{n} \mathrm{P}(x_i) \log \mathrm{P}(x_i)$$ ← Over the variable’s possible values

- Information Theory
  - *p(E)*: information content, also called the surprisal, of an event E
    - Surprisal of the event is low, p(E) is close to 1, if it is high, p(E) is close to 0.
  - *I(E)*: Information (or surprisal) of an event E:

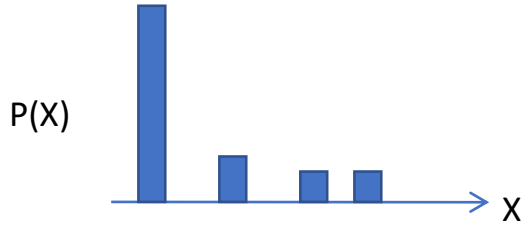
$$I(E) = \log_2\left(\frac{1}{p(E)}\right)$$

  - Entropy *H(X)*: expected value of the information

$$\mathrm{H}(X) = \mathrm{E}[\mathrm{I}(X)] = \mathrm{E}[-\log(\mathrm{P}(X))] = -\sum_{i=1}^{n} \mathrm{P}(x_i) \log_b \mathrm{P}(x_i)$$

Entropy

- P(X) encodes our uncertainty about X
  - Some variables are more uncertain than others



  - How can we quantify this intuition?
    - Information (or Surprise): $\log \frac{1}{p(x)}$
    - Entropy: average number of bits required to encode discrete R.V. X (expected value of the Surprise)

$$H_P(X) = E\left[\log \frac{1}{p(x)}\right] = \sum_x P(x) \log \frac{1}{P(x)} = -\sum_x P(x) \log P(x)$$

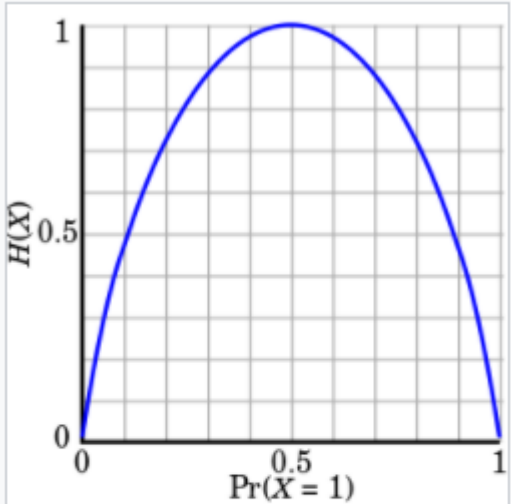
Binary Entropy

$$H_P(X) = E\left[\log \frac{1}{p(x)}\right] = \sum_x P(x) \log \frac{1}{P(x)} = -\sum_x P(x) \log P(x)$$

If $\Pr(X = 1) = p$, then $\Pr(X = 0) = 1 - p$ and the entropy of X (in shannons) is given by

$$\mathrm{H}(X) = \mathrm{H_b}(p) = -p \log_2 p - (1 - p) \log_2 (1 - p),$$

- Ex: Binary entropy:
  - In normal case, p(X=1) = p(X=0) = ½
  - If p=0.7: H(X) = -0.7*$\log_2$(0.7)-0.3*$\log_2$(0.3)=0.8816

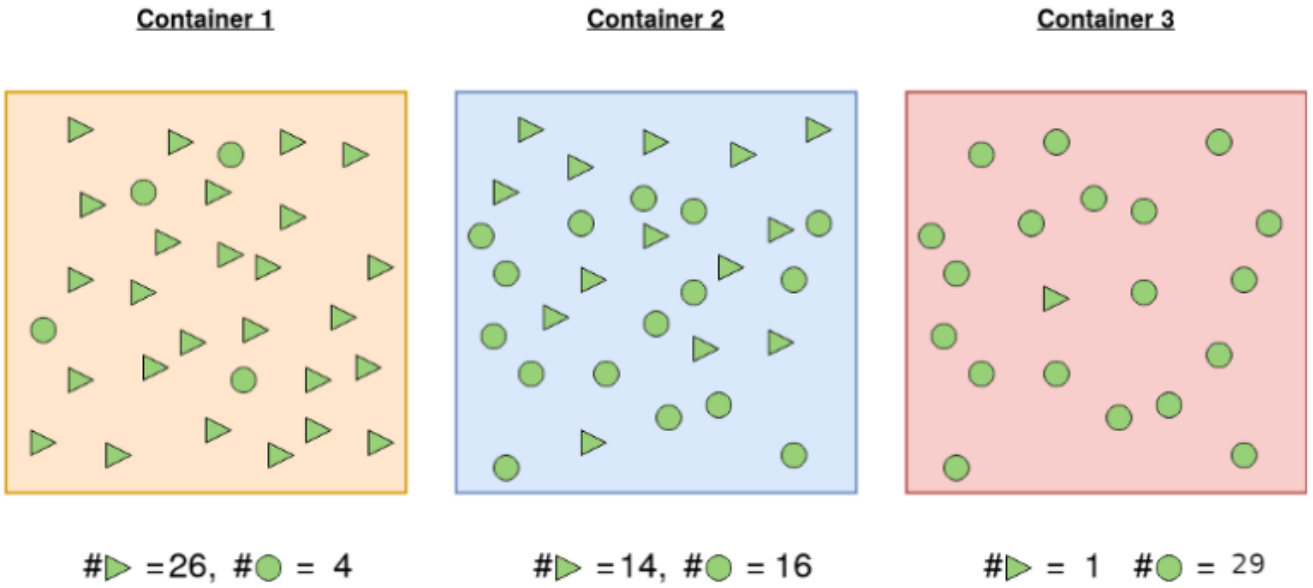


Entropy of a Bernoulli trial as a function of binary outcome probability, called the **binary entropy function.**

Ref: en.wikipedia.org

Entropy

- Can also be used a classification criteria (loss):



$$H(X) = -\sum_{x} p(x)\log(p(x))$$
$$= -[p(x_1)\log_2(p(x_1)) + p(x_2)\log_2(p(x_2))]$$
$$= -\left[\frac{26}{30}\log_2\left(\frac{26}{30}\right) + \frac{4}{30}\log_2\left(\frac{4}{30}\right)\right]$$
$$= 0.5665$$

H(X) = 0.9968

H(X) = 0.2108

- **We can use Entropy to quantify the similarity and difference.**

Cross Entropy, KL Divergence

- Cross Entropy (CE)
  - For discrete distribution *p* and *q* with the same support (the set of values that the random variable can take) X,

$$H(p, q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x)$$

- KL Divergence
  - Measure how one probability distribution P(x) is different from a second (reference distribution) Q(x)

$$D_{\mathrm{KL}}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \log\left(\frac{P(x)}{Q(x)}\right)$$

$$\begin{aligned} H(p, q) &= H(p) + D_{KL}(p \parallel q) \\ &= -\sum_{i=0}^{n} p(x_i) log(p(x_i)) + \sum_{i=0}^{n} p(x_i) log(p(x_i)) - \sum_{i=0}^{n} p(x_i) log(q(x_i)) \\ &= -\sum_{i=0}^{n} p(x_i) log(q(x_i)) \end{aligned}$$

(*) If *p, q* perfectly match, D_{KL}(p||q) =0, and the lower D_{KL} is, the better match.

Cross Entropy (CE) and CE Loss

- Cross Entropy (CE)
  - CE of the distribution *q* relative to a distribution *p* over a given set is defined:

$$H(p, q) = -\mathrm{E}_p[\log q]$$

  - It may be formulated using KL-divergence as:

$$H(p, q) = H(p) + D_{\mathrm{KL}}(p \parallel q)$$

  - For discrete probability distribution *p* and *q,* it means:

$$H(p, q) = -\sum_{x \in \mathcal{X}} p(x)\, \log q(x)$$

- CE Loss:
  - CE can be used to define a loss function in machine learning. For true probability p_i is the true label, and the given distribution q_i is the predicted value (called log loss):
  - For binary case:

$$H(p, q) \;=\; -\sum_i p_i \log q_i \;=\; -\,y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

Performance Metrics - Regression

- **MSE and MAE**
  - MSE(Mean squared error)
  - MAE(Mean absolute error)
  - MAE 가 이상치(outlier)에 대해서는 MSE 보다 robust 하다고 알려짐.

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 \qquad \mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

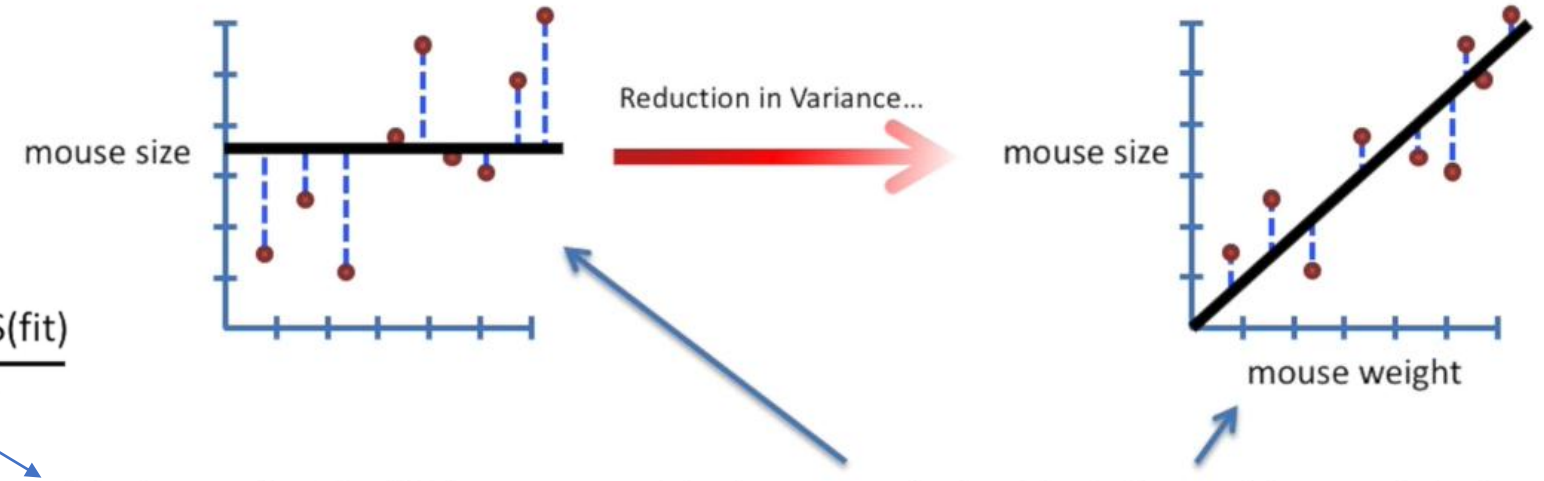
- **R Squared (R^2)**
  - 실제 출력 값에 대한 예측 출력 값 세트의 우수성 또는 적합성 표시
  - Numerator(MSE), denominator(variance)
  - What if all Yi is correctly predicted?
  - What if all Yi is predicted as the mean?

SS: sum of squares around mean, fit

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2}{\sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2} = \frac{\mathrm{SS(mean)} - \mathrm{SS(fit)}}{\mathrm{SS(mean)}}$$

- R^2=0 means that the model predicts the expected value of *y* disregarding the input features.

Performance Metrics – R-squared



$$\frac{SS(mean) - SS(fit)}{SS(mean)}$$

$$R^2 = \frac{Var(mean) - Var(fit)}{Var(mean)} \rightarrow \frac{Var(mouse\ size) - Var(after\ taking\ weight\ into\ account)}{Var(mouse\ size)}$$

$$R^2 = \frac{\text{The variation in mouse size explained by weight}}{\text{The variation in mouse size without taking weight into account}}$$

Proportion of variance (of y) that has been explained by the feature variables in the model.

https://www.youtube.com/watch?v=nk2CQITm_eo&list=PLblh5JKOoLUIzaEkCLIUxQFjPIlapw8nU&index=2 (StatQuest with Josh Stammer)

Performance Metrics - Regression

- Adjusted **R^2**
  - One limitation of R^2 : it increases by adding feature variables -> may be misleading since some added variables might be useless.
  - Adjusted R^2 avoids this by giving penalty if we make an attempt to add feature variable that does not improve the model (not solely based on the number of features)
    - Penalty is best understood bas the balance between the number of feature variables and the number of observations.
  - Adjusted R^2 takes into account the number of predictors in the model.
  - If useless feature added -> it will decrease, and if useful feature added -> it will increase.
  - In statistical terms, adding a feature is a loss of one degree of freedom and that carries a cost.

$$R_a^2 = 1 - (1 - R^2)\frac{n-1}{n-p-1}$$

p : number of feature variables
n : number of samples
n-p-1 : degree of freedom

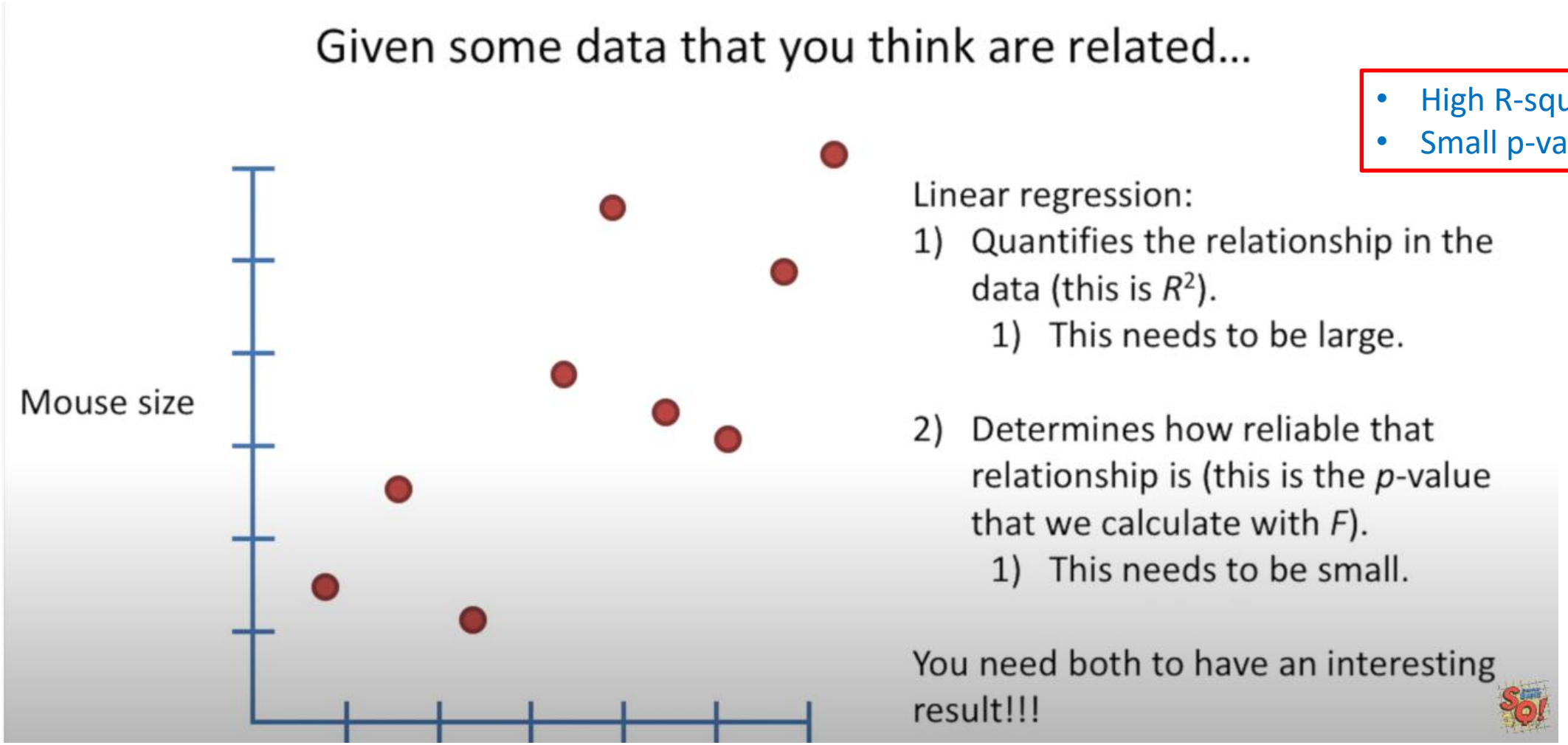
The R^2 is statistically significant? -> *p-value*

- **F-Test in regression**
  - Unlike t-tests that can assess only one regression coefficient at a time, the F-test can assess multiple coefficients simultaneously.
  - The F-test of the overall significance is a specific form of the F-test. It compares a model with no predictors to the model that you specify. A regression model that contains no predictors is also known as an intercept-only model.
  - Hypothesis for the F-test of the overall significance:

    - **H0**: The fit of the intercept-only model and your model are equal.
    - **H1**: The fit of the intercept-only model is significantly reduced compared to your model.
    - p-value < 0.05 means to reject H0;
      - the feature is dependent (coefficient not zero)
      - the feature is significant

  - While R-squared provides an estimate of the strength of the relationship between your model and the target variable, it does not provide a formal hypothesis test for this relationship. The overall F-test determines whether this relationship is statistically significant. If the P value for the overall F-test is less than your significance level, you can conclude that the R-squared value is significantly different from zero.

p-value in Regression



- High R-squared
- Small p-value

https://www.youtube.com/watch?v=nk2CQITm_eo&list=PLblh5JKOoLUIzaEkCLIUxQFjPIlapw8nU&index=2 (StatQuest with Josh Stammer)

Performance Metrics - classification

- **Classification – static, dynamic**
- **Static: confusion matrix (a.k.a. Error matrix)**
  - Tabular visualization of the model prediction vs. ground-truth labels
  - Row: the instances in a predicted class
  - Column: the instances in an actual class

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

  - True-positive (100), false-negative (5)
  - true-negative (50), false-positive (10)

Performance Metrics - classification

- **Accuracy**
  - Number of correct predictions divided by the total number of predictions
  - (ex) accuracy = (100+50)/165
- **Precision**
  - In some cases, accuracy is not a good indicator of your model performance, for example, when your class distribution is imbalanced.
  - Precision_yes = 100/110, Precision_noncat = 50/55
  - Says "**How reliable your prediction is…**" or "how much I can trust…"
- **Recall**
  - Recall_yes = 100/105
  - Recall_no = 50/60
  - Says "**how many actual class samples are correctly predicted**…"
- **F1-Score**
  - Combine the above two metrics (precision and recall) as harmonic mean:

    F1-score = 2*Precision*Recall / (Precision+Recall)

Performance Metrics - classification

- **Dynamic: ROC Curve (Receiver Operating Characteristic curve)**
  - Shows the performance of a binary classifier as function of its cut-off threshold
  - It essentially shows the true positive rate(tpr) against the false positive rate(fpr) for various threshold values.
- **As an example,**
  - Suppose your model predicts 4 sample images with probabilities [0.45, 0.6, 0.7, 0.3].
  - Then, depending on the threshold, you will get different labels:

    cut_off=0.5: predicted_value=[0,1,1,0] (default threshold)
    cut_off=0.2: predicted_value=[1,1,1,1]
    cut_off=0.8: predicted_value=[0,0,0,0]

  - Making different confusion matrix depending on the threshold.

Performance Metrics (example)

환자번호	성별	점수	순위	실제 값		
7	F	0.98	1	N (0)	FP	
125	M	0.96	2	C (1)	TP	
4	F	0.95	3	N	FP	
199	M	0.86	4	C	TP	
2	F	0.84	5	N	FP	
200	M	0.82	6	C	TP	
176	M	0.81	7	C	TP	
73	M	0.80	8	N	FP	
82	M	0.79	9	C	FN	TP
3	F	0.77	10	N	TN	FP
123	F	0.76	11	N	TN	FP
		...		C	FN	TP
43	F	0.48	198	N	TN	FP
93	M	0.42	199	N	TN	
120	F	0.40	200	N	TN	

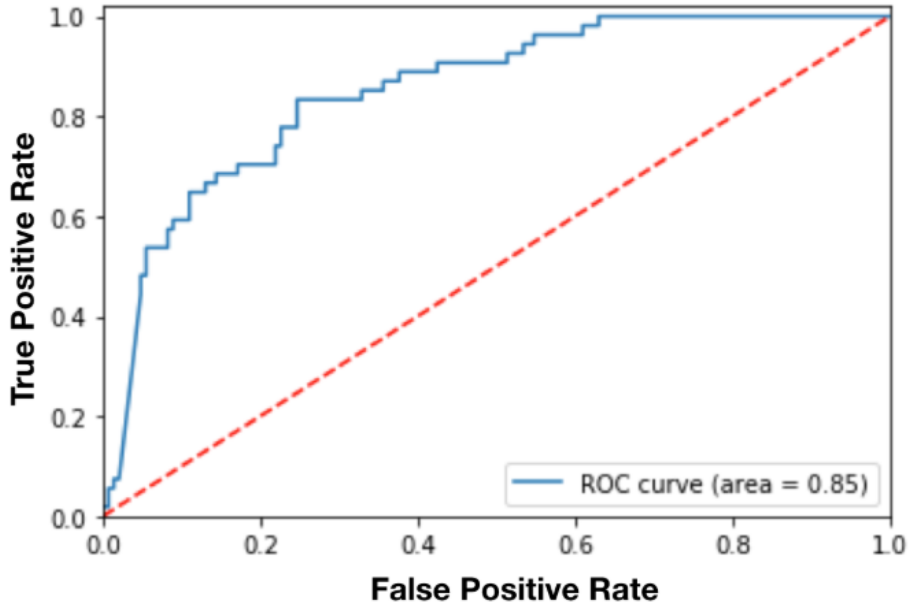
conservative

Different Confusion Matrices depending on the threshold

ROC/AUC (Example)

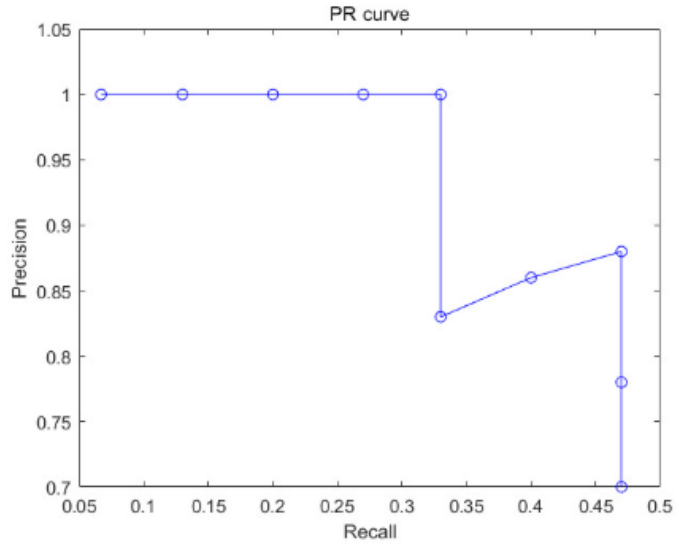
환자번호	성별	점수	순위	실제 값	TPr	FPr
7	F	0.98	1	N (0)	0	1/m
125	M	0.96	2	C (1)	1/n	
4	F	0.95	3	N		2/m
199	M	0.86	4	C	2/n	
2	F	0.84	5	N		3/m
200	M	0.82	6	C	3/n	
176	M	0.81	7	C	4/n	
73	M	0.80	8	N		4/m
82	M	0.79	9	C	5/n	
3	F	0.77	10	N		5/m
123	F	0.76	11	N		6/m
		...		C	6/n	
43	F	0.48	198	N	..	7/m
93	M	0.42	199	N	..	..
120	F	0.40	200	N	1	1

(*) score : probability of cancer
(*) depending on the threshold, you will get different confusion matrix

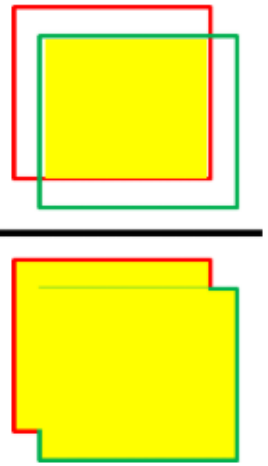


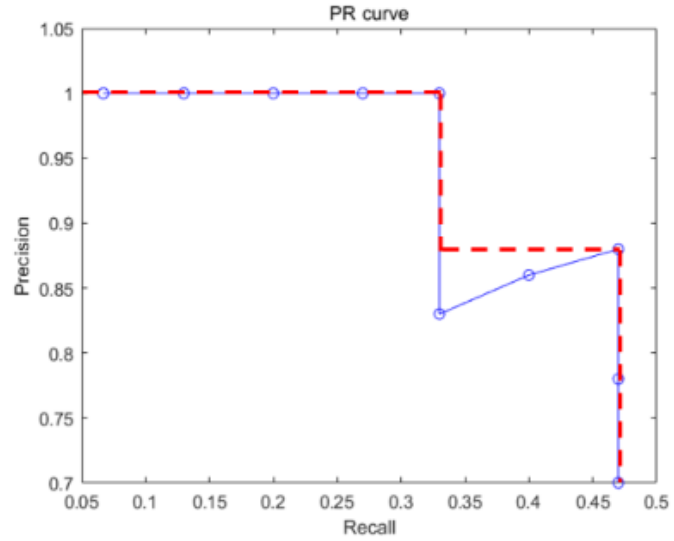
Performance Metrics (IoU and mAP)

- **Object detection and Image Classification**
  - IOU (Intersection over Union)
  - Average Precision (AP): average of precisions for Recall=0.1,0.2,…,1.0 (빨간선 아래 면적)
  - mAP (mean Average Precision) : mean of AP's of multiple objects



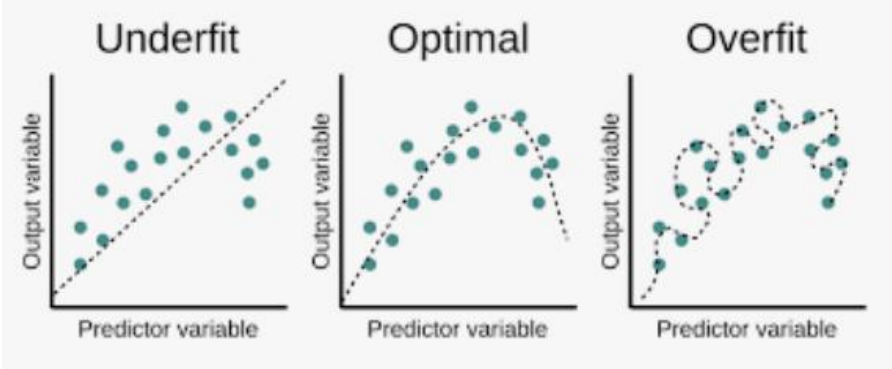
$$IoU = \frac{area(B_{gt} \cap B_p)}{area(B_{gt} \cup B_p)} =$$

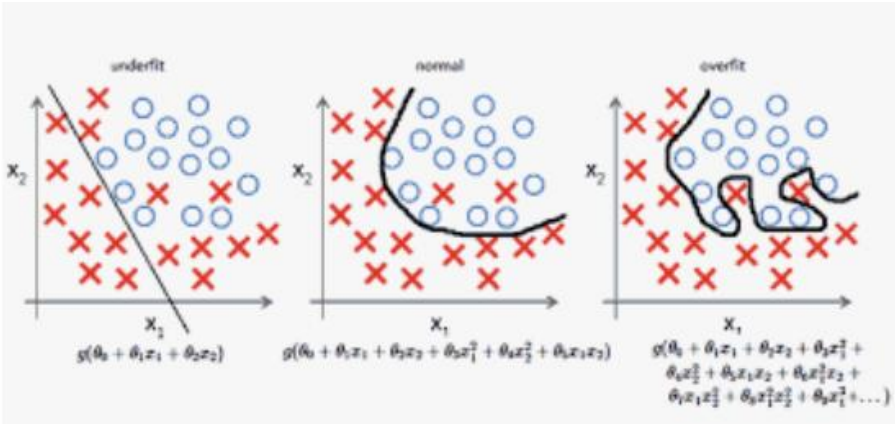




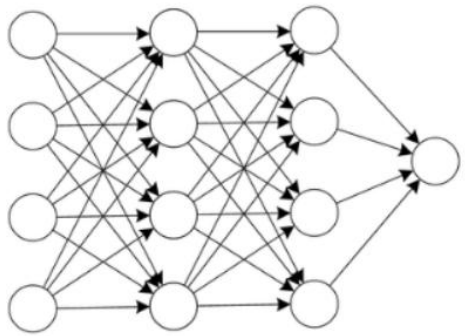
Overfitting and Underfitting

- **Overfitting** and **Underfitting**

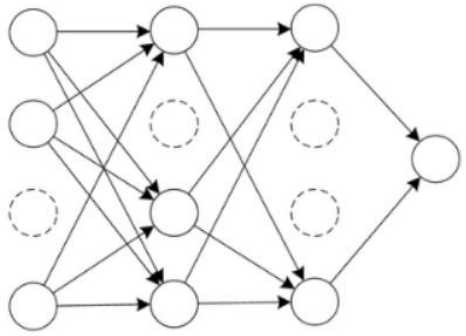




- **How to reduce overfitting?**
  - **More data**
  - **Simplify the model**
  - **Feature selection**
  - **Data augmentation**
  - **Regularization**
  - **Early stopping**
  - **Dropouts**



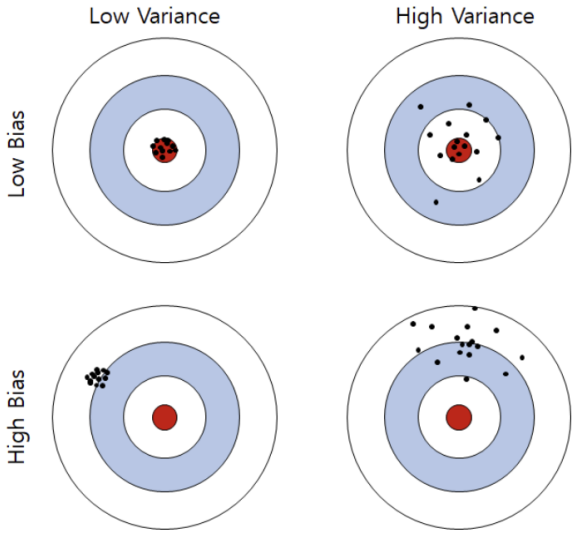
(a) Standard Neural Network

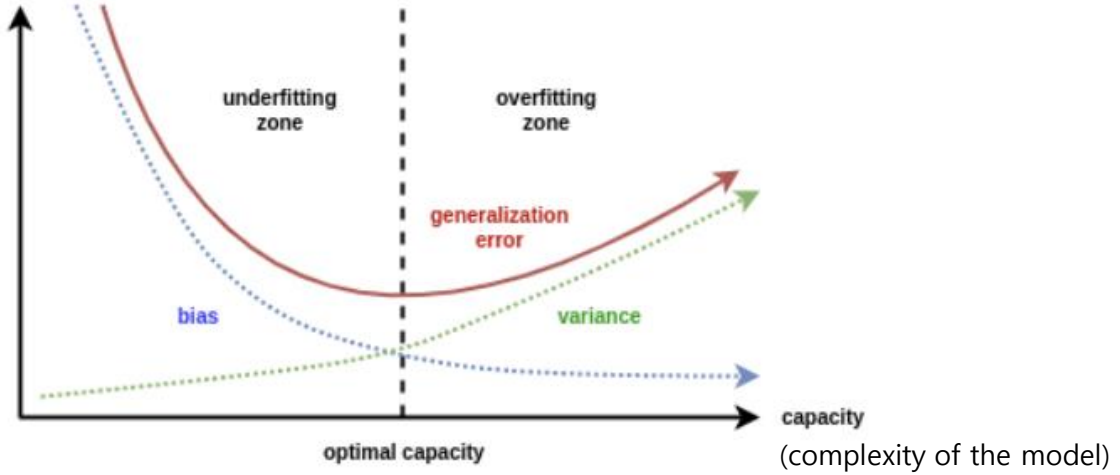


(b) Network after Dropout

Bias and Variance

- **Bias-Variance tradeoff (편향과 분산)**
  - Bias: difference between the average prediction of the model and the correct value (wrong model -> high bias -> underfitting)
  - Variance: variability of model prediction (noisy dataset -> high variance -> overfitting)
  - total error = Bias + Variance + noise

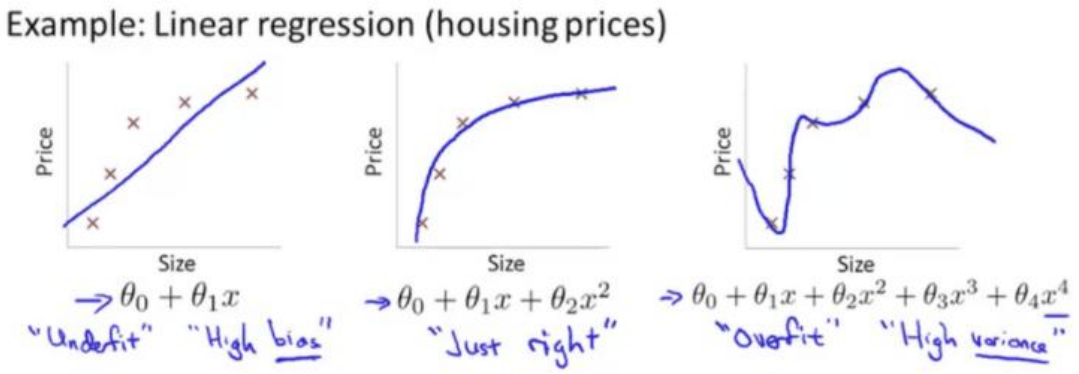




Bias-Variance tradeoff

Regularization

- **Regularization (규제화)**
  - Add information in objective function to reduce model complexity for reducing overfitting (regression and classification)
  - **Ridge** (L2): give more penalties on large-valued coefficients
  - **Lasso** (L1) (Least Absolute Shrinkage and Selection Operator): shrinks the less important features' coefficient to zero (good for **feature selection**)
  - **Elastic net**: use the both



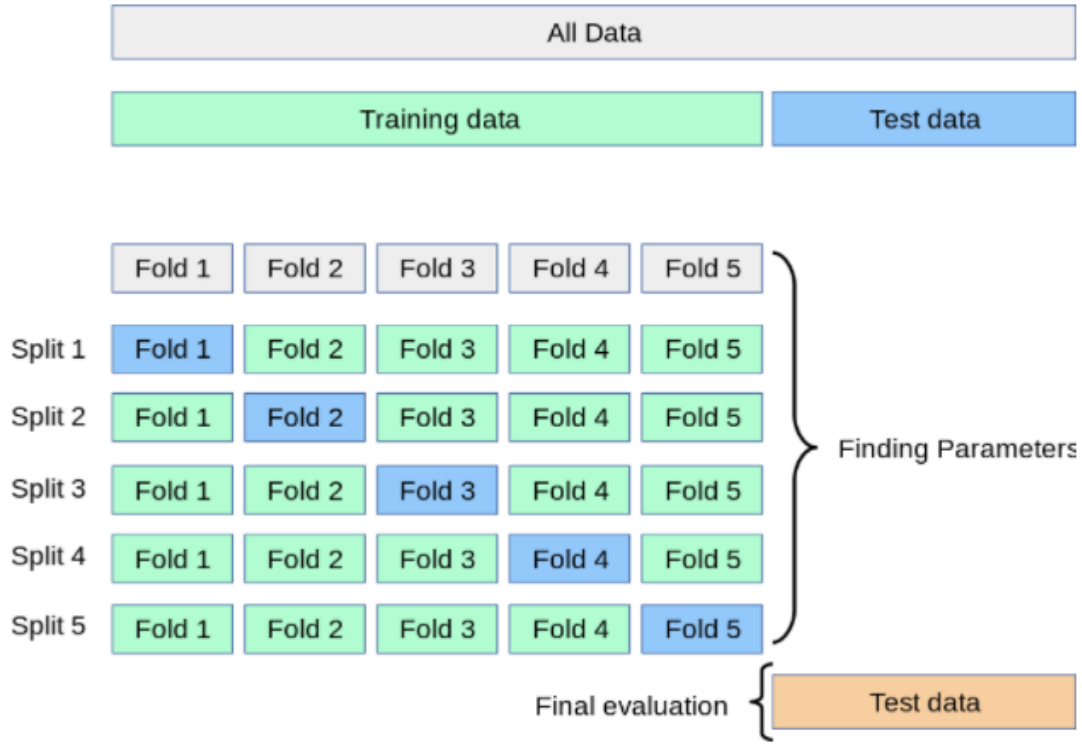
$$J(W) = MSE(W) + \alpha \frac{1}{2} \sum_{i=1}^{n} W_i^2$$

$$J(W) = MSE(W) + \alpha \sum_{i=1}^{n} |W_i|$$

$$J(\theta) = MSE(\theta) + \gamma\alpha \sum_{i=1}^{n} |\theta_i| + \frac{1-\gamma}{2} \alpha \sum_{i=1}^{n} \theta_i^2$$

K-Fold Cross Validation

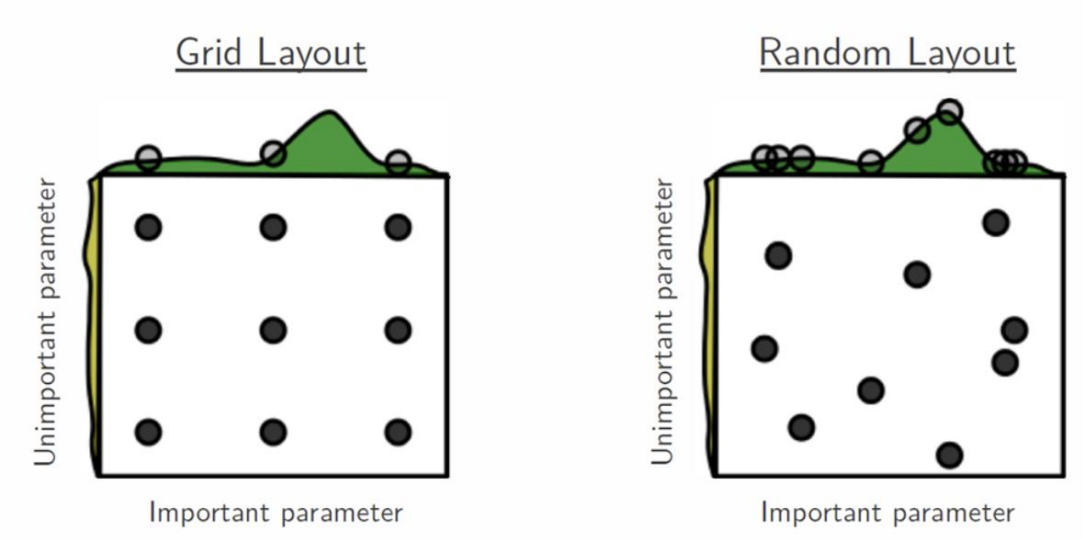
- **(stratified) K-Fold Cross Validation**
  - Helps to generalize the model (average)
  - Can see how the model is robust, and data is reliable




```
>>> from sklearn.model_selection import cross_val_score
>>> clf = svm.SVC(kernel='linear', C=1, random_state=42)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores
array([0.96..., 1. , 0.96..., 0.96..., 1. ])
```

Hyperparameter Tuning

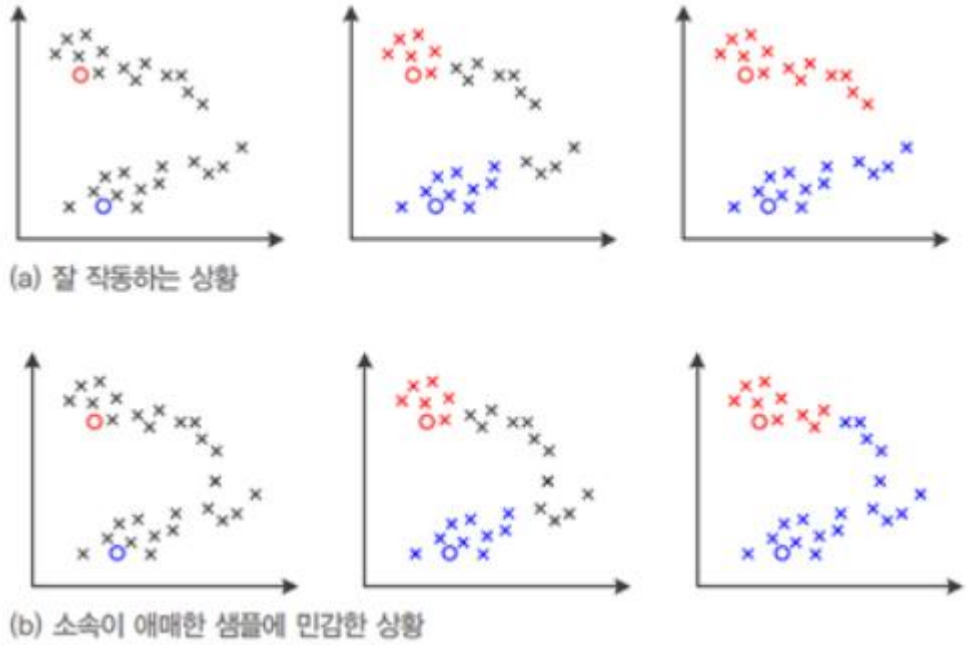
- **Hyperparameter tuning**
  - Grid Search: select the best among possible combination of hyperparameters
  - Random search: provide a statistical distribution or ranges for search
  - Fine-tuning: do the fine-tuning around the candidate points



6. Other Machine Learning Concepts

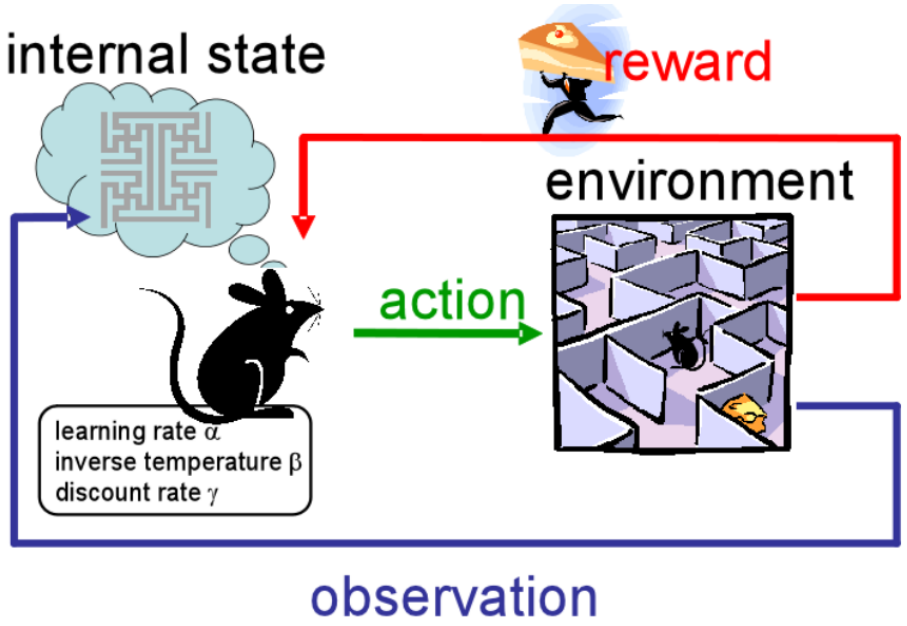
Semi-supervised Learning

- **Semi-supervised**
  - **모델이 스스로** 레이블이 없는 대량의 데이터를 활용하여 학습을 개선.
  - Extensive unlabeled data with small labeled data
  - Will unlabeled data be helpful? Yes or No
  - Self-training:
    - Train with labeled data
    - Classify unlabeled data
    - Select samples with high confidence and include them in labeled data
    - Retrain the classifier
    - Repeat
  - Using GAN and many others



Reinforcement Learning

- **Reinforcement learning**
  - A computer learns to perform a task through repeated trial-and-error interactions with a dynamic environment.
  - It enables the computer to make a series of decisions that maximize a reward (with human intervention and explicit program).



Practical issues in machine learning

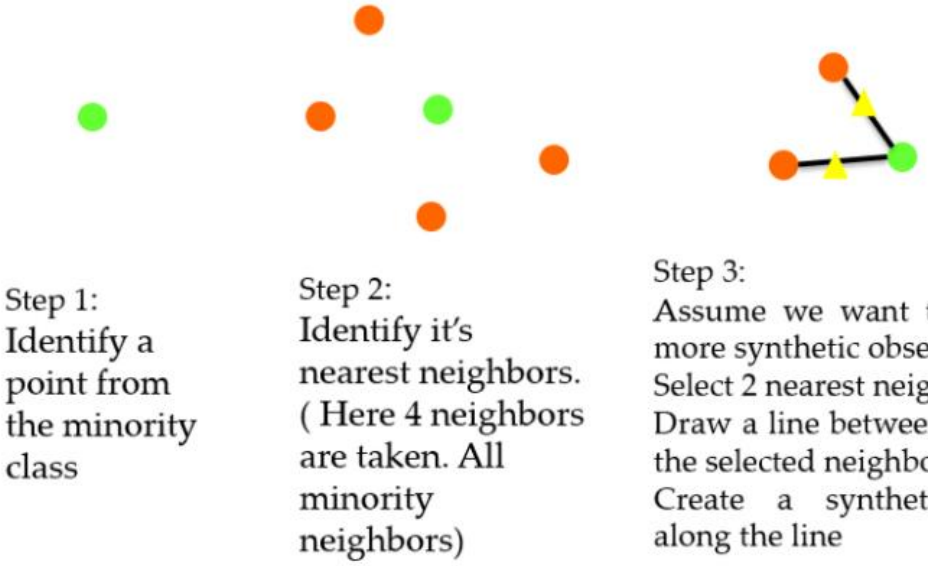
issue	result	method
Data volume, velocity, and scalability	• May be infeasible due to constraints in algorithms and hardware	• Data sampling (stratified sampling, varying sample sizes)
Data quality and noise (missing values, duplicate values, incorrect values, Incorrect formatting)	• Incorrect or incomplete model	• data cleaning
Imbalanced data	• affects the choice of learning, the process of selecting algorithms, model evaluation and verification • May suffer large biases	• cost-sensitive learning, ensemble learning, outlier detection
Overfitting	• Poor performance (to unseen data)	• More data, simple model, regularization, early stopping, dropout
Curse of dimensionality (too many features)	• Introduce **sparsity** (fewer data points on average per unit volume of feature space), hence poor performance (in distance-based models)	• Dimension reduction • Feature selection • Feature engineering

Imbalance Problems

- **Class imbalance problem**
  - Class distributions are highly imbalanced in the training dataset
  - Tend to have low prediction accuracy for the infrequent (minority) class
  - Exists in many real word classification problems, such as fraud detection, spam detection, threat-object detection, anomaly detection, etc.
  - Causes: properties of the domain, biased sampling, measurement error
- **How to reduce the imbalance problem?**
  - Artificial resampling: over-sampling (replicating minority class), under-sampling of majority class
  - SMOTE(Synthetic Minority Oversampling TEchnique): make synthetic data points by finding the nearest neighbors to each minority sample
  - Augmentation or Use generative model for synthetic data
  - More weights on minority samples
  - Majority sample selection based on RL
  - Resampling is to be done only on Train dataset (not Test dataset !)
  - Still a hot research topic

Imbalance Problem

- **SMOTE (**Synthetic Minority Oversampling Technique**)**

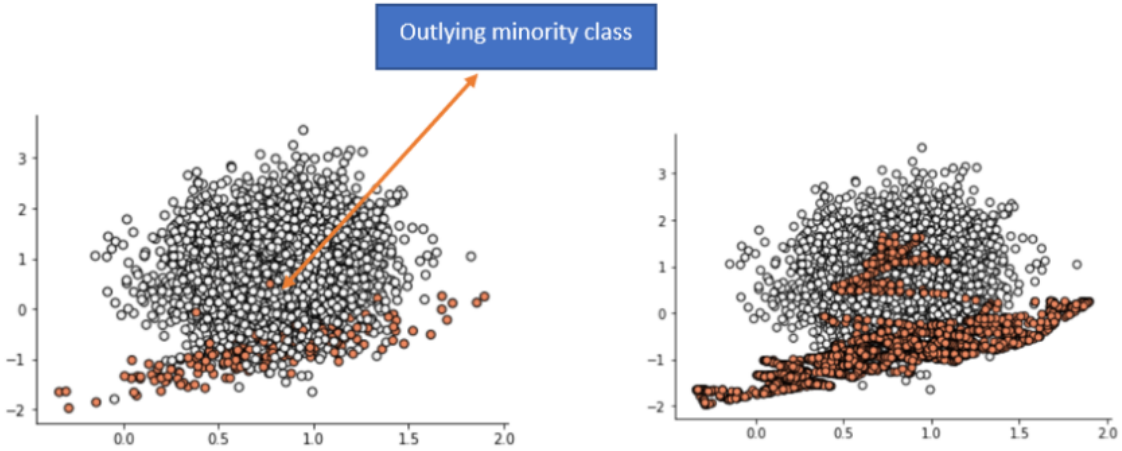


Step 1:
Identify a point from the minority class

Step 2:
Identify it's nearest neighbors. (Here 4 neighbors are taken. All minority neighbors)

Step 3:
Assume we want to add 2 times more synthetic observations
Select 2 nearest neighbor randomly
Draw a line between the point and the selected neighbors
Create a synthetic observation along the line

SMOTE, Synthetic Minority Observation Generation Process (Source: Author)

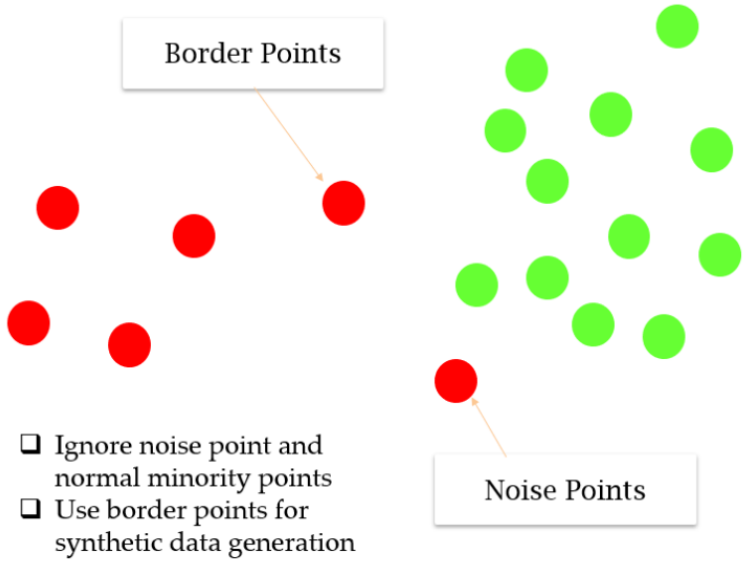


Left Side: Original Data Right Side: Data after SMOTE is Applied (Image Source: Author)

- If there are outlying minority classes and appear in the majority class, it creates a line bridge with the majority class. (problem!)

Imbalance Problem

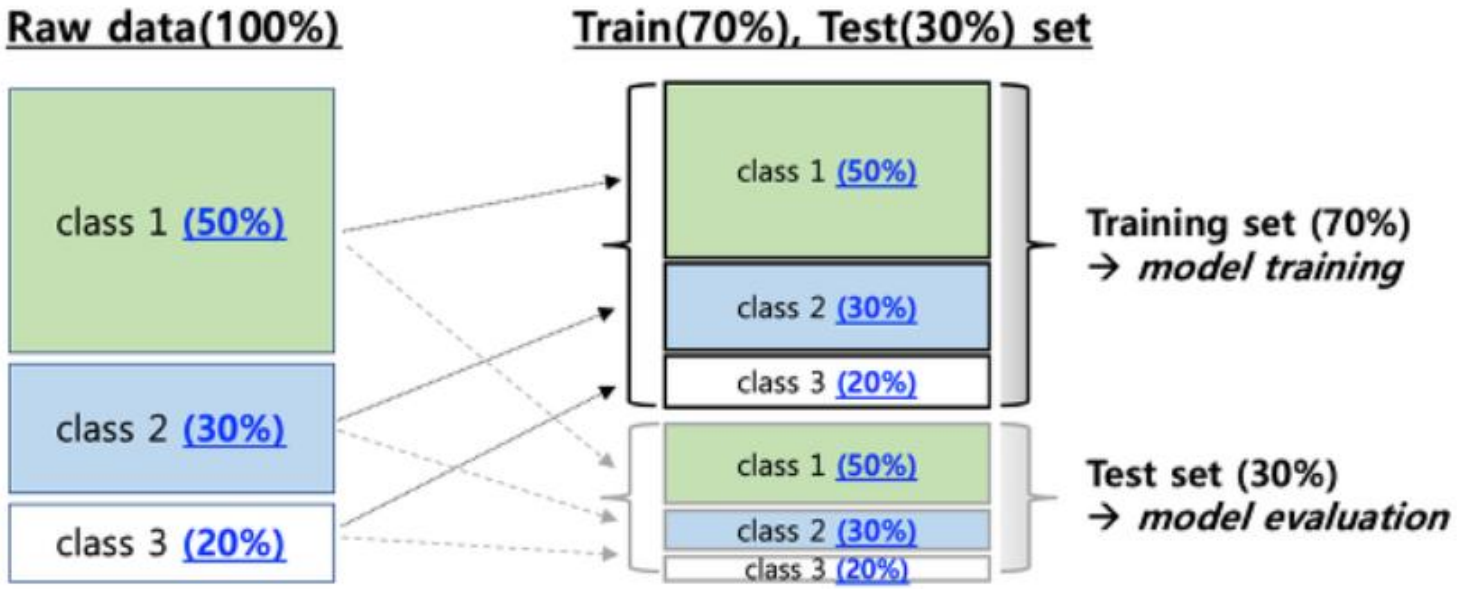
- **Borderline SMOTE**
  - Classify minority classes as noise point if all neighbors are the majority class – ignored.
  - Classifies a few points as border points that have both majority and minority class.
  - Resample only from border points.
  - **End up giving more attention to extreme observations.**
- More variants
  - ADASYN: generating more synthetic samples in areas where classification is difficult, such as where the density of minority examples is low.
  - and more …



Border Line SMOTE : (Image Source Author)

Imbalance Problem

- **Splitting dataset for Training and Testing**



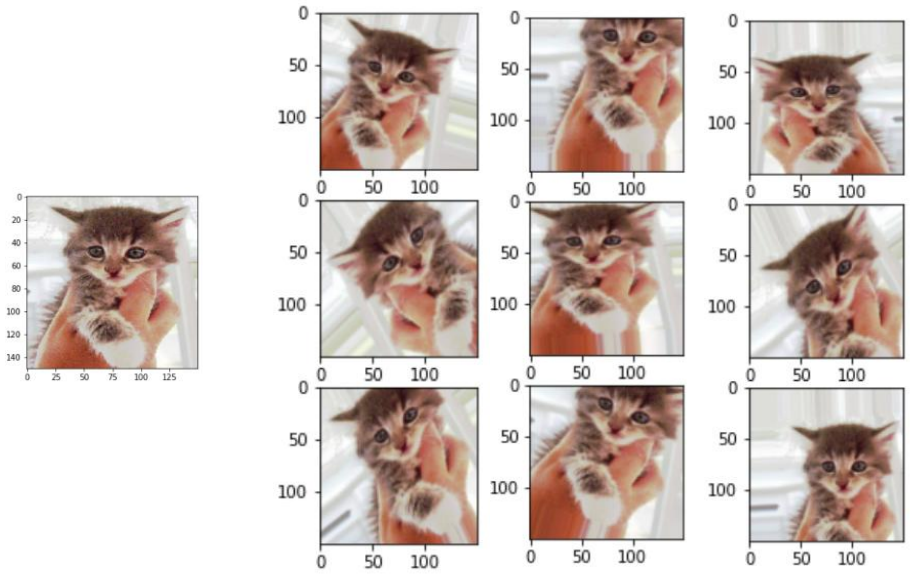
sklearn.model_selection.train_test_split(X, y, test_size=0.3, stratify=stratum_col)
→ *returns X_train, X_test, y_train, y_test set*

sklearn.model_selection.StratifiedShuffleSplit(n_splits=1, test_size=0.3)
→ *returns train/test set indices*

Ref: https://rfriend.tistory.com/520

Augmentation

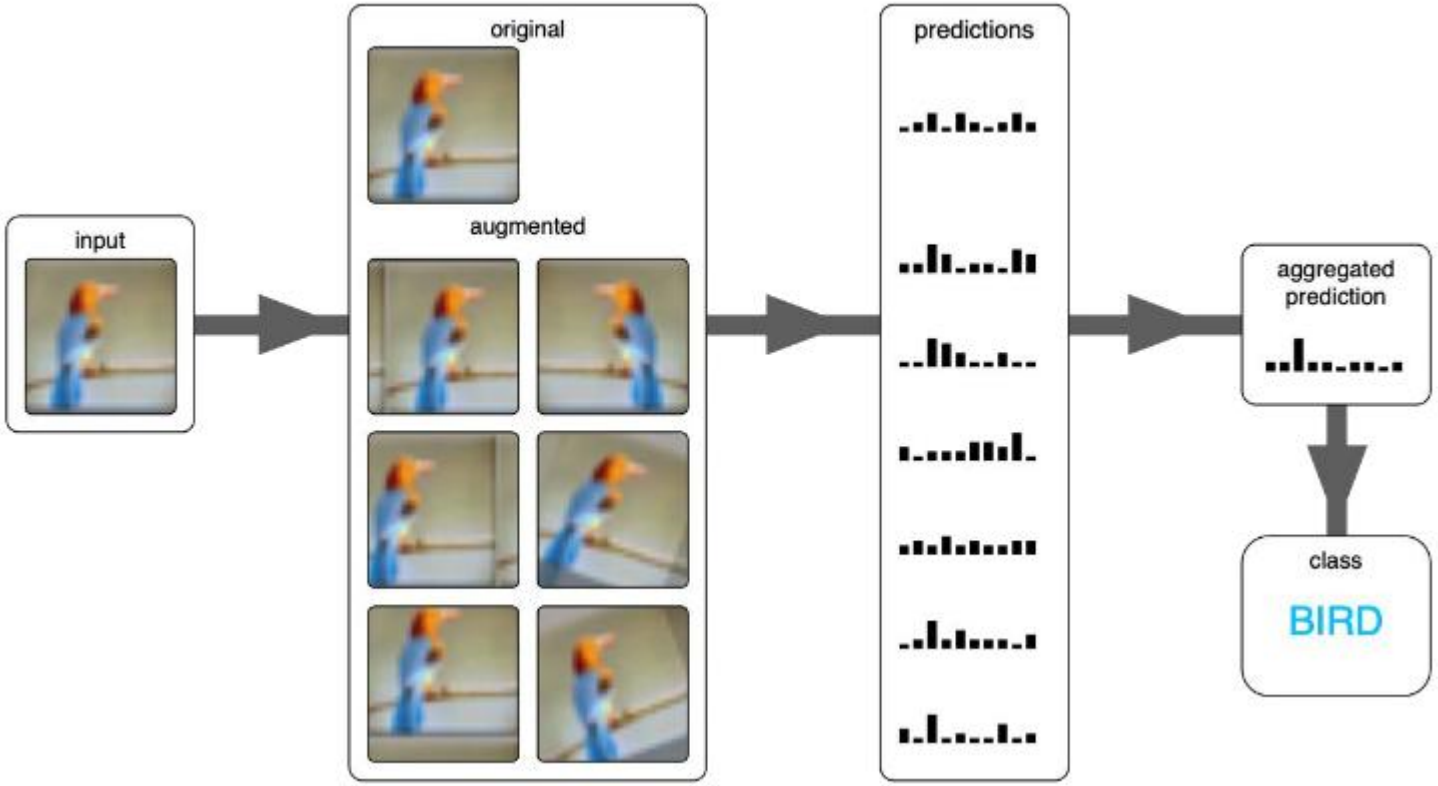
- **Augmentation (증강 or 확장)**
  - Increase the amount of data by adding slightly modified copies of existing data or newly created synthetic data from existing data
  - Introducing new synthetic images: transformation, GAN, image synthesis
  - Data augmentation for speech recognition based on RNN



```
train_datagen = ImageDataGenerator(
    rescale= 1./255,
    rotation_range = 40,
    width_shift_range = 0.2,
    height_shift_range = 0.2,
    shear_range=0.2,
    zoom_range=0.2,
    horizontal_flip = True)
```

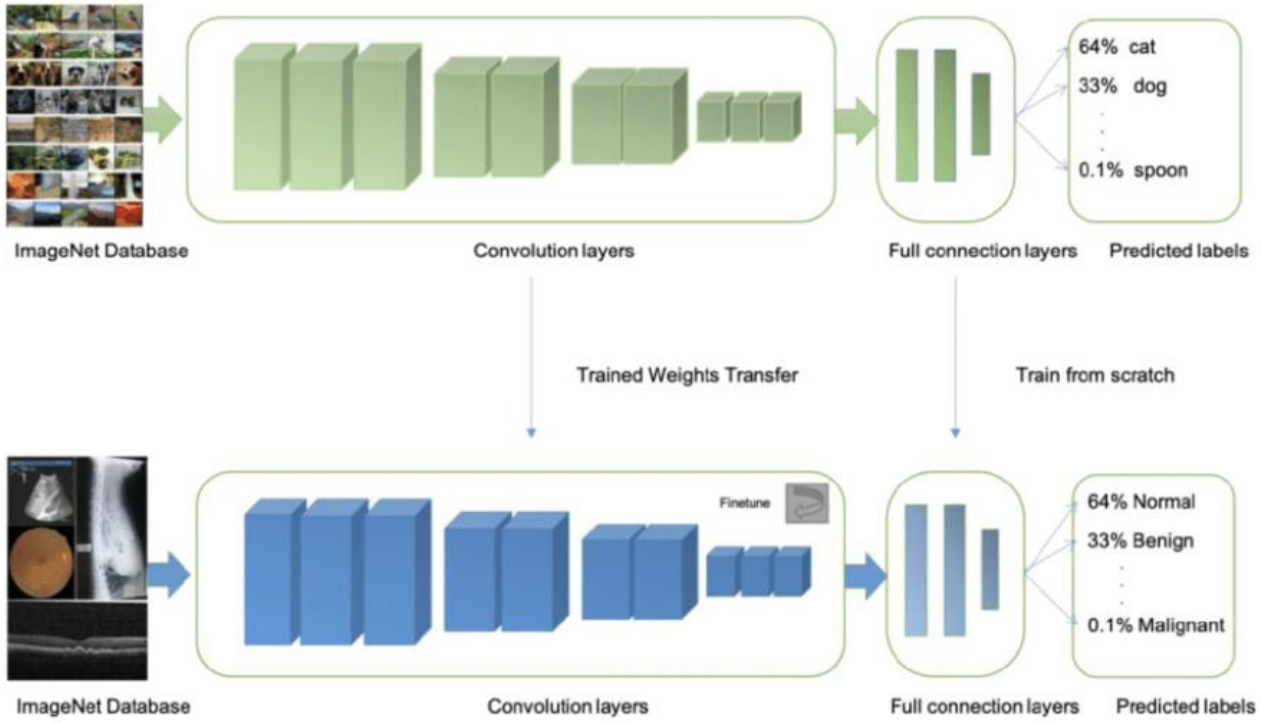
Test Time Augmentation

- **TTA (Test Time Augmentation)**
  - Use augmentation at Test time
  - Usually gives somewhat better performance



Transfer Learning

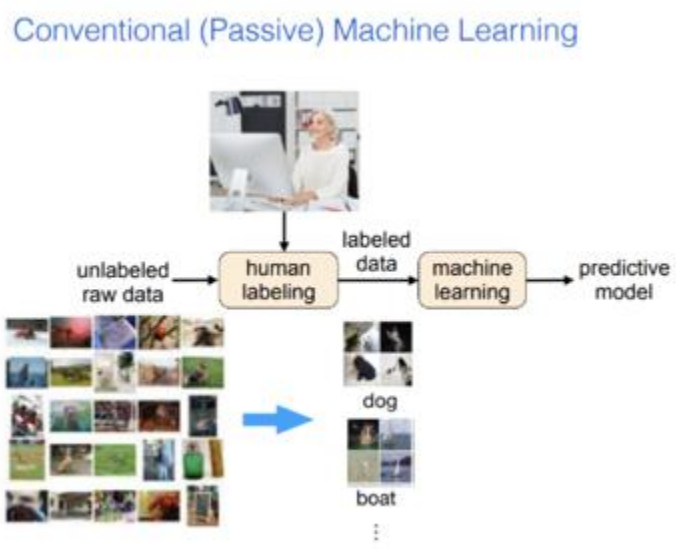
- **Transfer Learning (전이학습)**
  - A model trained on one task is reused on a second related task
  - Examples for image: Oxford VGG model, Google Inception model, Microsoft ResNet model
  - Examples for language data: Google's word2vec model, Stanford's Glove model

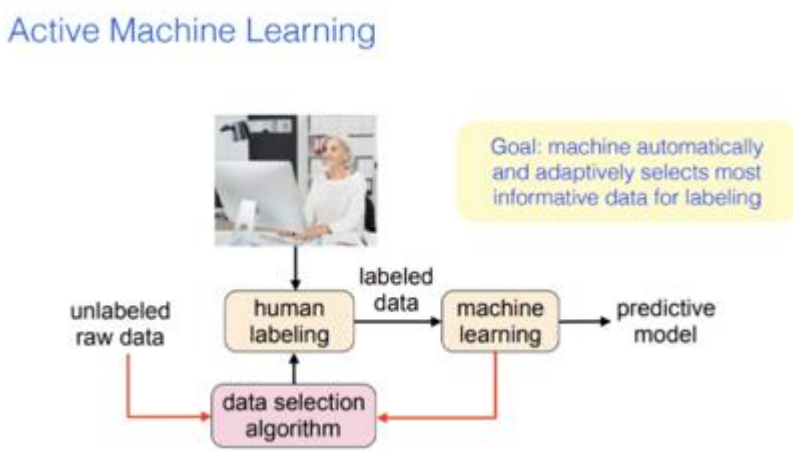


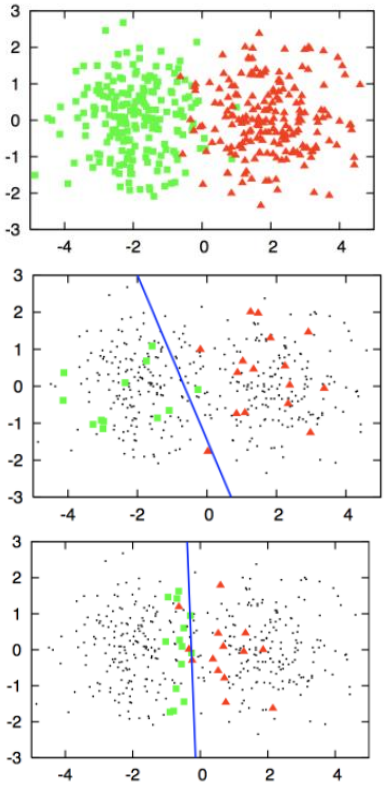
[ref: https://www.researchgate.net/figure/]

Active Learning

- **Active learning**
  - Semi-supervised 와 유사하지만 인간의 개입이 들어감.
  - Machine may do better labeling than human, or we may have many unlabeled samples.
  - Machine automatically and adaptively selects most informative data for labeling.
  - Many query (selection) strategies







poor selection

better selection

[ref: https://www.datacamp.com/community/tutorials/active-learning]

7. Machine Learning Libraries

Scikit-Learn design principle

- **Consistency**
  - **Estimators**: **estimate some parameters based on dataset**
    - `fit(X [,y])` method with some hyper-parameters
  - **Transformers: some estimators can transform a dataset**
    - `transform(X)` method
    - `fit_transform(X [,y])`: equivalent to calling `fit()` and `transform()`
  - **Predictors: making predictions**
    - `predict()` method : returns a dataset of corresponding predictions
    - `score()` method : measure the quality of the predictions
- **Inspection**
  - **Hyper-parameters** are accessed via instance variable (e.g. `imputer.strategy`)
  - Estimator's **learned parameters** are accessed via instance variable with an underscore suffix (e.g. `imputer.statistics_`)

Scikit-Learn design principle

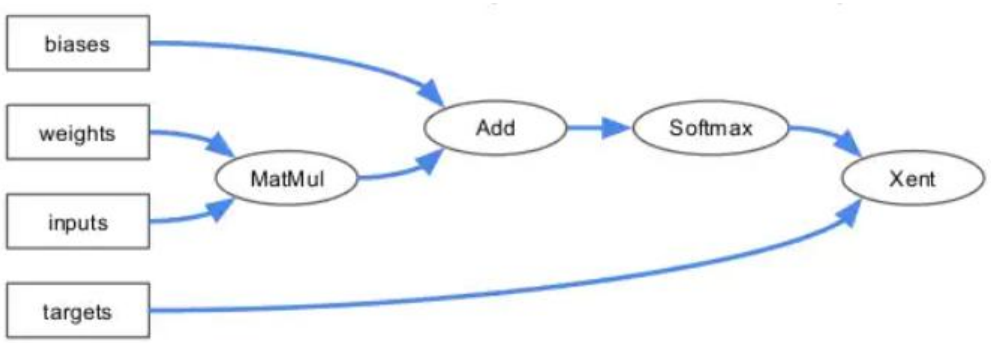
- **Nonproliferation of classes**
  - Datasets are represented as Numpy arrays or Scipy sparse matrices.
  - Hyper-parameters are just regular Python strings or numbers
- **Composition**
  - Existing building blocks are reused as much as possible.
  - For example, it is easy to create a `Pipeline` estimator from an arbitrary sequence of transformers followed by a final estimator.
- **Sensible defaults**
  - Provides reasonable default values for most parameters

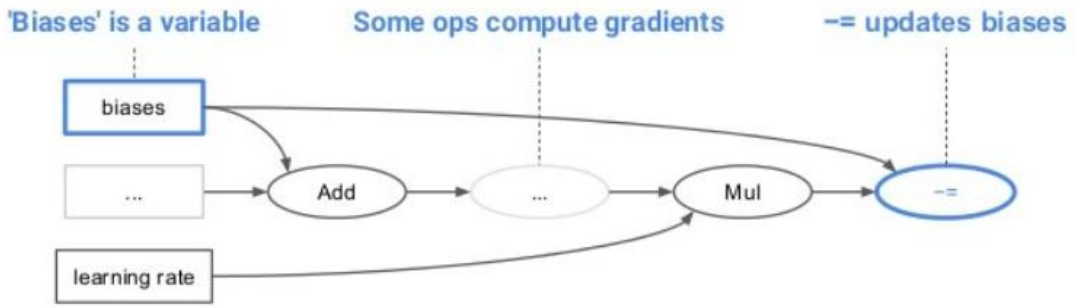
Tensorflow

- Google's open source library for machine learning
- Tensor: N-dimensional array
- Flow: data flow computation framework
- http://tensorflow.org
- Machine learning Framework based on data flow graph, automatic differentiation
- Tensorflow 0.5 Release (2015.11)
- C++ Core, Python API
- Several High-level API including Keras
- Define and Run (Graph and Session)

Tensorflow

- **Computation as a Dataflow Graph**
  - Graph of Nodes, also called operations (ops)





Forward:
- Edges are N-dimensional arrays: Tensors

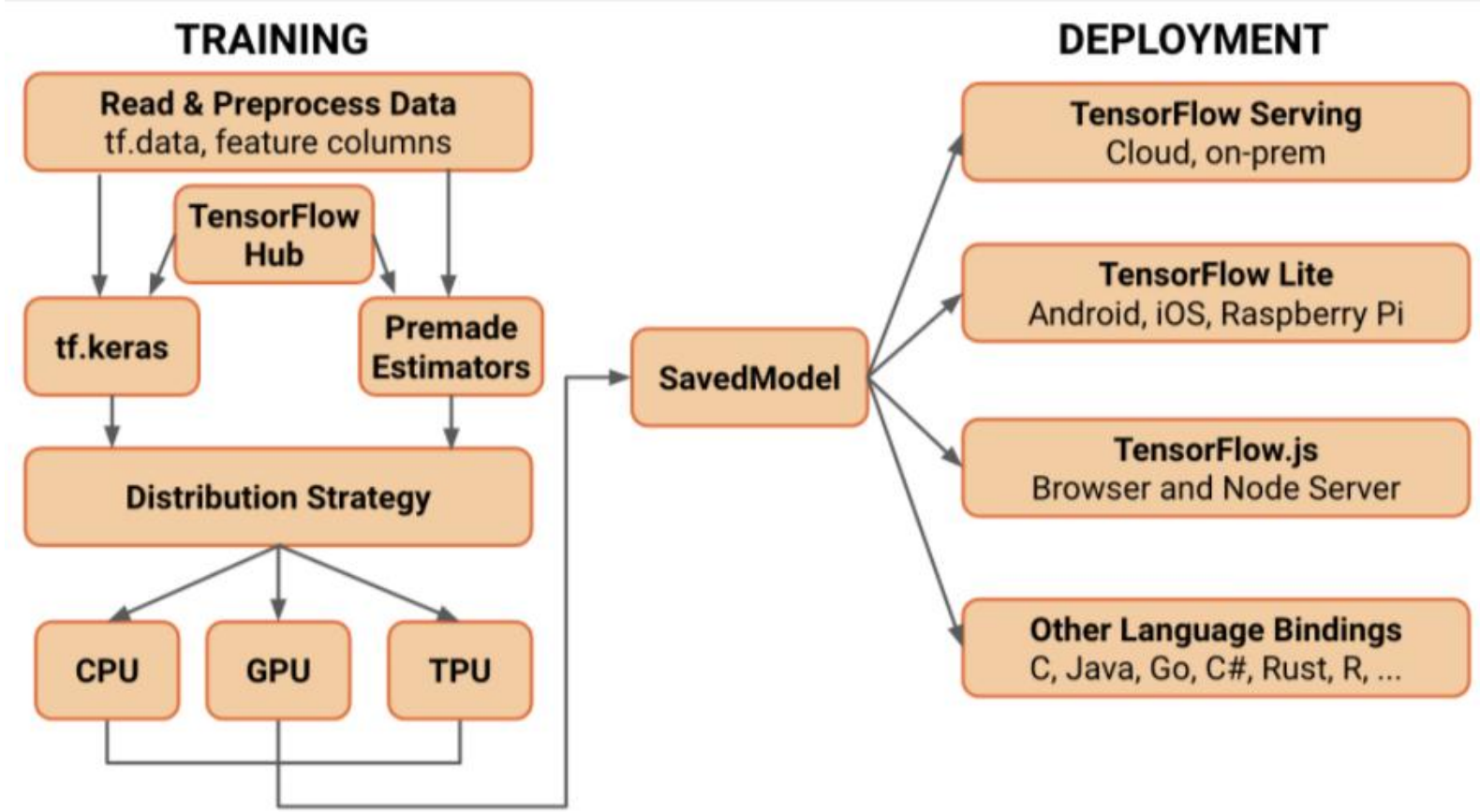
Backward graph and updates:
- Backward graph and update are added automatically to graph

Tensorflow 2.0

- Eager Execution (Define by Run):
  - easy debug
  - and rapid development
  - Autograph to boost performance
- Functions, not Session
- Keras Python API
- API Cleanup
- No more Globals
- Default since 2019
- Standard SavedModel file format
  - TensorFlow Serving (ML Servers)
  - Tensorflow Lite (for Mobiles or IoT)
  - TensorFlow.js (in JavaScript, and for browser)

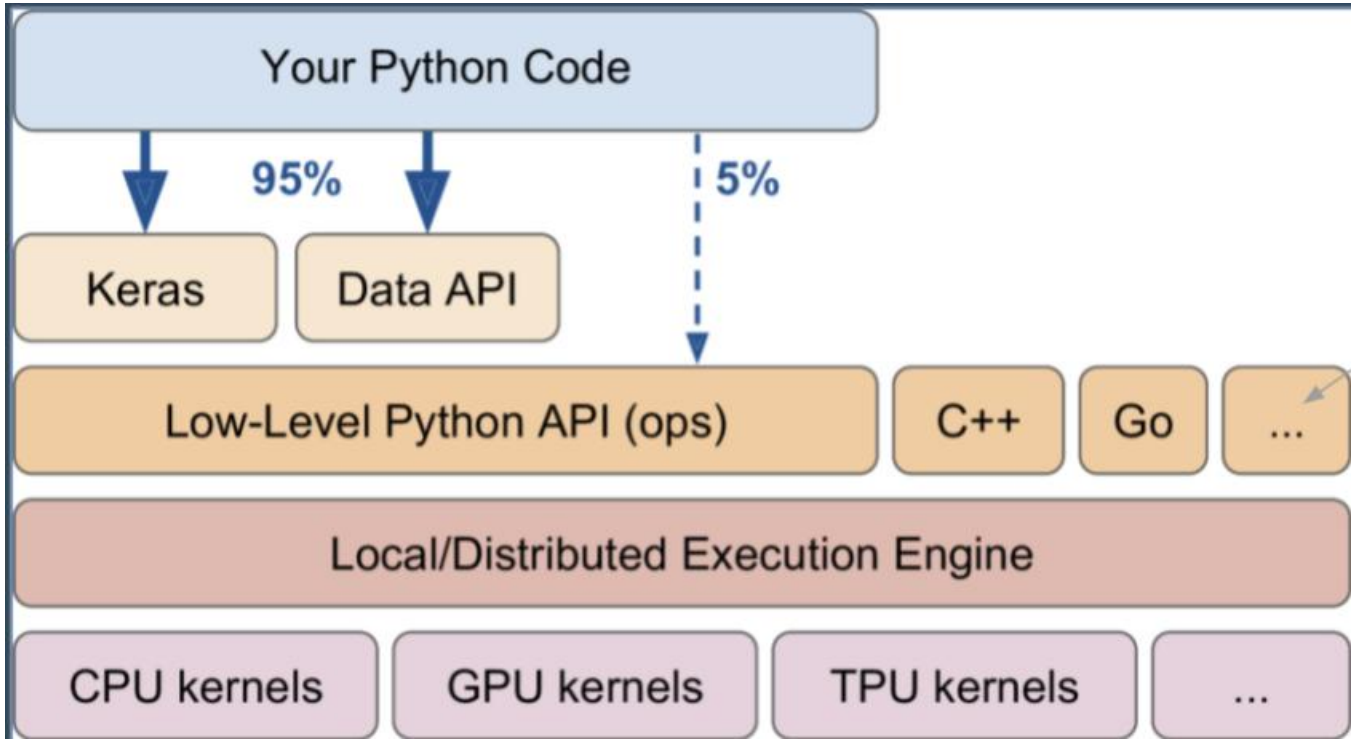
Tensorflow 2.0

- **TF2.0 Concept Diagram**



Keras

- High-level Neural Networks Specification (https://keras.io) (2015)
- Python API for TensorFlow 2.0 (2020)
- Deprecated tf.layer, tf.contrib.layers(Slim)



Tensorflow Keras

- **Sequential API**
  - Plain stack of layers (one input and one output tensor)

```
model = keras.Sequential(
    [
        layers.Dense(2, activation="relu"),
        layers.Dense(3, activation="relu"),
        layers.Dense(4),
    ]
)
```

```
model = keras.Sequential()
model.add(layers.Dense(2, activation="relu"))
model.add(layers.Dense(3, activation="relu"))
model.add(layers.Dense(4))
```

  - (ex) Transfer learning

```
# Load a convolutional base with pre-trained weights
base_model = keras.applications.Xception(
    weights='imagenet',
    include_top=False,
    pooling='avg')

# Freeze the base model
base_model.trainable = False

# Use a Sequential model to add a trainable classifier on top
model = keras.Sequential([
    base_model,
    layers.Dense(1000),
])

# Compile & train
model.compile(...)
model.fit(...)
```

Tensorflow Keras

- **Keras model**

```
from tensorflow import tf

model = tf.keras.Sequential()
# 64개의 유닛을 가진 완전 연결 층을 모델에 추가합니다:
model.add(tf.keras.layers.Dense(64, activation='relu'))
# 또 하나를 추가합니다:
model.add(tf.keras.layers.Dense(64, activation='relu'))
# 10개의 출력 유닛을 가진 소프트맥스 층을 추가합니다:
model.add(tf.keras.layers.Dense(10, activation='softmax'))

# 컴파일
model.compile(optimizer=tf.keras.optimizers.Adam(0.001),
              loss='categorical_crossentropy',
              metrics=['accuracy'])

# 모델 훈련
model.fit(train_data, labels, epochs=10, batch_size=32)
# 모델 평가
model.evaluate(test_data, labels)
# 샘플 예측
model.predict(new_sample)
```

```
model = tf.keras.Sequential([
    tf.keras.layers.Dense(64),
    tf.keras.layers.Dense(64),
    tf.keras.layers.Dense(10),
])
```

Tensorflow Keras

- **Functional API**
  - to create models in more flexible way
  - Can handle non-linear topology, shared layers, and multiple inputs or outputs
  - All Layers and Models are callable
  - Manipulate complex graph topologies
- **Built-in layers in Keras:**
  - Convolutional layers: Conv1D, Conv2D, Conv3D, Conv2DTranspose
  - Pooling layers: MaxPooling1D, maxPooling2D, AveragePooling1D
  - SimpleRNN, GRU, LSTM, ConvLSTM2D
  - BatchNormalization, Dropout, Embedding, etc.

```
encoder_input = keras.Input(shape=(28, 28, 1), name="original_img")
x = layers.Conv2D(16, 3, activation="relu")(encoder_input)
x = layers.Conv2D(32, 3, activation="relu")(x)
x = layers.MaxPooling2D(3)(x)
x = layers.Conv2D(32, 3, activation="relu")(x)
x = layers.Conv2D(16, 3, activation="relu")(x)
encoder_output = layers.GlobalMaxPooling2D()(x)

encoder = keras.Model(encoder_input, encoder_output, name="encoder")
encoder.summary()

decoder_input = keras.Input(shape=(16,), name="encoded_img")
x = layers.Reshape((4, 4, 1))(decoder_input)
x = layers.Conv2DTranspose(16, 3, activation="relu")(x)
x = layers.Conv2DTranspose(32, 3, activation="relu")(x)
x = layers.UpSampling2D(3)(x)
x = layers.Conv2DTranspose(16, 3, activation="relu")(x)
decoder_output = layers.Conv2DTranspose(1, 3, activation="relu")(x)

decoder = keras.Model(decoder_input, decoder_output, name="decoder")
decoder.summary()

autoencoder_input = keras.Input(shape=(28, 28, 1), name="img")
encoded_img = encoder(autoencoder_input)
decoded_img = decoder(encoded_img)
autoencoder = keras.Model(autoencoder_input, decoded_img, name="autoencoder")
autoencoder.summary()
```