

Machine Learning

2021. 8

Yongjin Jeong, KwangWoon University

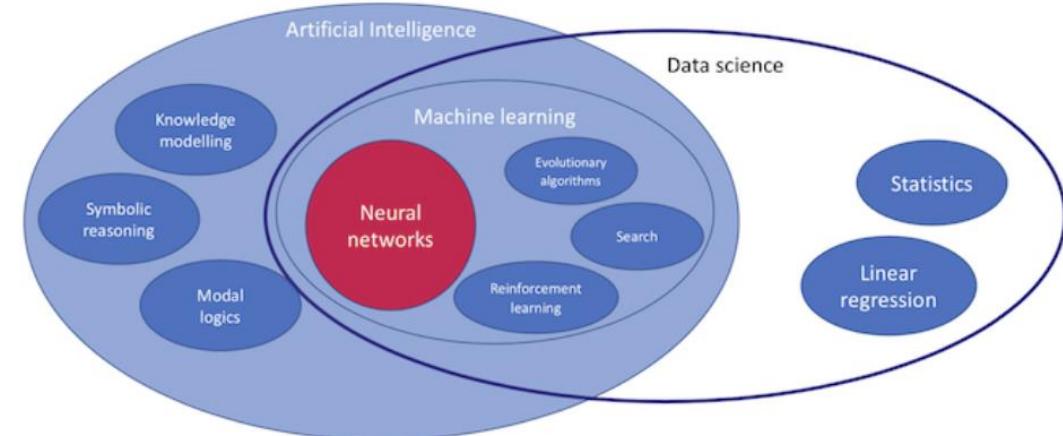
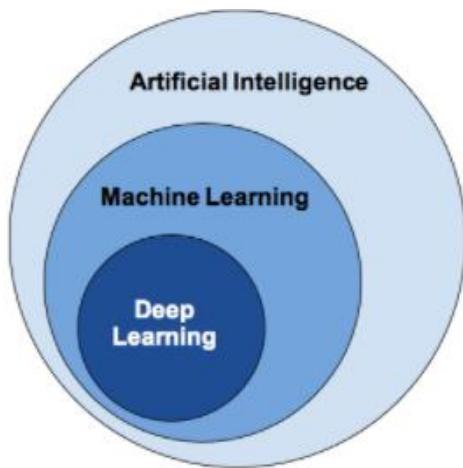
[참고] 본 자료에는 인터넷에서 다운받아 사용한 그림이나 수식들이 일부 있으니 다른 용도로 사용하거나 외부로 유출을 금해 주시기 바랍니다.

Contents

- What is machine Learning
- Supervised Learning
 - ✓ Regression
 - ✓ Classification
- Unsupervised Learning
 - Clustering
 - Dimension reduction (SelectPercentile, PCA, t-SNE)
- Anomaly Detection
- Problems in Machine Learning
 - Overfitting and Underfitting
 - Regularization
- Validation and Testing
 - Hyper-parameter Tuning
 - K-Fold Cross Validation

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/>

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



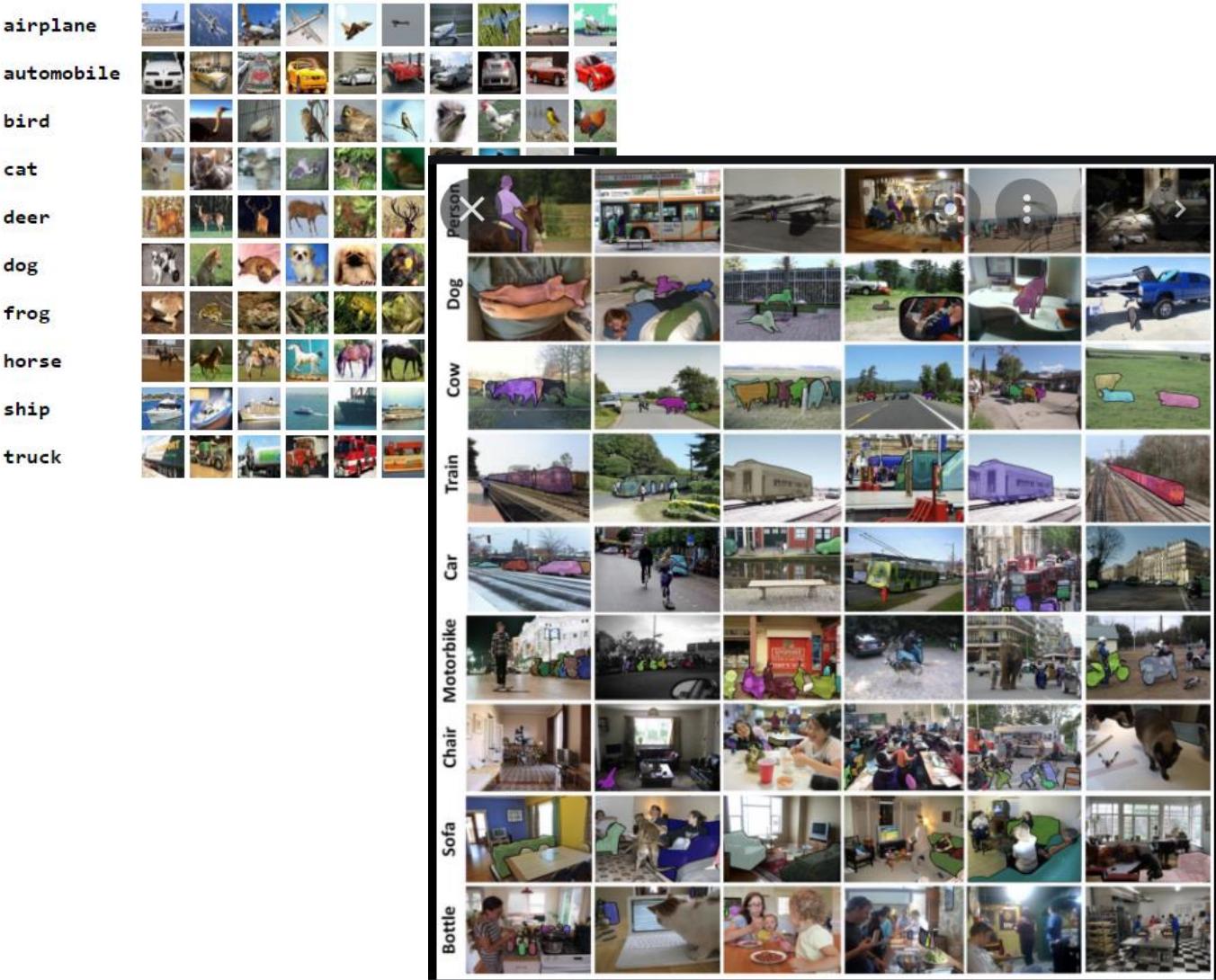
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 0 | 4 | 1 | 9 | 2 | 1 | 3 | 1 | 4 |
| 3 | 5 | 3 | 6 | 1 | 7 | 2 | 8 | 6 | 9 |
| 4 | 0 | 9 | 1 | 1 | 2 | 4 | 3 | 2 | 7 |
| 3 | 8 | 6 | 9 | 0 | 5 | 6 | 0 | 7 | 6 |
| 1 | 8 | 1 | 9 | 3 | 9 | 8 | 5 | 9 | 3 |
| 3 | 0 | 7 | 4 | 9 | 8 | 0 | 9 | 4 | 1 |
| 4 | 4 | 6 | 0 | 4 | 5 | 6 | 1 | 0 | 0 |
| 1 | 7 | 1 | 6 | 3 | 0 | 2 | 1 | 1 | 7 |
| 9 | 0 | 2 | 6 | 7 | 8 | 3 | 9 | 0 | 4 |
| 6 | 7 | 4 | 6 | 8 | 0 | 7 | 8 | 3 | 1 |



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

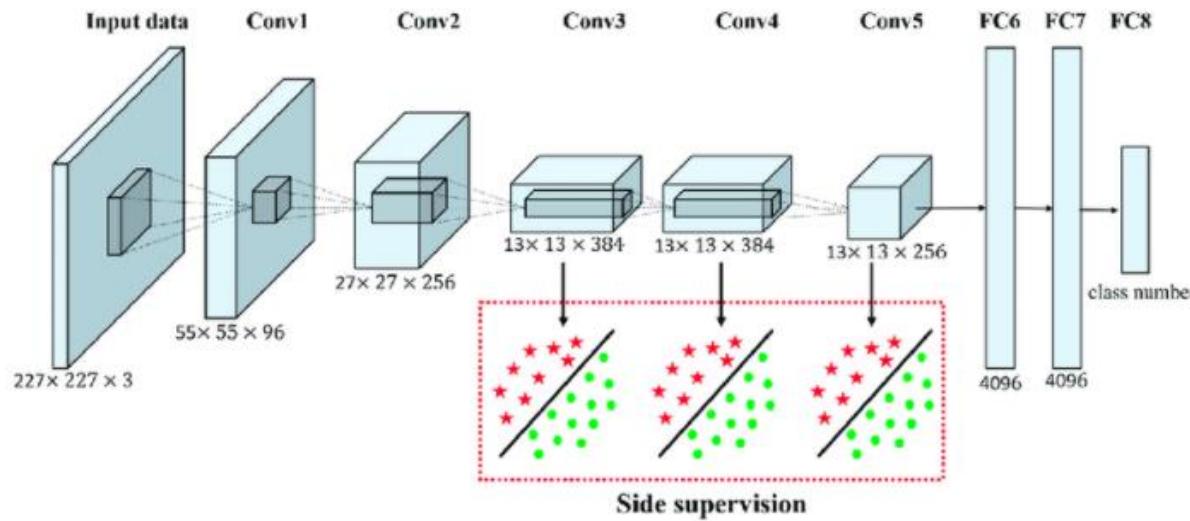
- **ILSVRC**

- 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



ILSVRC Winners

- **ALexNet – 2012 Winner (top-5 error rate 15.3%)**
 - Use CNN (prior to 2012, the classification model error was 25%)
 - Regarded as a Pioneer of CNN and starting point of the Deep learning
 - 60 million parameters
 - Used ReLU activation function, data augmentation, dropout, and overlapped pooling layers



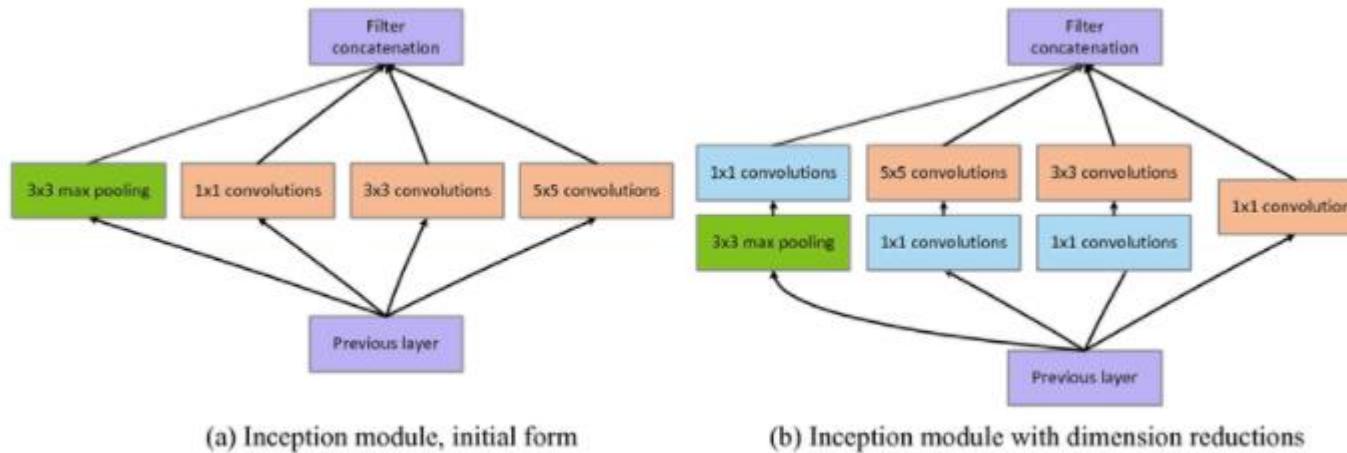
ImageNet Challenge (2012) – AlexNet ([Source](#))

(*) top-5 error: The model is considered to have classified a given image correctly if the target label is one of the model's top 5 predictions. (image classification)

ILSVRC Winners

- **Inception V1 (GoogleNet) – 2014 Winner (top-5 error rate 6.67%)**

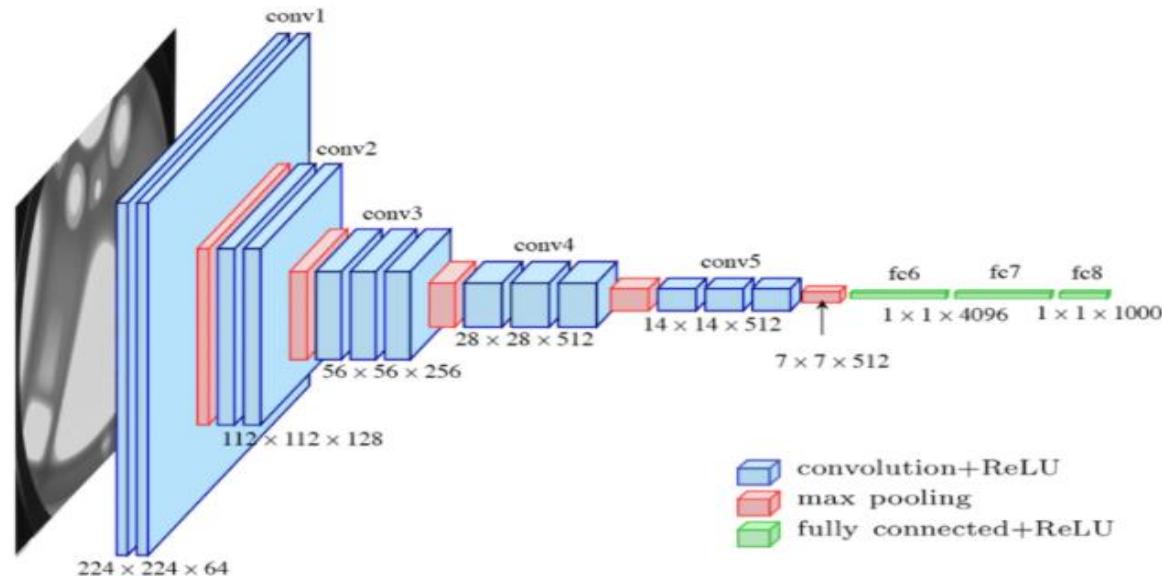
- The v1 stands for 1st version and later there were further versions v2, v3, etc. It is also popularly known as GoogLeNet.
- Deep with 22 layers.
- Used multiple types of filter size, instead of being restricted to a single filter size, in a single image block, which we then concatenate and pass onto the next layer.
- Used 1x1 convolutional with ReLU to reduce dimensions and number of operations.



ImageNet Challenge (2014)- Inception-V1 (GoogLeNet) [Source](#)

ILSVRC Winners

- **VGG-16 (University of Oxford) – 2014 Runners-Up (top-5 error rate 7.3%)**
 - Despite not winning the competition, VGG-16 architecture was appreciated and went on to become one of the most popular image classification models.
 - instead of using large-sized filters like AlexNet, it uses several 3×3 kernel-sized filters consecutively. The hidden layers of the network leverage ReLU activation functions.
 - VGG-16 is however very **slow to train** and the network weights, when saved on disk, occupy a **large** space.

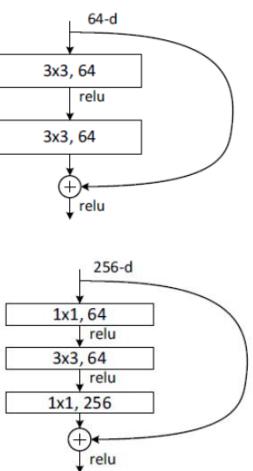


ImageNet Challenge (2014) – VGG-16 ([Source](#))

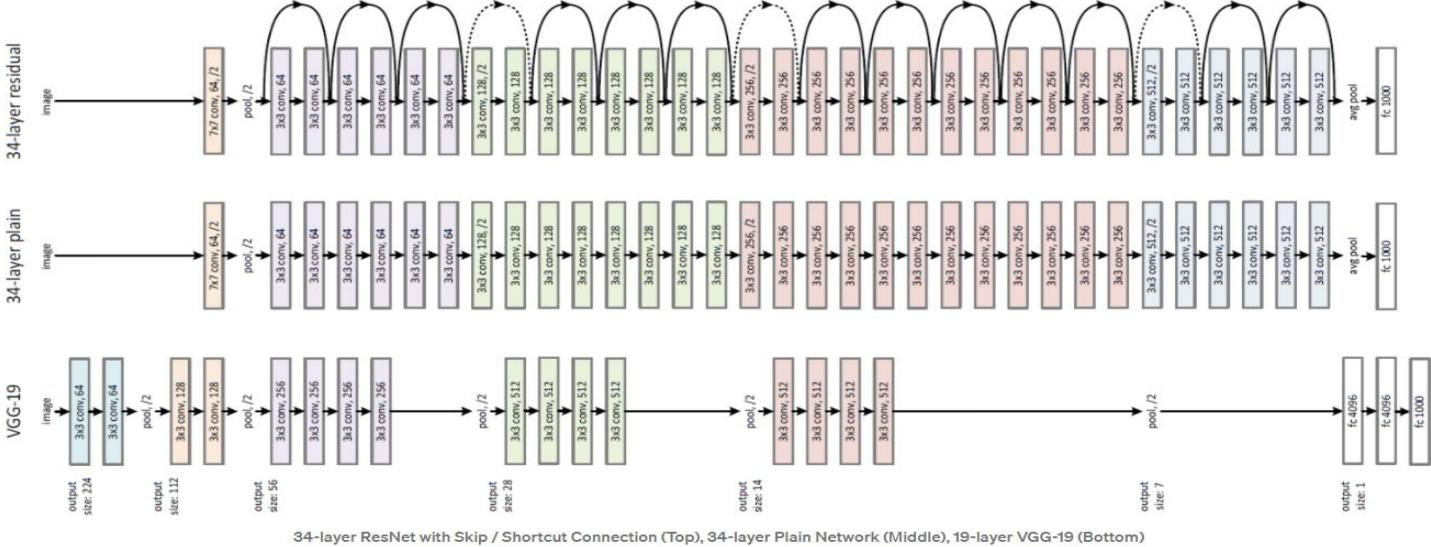
ILSVRC Winners

- **ResNet – 2015 Winner (top-5 error rate 3.57%)**

- ResNet ([Residual Network](#)) was created by the Microsoft Research team.
- To solve the problem of vanishing/exploding gradients, a [skip/shortcut connection](#) is added to add the input x to the output after few weight layers as below:
- 1×1 Conv can reduce the number of connections (parameters) while not degrading the performance of the network so much. (as in Inception-V1)
- ResNet-18/34/50/101/152 has 1.8/3.6/3.8/7.6/11.3 GFLOPs (lower than VGG-16/19 with 15.3/19.6 GFLOPS)



The Basic block (top) and the Proposed Bottleneck design (bottom)

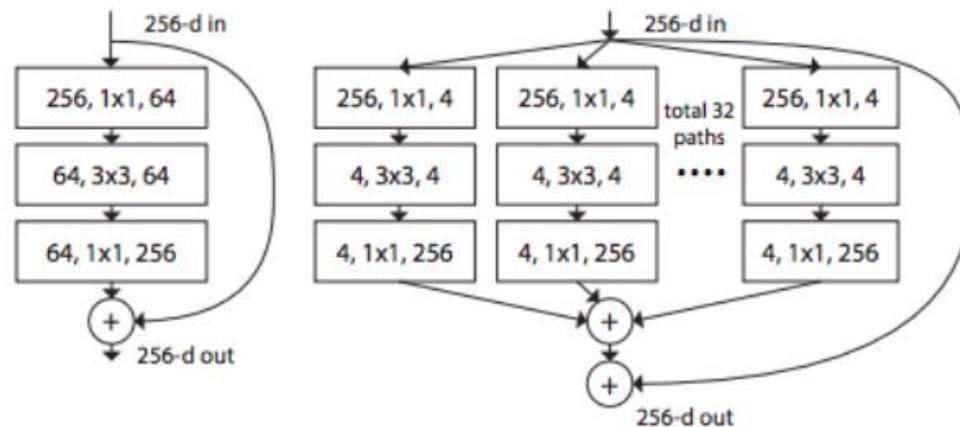


(*) VGG-19 (bottom): state-of-the-art approach in 2014
middle: deeper network of VGG-19 (i.e. more Conv layers)

ILSVRC Winners

- **ResNeXt – 2016 Runners-Up (top-5 error rate 4.1%)**

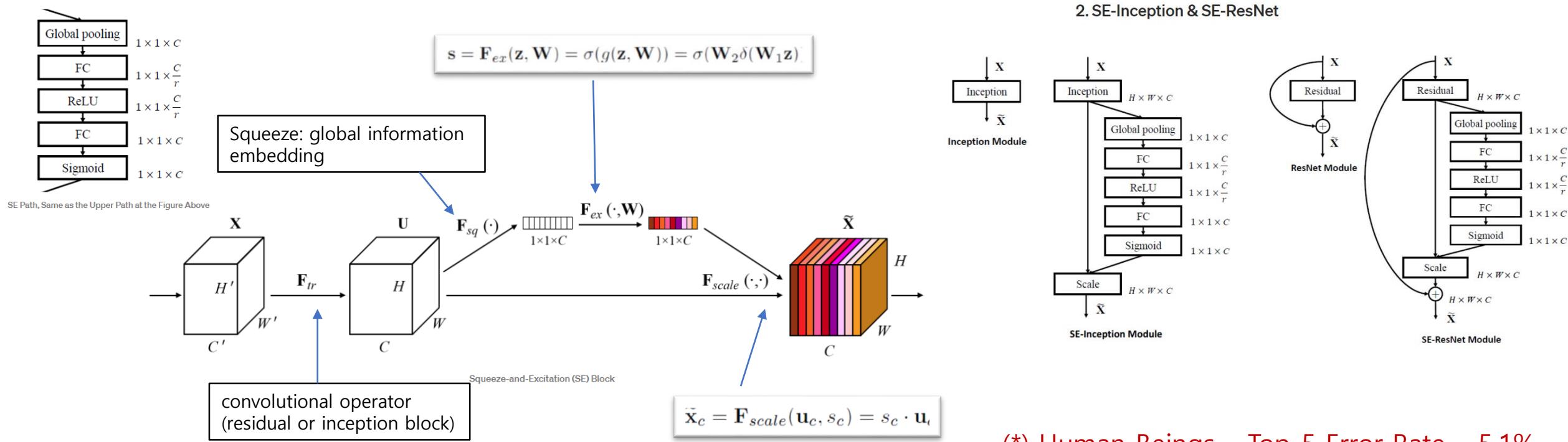
- Developed in the collaboration of the Researchers from UC San Diego and Facebook [AI](#) Research.
- Inspired by (ResNet + VGG + Inception).
- Still it became a popular model.
- stacks the blocks and then use the ResNet approach of residual blocks. Here the hyper-parameters such as width and filters were also shared.



ImageNet Challenge (2016)- ResNeXt ([Source](#))

ILSVRC Winners

- **SENet(Squeeze-and-Excitation Network) – 2017 Winner (top-5 error rate 2.251%)**
 - Developed in University of Oxford.
 - With “Squeeze-and-Excitation” (SE) block that **adaptively recalibrates channel-wise feature responses by explicitly modelling interdependencies between channels**, SENet is constructed.
 - SE block can be added to both Inception and [ResNet](#) block easily as **SE-Inception** and **SE-ResNet**. (achieved the best 2.25%).

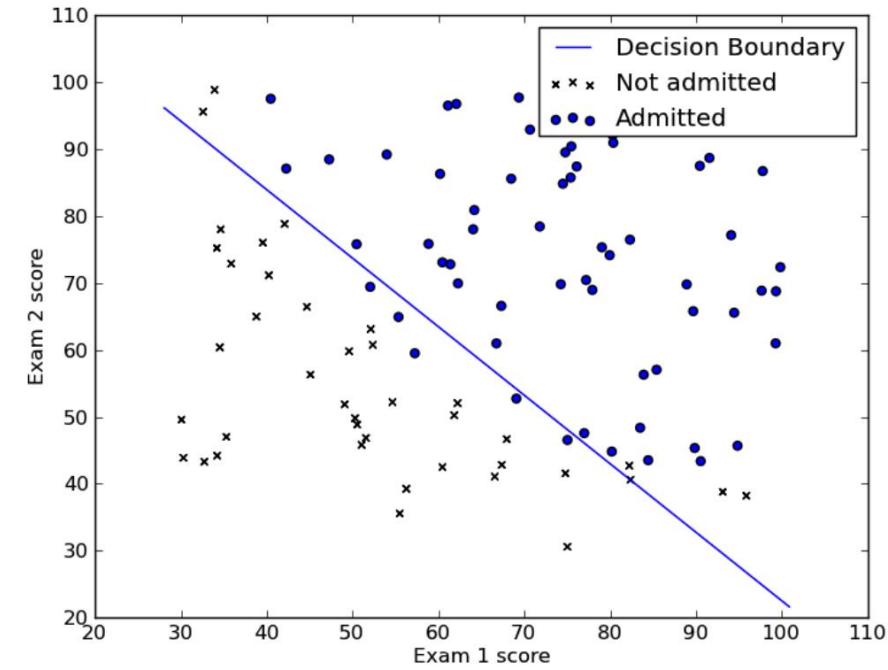
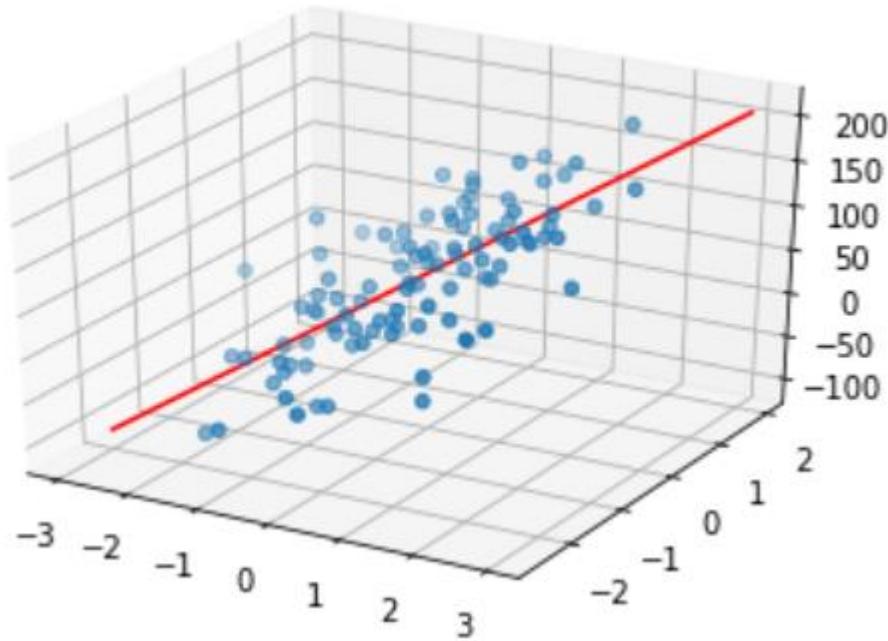


Machine Learning

- **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)

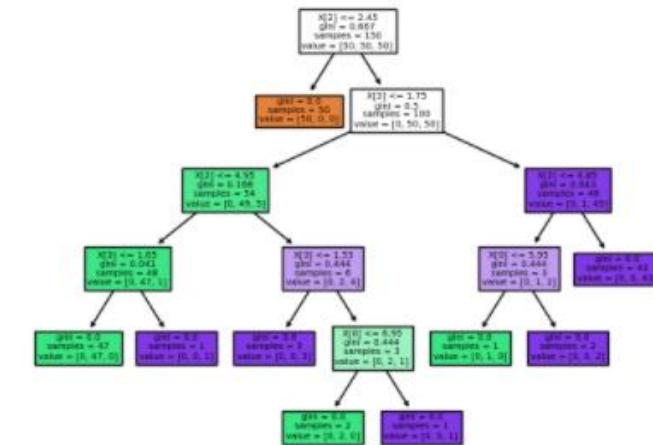
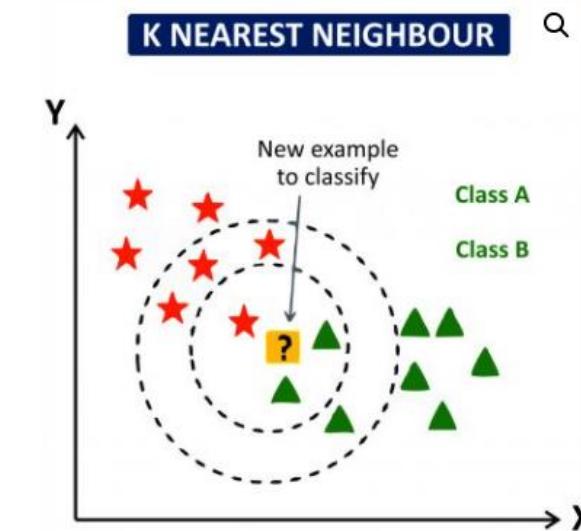
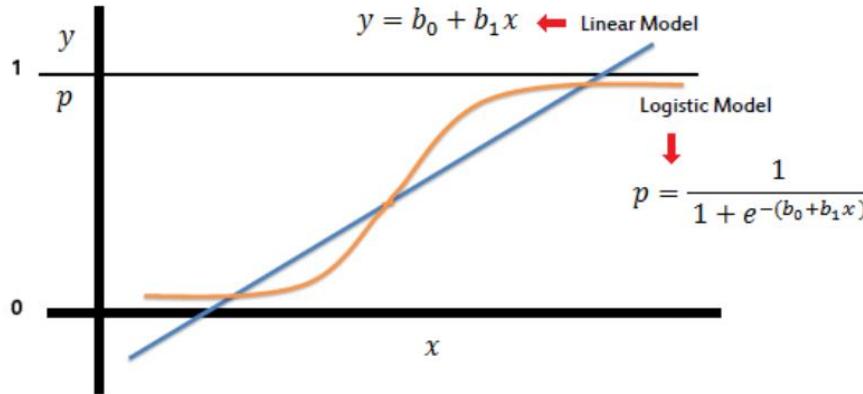
Supervised Learning

- **Linear Regression and Linear Classification**
 - (regression) $y = w_1 \cdot x_1 + w_2 \cdot x_2 + b$
 - (classification) $w_1 \cdot x_1 + w_2 \cdot x_2 + b = 0$



Supervised Learning

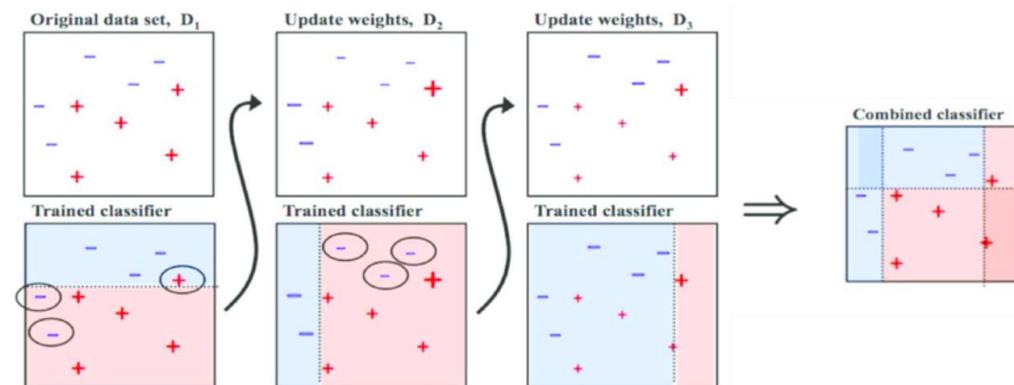
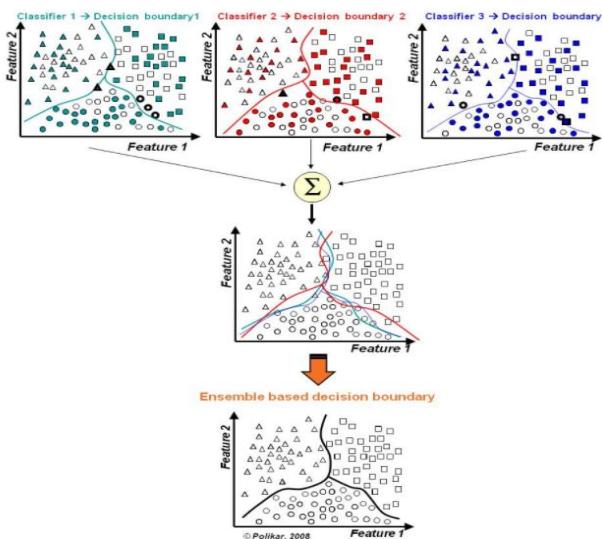
- Other algorithms (linear and nonlinear)
 - Logistic Regression Classifier
 - Knn (k-nearest neighbor)
 - Decision Tree



Supervised Learning

- **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)

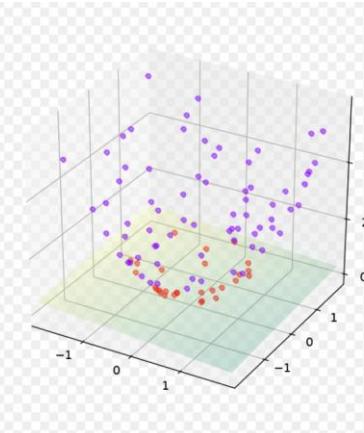
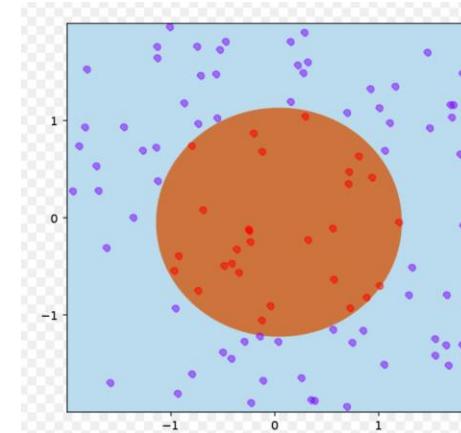
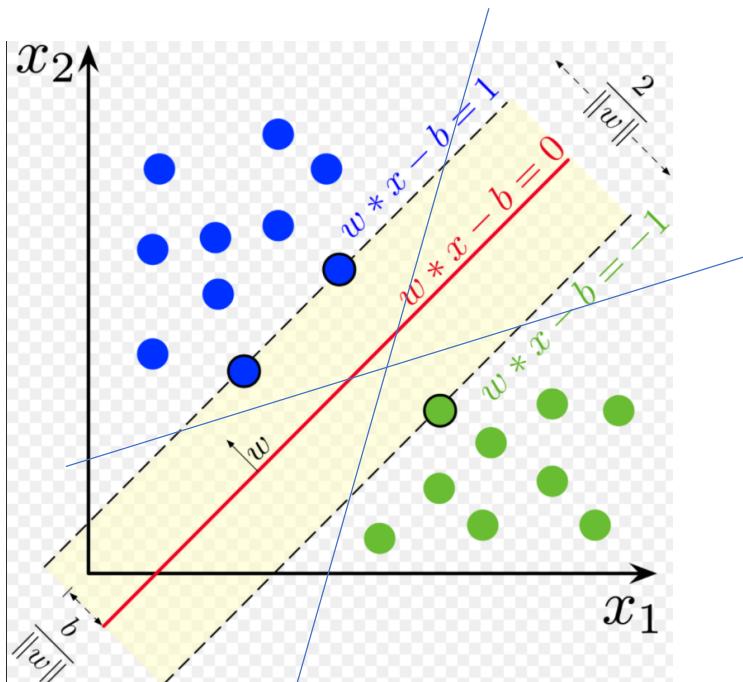


출처: Medium (Boosting and Bagging explained with examples)

Supervised Learning

- **SVM (Support Vector Machine)**

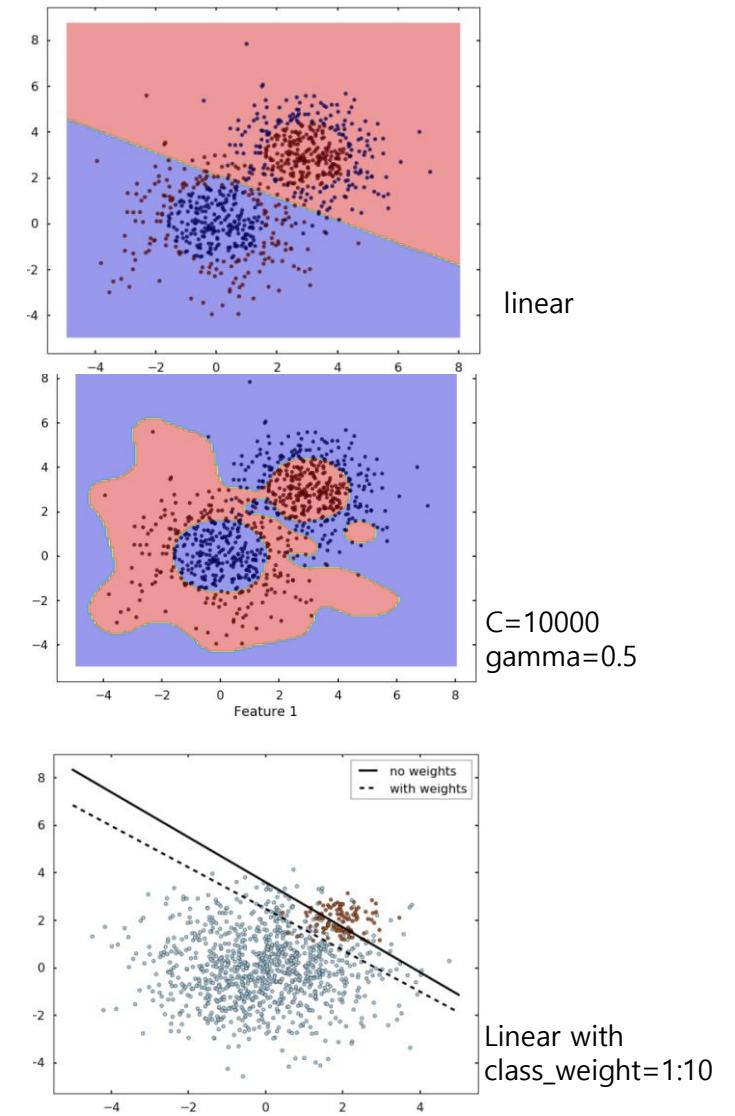
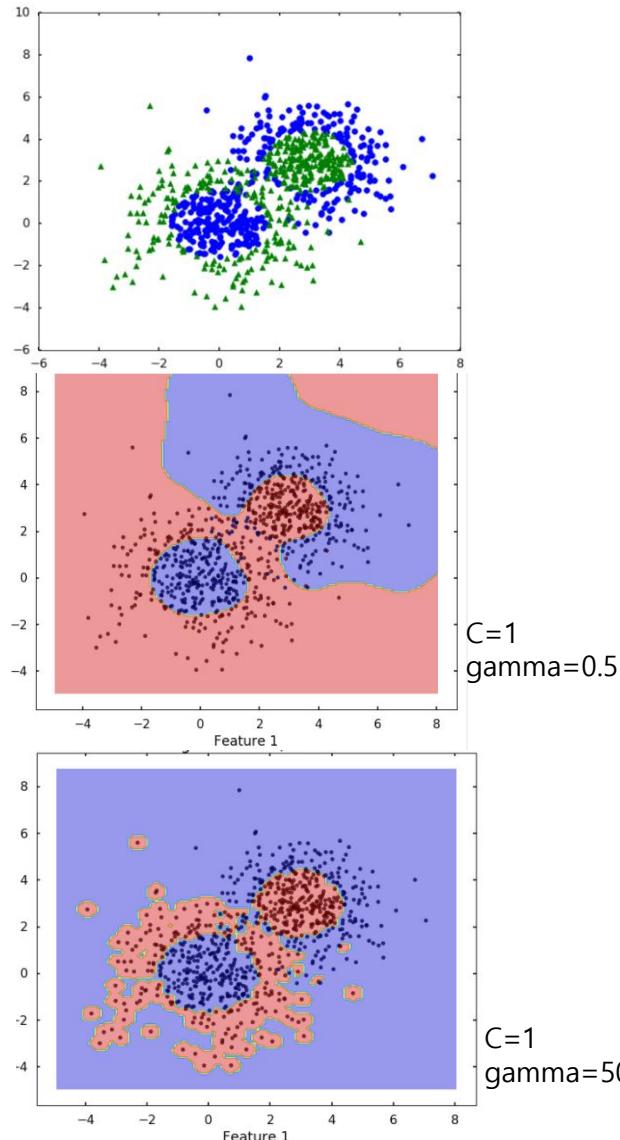
- Finds a maximum-margin hyperplane
- Linear SVM
- Nonlinear SVM: use kernel (polynomial, sigmoid, rbf)



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

Supervised Learning

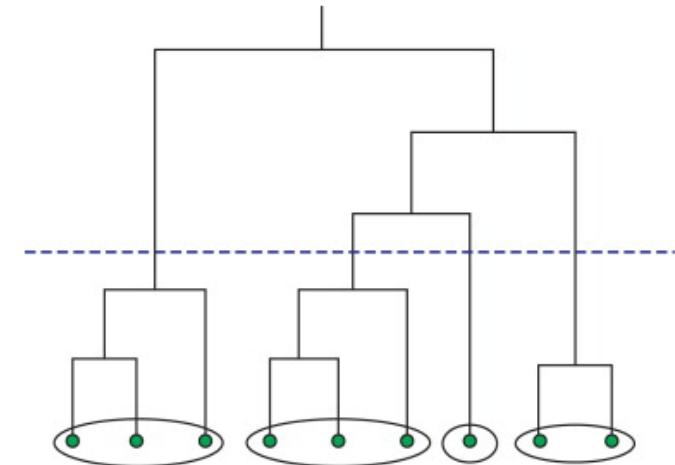
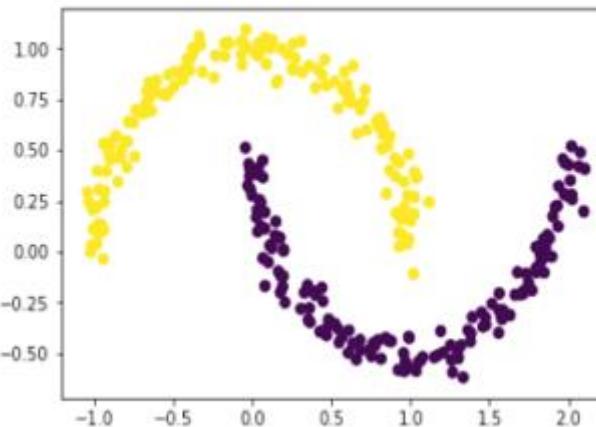
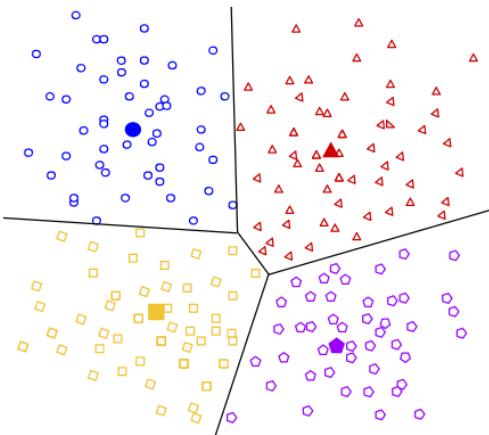
- **SVM (continued)**
 - 'rbf' kernel (hyperparameters: C and gamma)
 - **C**: tradeoff between classification error and simplicity of the boundary
 - **gamma**: defines how far the influence of a single example reaches (high value is 'close')
 - `class_weight`: imbalance cases



Unsupervised Learning

- **Clustering (or Grouping)**

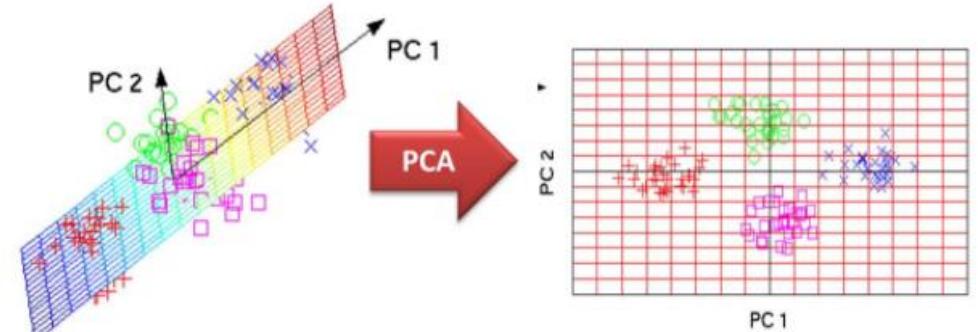
- Divide the data points into several clusters based on similarity (유사도)
- Need scaling as a preprocessing step
- Applications: detect hackers and criminal activity, identifying fake news, etc.
- Centroid-based ([K-means](#))
- Density-based ([DBSCAN](#))
- Hierarchical (ex: [dendrogram](#))



Unsupervised Learning

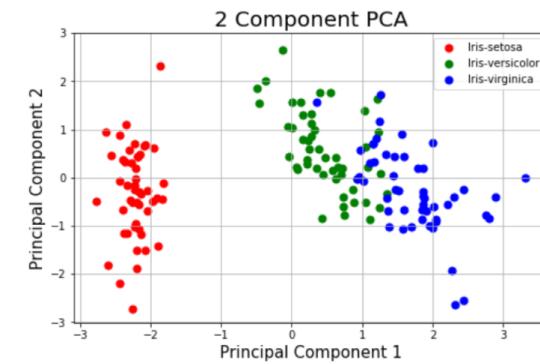
- Dimension reduction by **PCA**

- 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, [SelectPercentile\(\)](#), [tSNE\(\)](#)



| | 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-virgi |
| 147 | 6.5 | 3.0 | 5.2 | 2.0 | Iris-virgi |
| 148 | 6.2 | 3.4 | 5.4 | 2.3 | Iris-virgi |
| 149 | 5.9 | 3.0 | 5.1 | 1.8 | Iris-virgi |

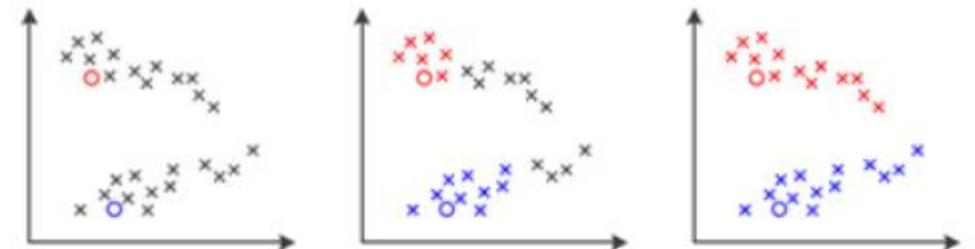
| | principal component 1 | principal component 2 | species |
|---|-----------------------|-----------------------|-------------|
| 0 | -2.264542 | -0.505704 | Iris-setosa |
| 1 | -2.086426 | 0.655405 | Iris-setosa |
| 2 | -2.367950 | 0.318477 | Iris-setosa |
| 3 | -2.304197 | 0.575368 | Iris-setosa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



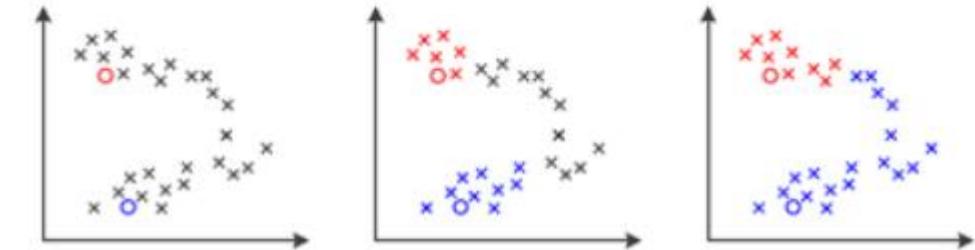
Semi-supervised Learning

- **Semi-supervised**

- large 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
- Many others



(a) 잘 작동하는 상황

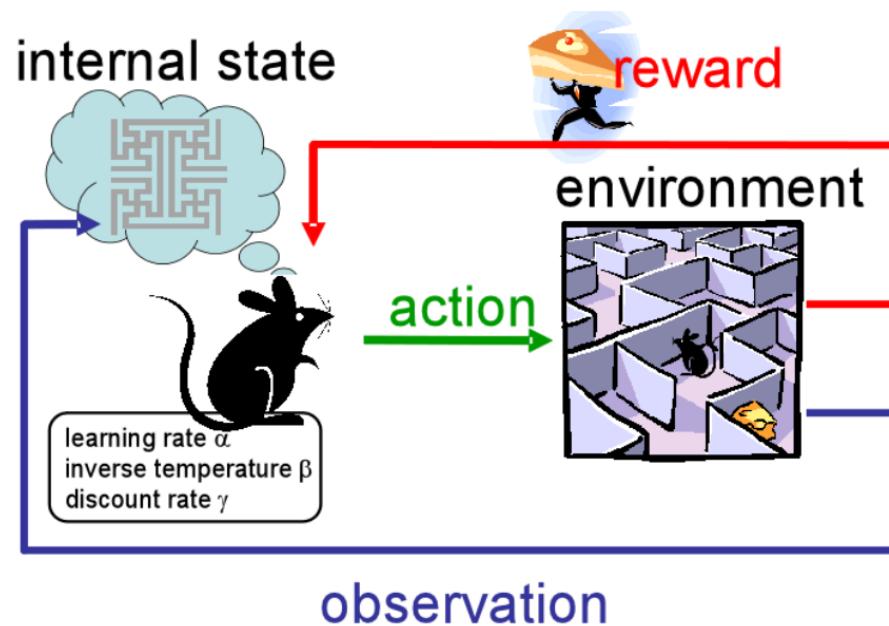


(b) 소속이 애매한 샘플에 민감한 상황

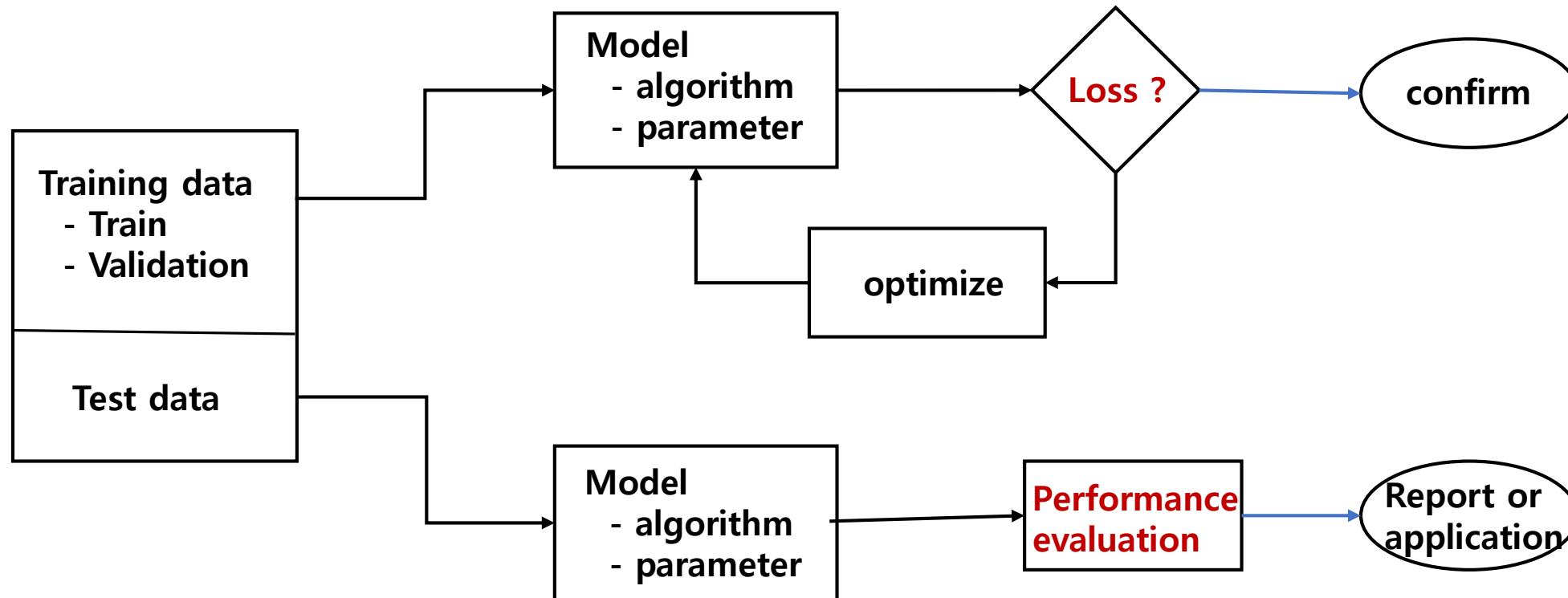
Reinforcement Learning

- **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).



Machine Learning Model (supervised)

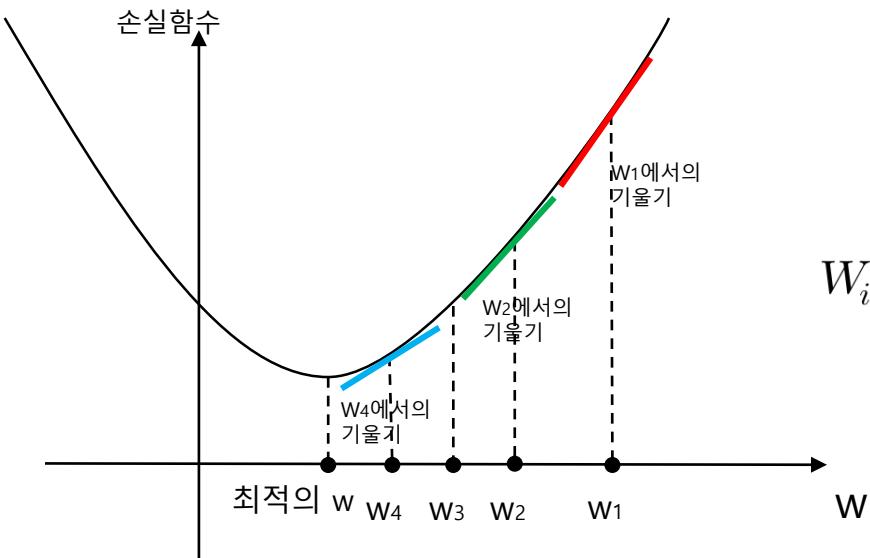


- (model) Parameter: estimated from the dataset (learned during training from the historical data sets)
- Hyper-parameter: external to the model (defined manually before the model training by trial-error)

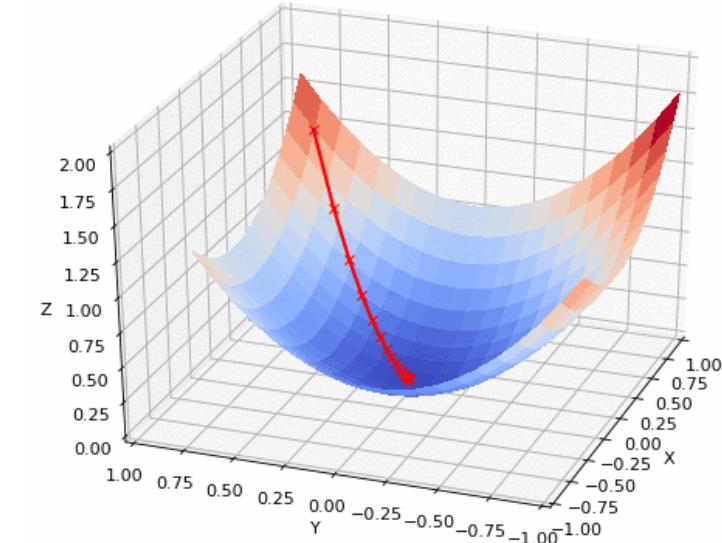
Gradient Descent (GD) algorithm

- **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



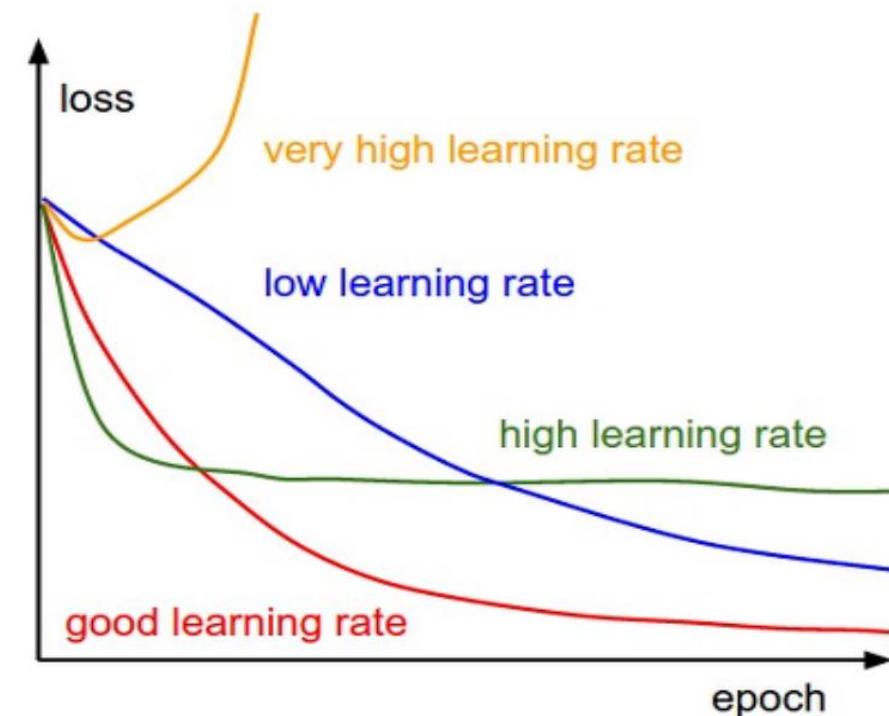
$$W_i = W_{i-1} - \eta \text{Grad}(i)$$



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**

$$CE = \sum_i p_i \log\left(\frac{1}{p_i}\right) \quad Gini = 1 - \sum_{k=1}^m p_k^2$$

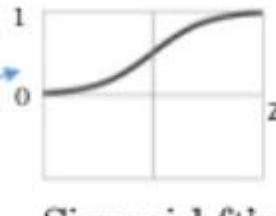
- Binary case:

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

Loss Function

- Binary Cross Entropy

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

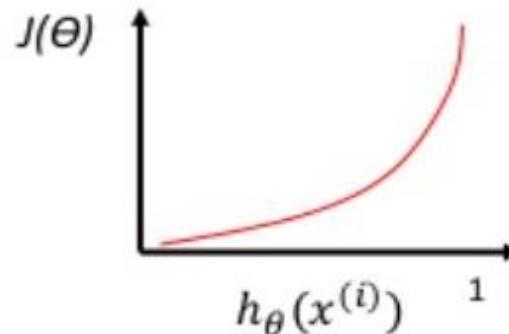
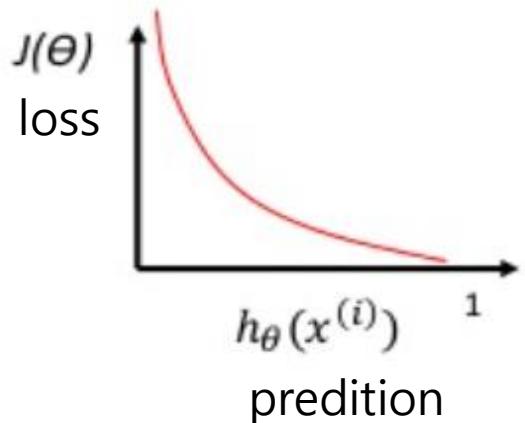


For $y^{(i)} = 1$ case

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

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: $f(x_i) \rightarrow +$ (likely +1)

$\rightarrow -$ (likely -1)

- $y_i f(x_i)$ 가 negative 일 때 얼마나 penalty 를 줄 것인지.

- 0/1 Loss

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

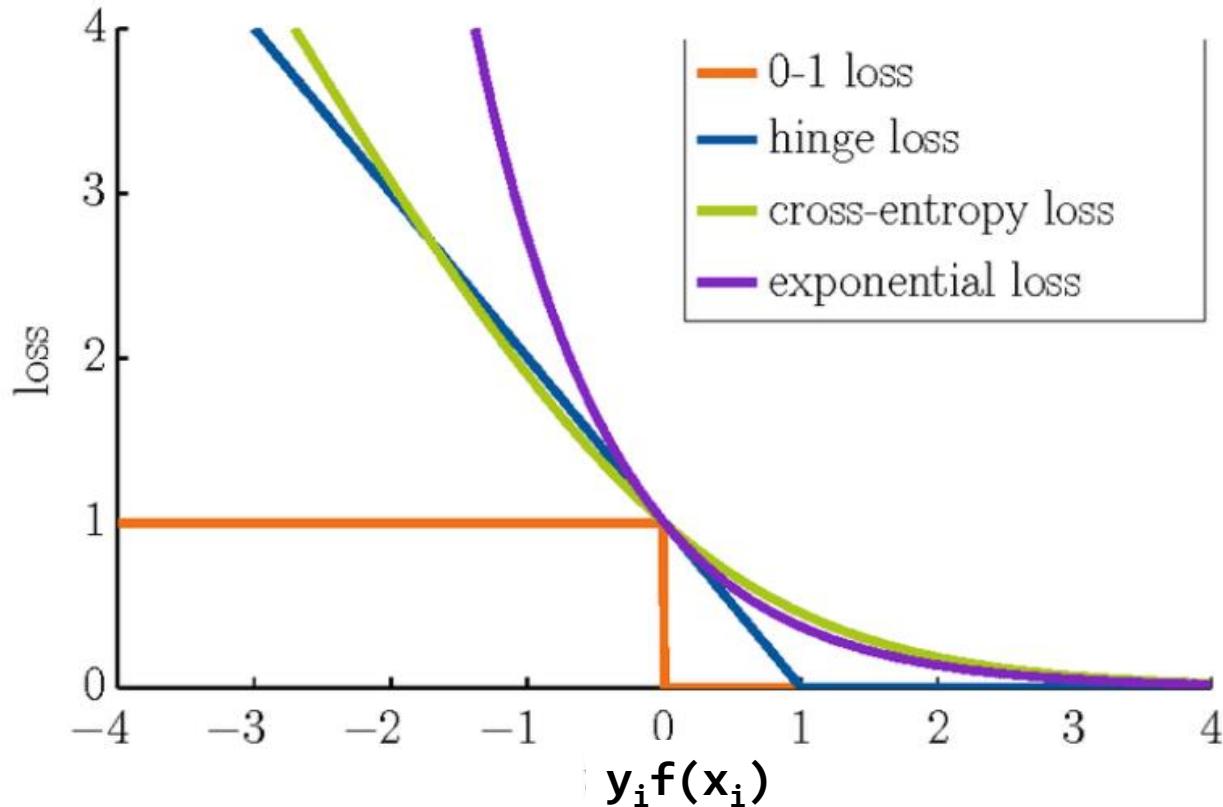
- Exponential loss

- $\bullet e^{-y_i f(x_i)}$

- Hinge Loss (SVM Loss)

- $\bullet \text{Max } [0, 1 - y_i f(x_i)]$

- Cross Entropy (Log loss)



Classification Loss Functions

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

$\rightarrow -$ (likely -1)

- $y_i f(x_i)$ 가 negative 일 때 얼마나 penalty 를 줄 것인지.

- 0/1 Loss

$$L_i = 0, \text{ if } y_i f(x_i) \geq 0 \\ 1, \text{ if } y_i f(x_i) < 0$$

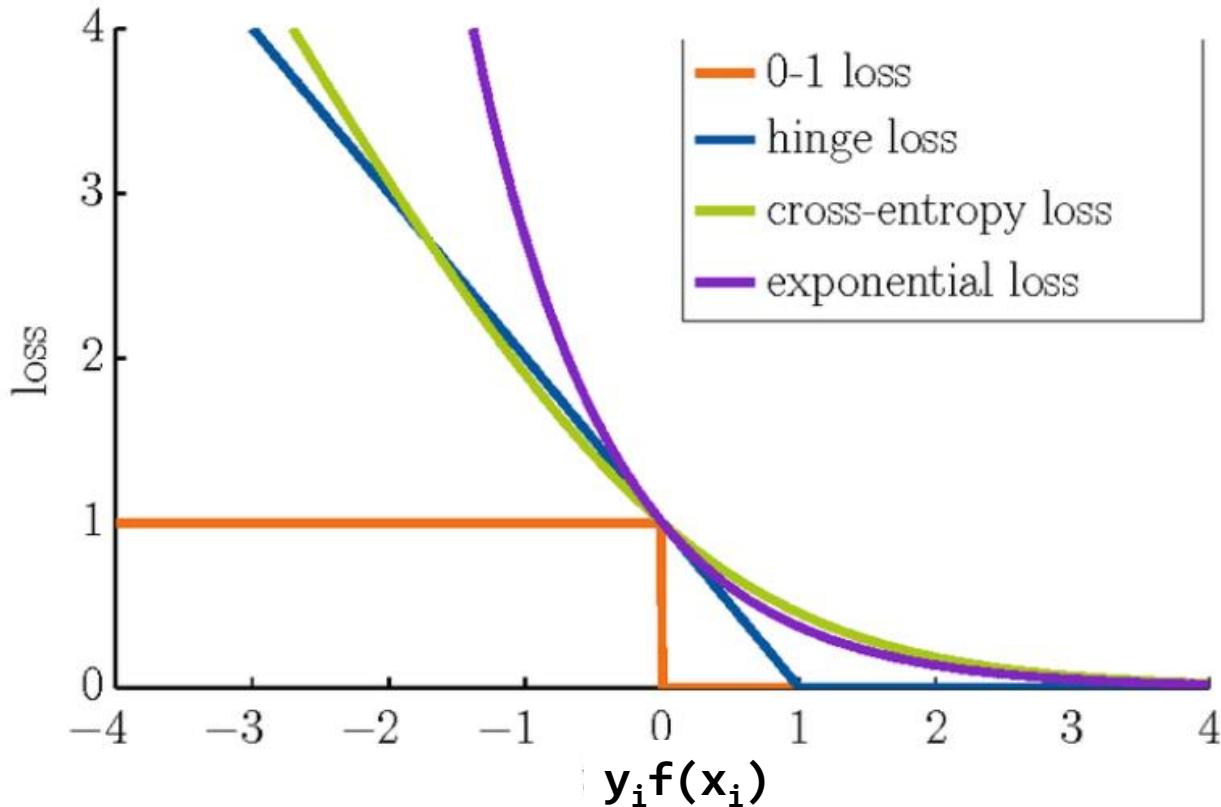
- Exponential loss

- $\bullet e^{-y_i f(x_i)}$

- Hinge Loss (SVM Loss)

- $\bullet \text{Max} [0, 1 - y_i f(x_i)]$

- Cross Entropy (Log loss)



Sub-gradient Descent

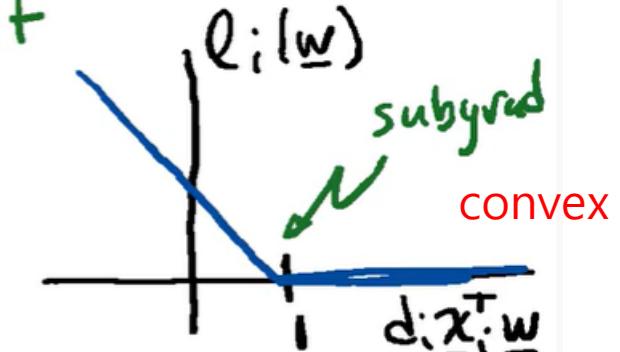
Gradient descent for SVMs

6

$$\ell(\underline{w}) = \sum_{i=1}^N (1 - d_i \underline{x}_i^\top \underline{w})_+ \rightarrow \text{subgradient}$$

$$\ell_i(\underline{w}) = (1 - d_i \underline{x}_i^\top \underline{w})_+ = \begin{cases} 1 - d_i \underline{x}_i^\top \underline{w} & d_i \underline{x}_i^\top \underline{w} < 1 \\ 0 & d_i \underline{x}_i^\top \underline{w} \geq 1 \end{cases}$$

Subgradient



$$\nabla \ell_i(\underline{w}) = \begin{cases} -d_i \underline{x}_i & d_i \underline{x}_i^\top \underline{w} < 1 \\ 0 & d_i \underline{x}_i^\top \underline{w} \geq 1 \end{cases} = -d_i \underline{x}_i I_{\{d_i \underline{x}_i^\top \underline{w} < 1\}}$$

indicator function

$$\text{Cost } f(\underline{w}) = \ell(\underline{w}) + \lambda \|\underline{w}\|_2^2$$

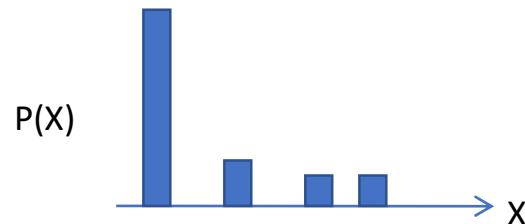
$$\Rightarrow \nabla f(\underline{w})|_{\underline{w}^{(k)}} = \sum_{i=1}^N (-d_i \underline{x}_i I_{\{d_i \underline{x}_i^\top \underline{w}^{(k)} < 1\}}) + 2\lambda \underline{w}^{(k)}$$

Gradient descent

$$\underline{w}^{(k+1)} = \underline{w}^{(k)} - \tau \nabla f(\underline{w})|_{\underline{w}^{(k)}}$$

Entropy

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



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

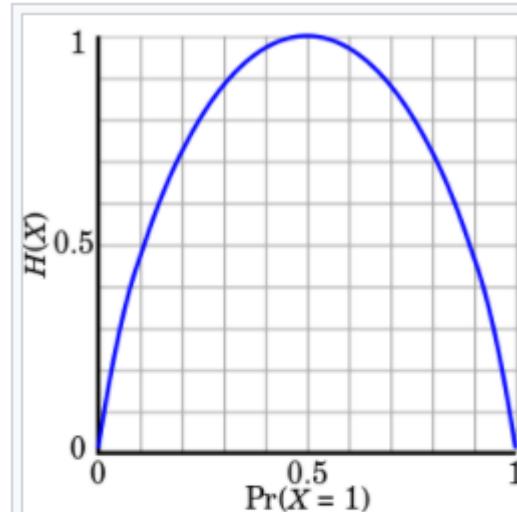
$$H_p(X) = E\left[\log \frac{1}{P(x)}\right] = \sum_x P(x) \log \frac{1}{P(x)} = -\sum_x P(x) \log P(x)$$

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

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



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

Cross Entropy, KL Divergence

- Cross Entropy (CE)
 - For discrete distribution p and q with the same support 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) $Q(x)$

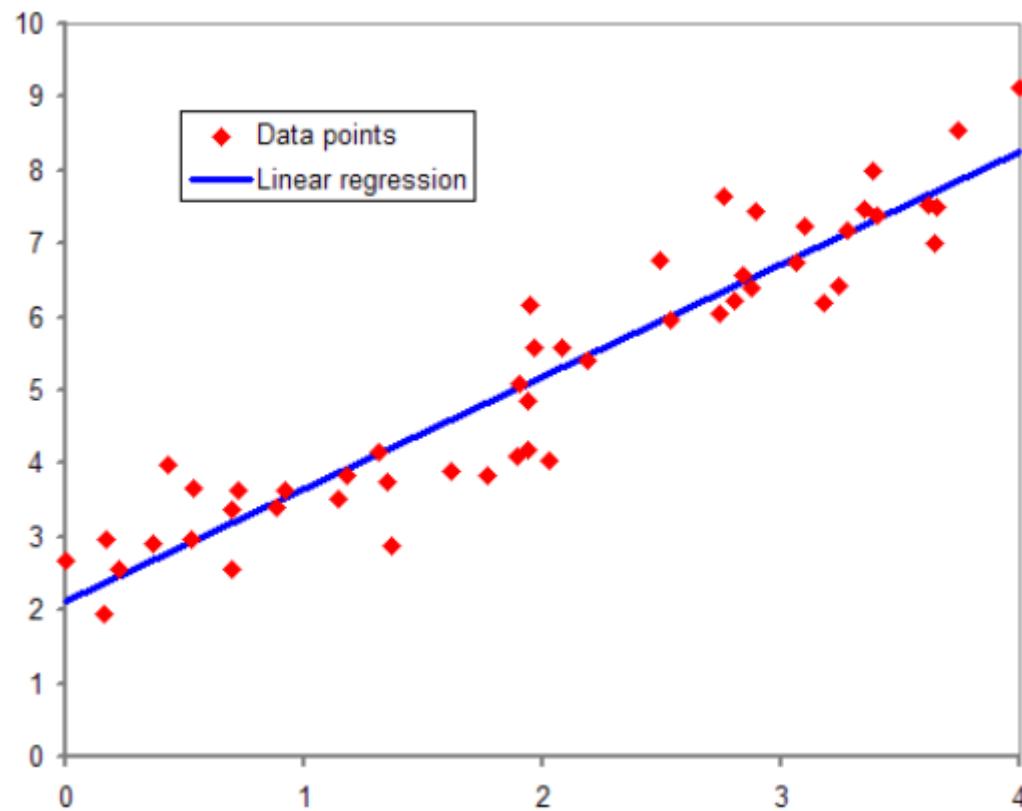
$$D_{KL}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \log\left(\frac{P(x)}{Q(x)}\right)$$

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

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

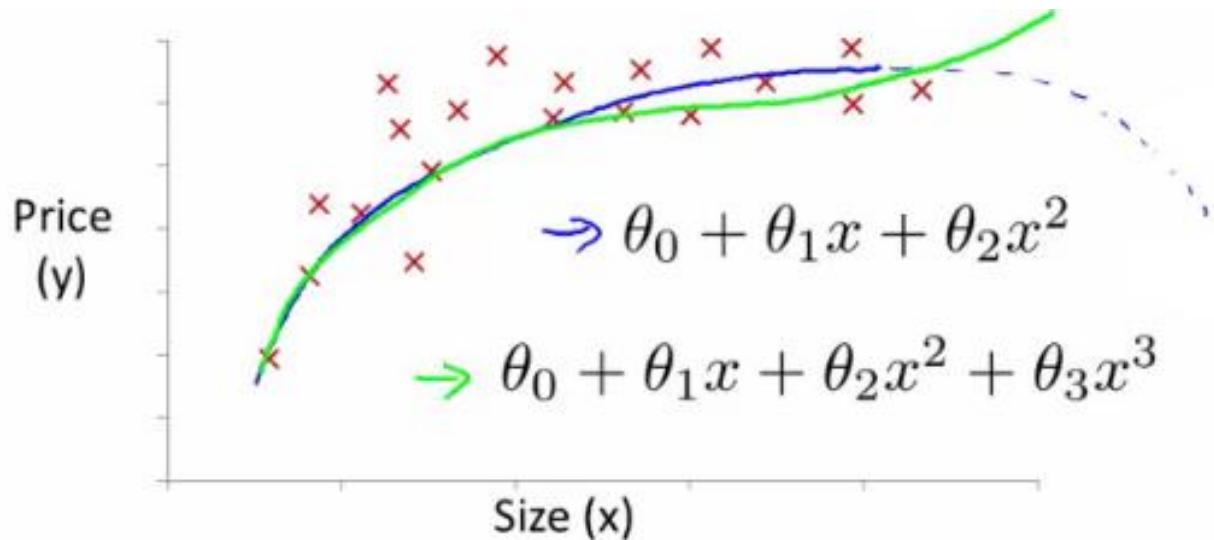
Linear Regression

- Linear regression



Linear Regression

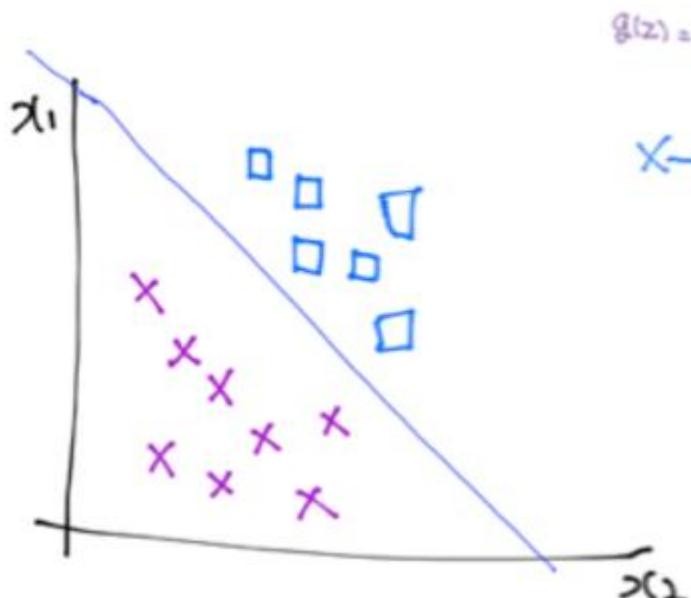
- **Polynomial Regression**



- 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

Linear Classification

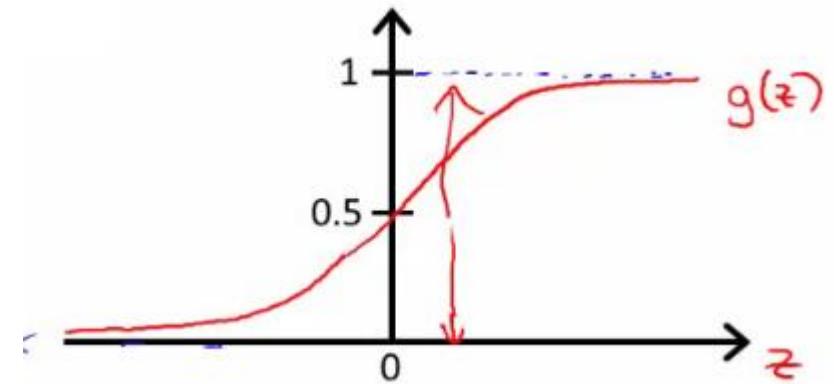
- Logistic Regression classifier (binary)



$$g(z) = \frac{1}{1 + e^{-z}} \quad H_\theta(x) = g(H_\theta(x))$$

$x \rightarrow \begin{matrix} w \\ \times \end{matrix} \rightarrow z \rightarrow \begin{matrix} g \\ \circ \end{matrix} \rightarrow \tilde{Y}$

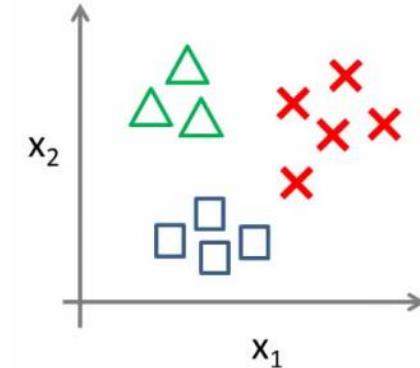
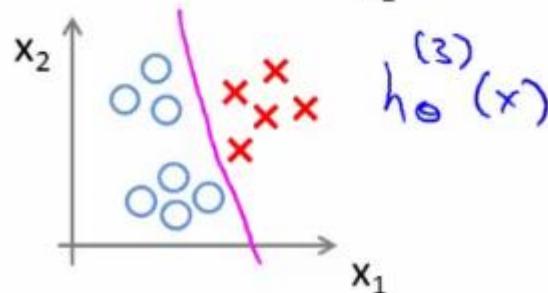
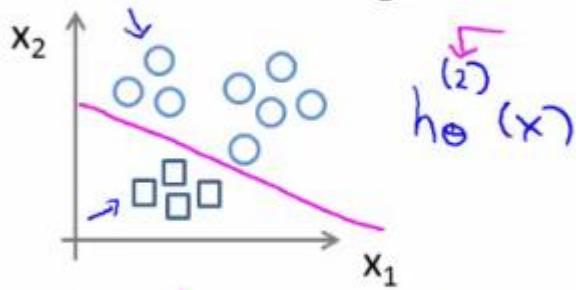
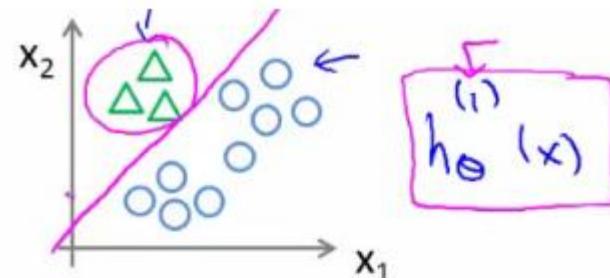
The diagram illustrates the logistic regression model architecture. An input vector x is multiplied by a weight vector w to produce a weighted sum z . This sum is then passed through a sigmoid function g to produce the final output \tilde{Y} .



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

Linear Classification

- Multinomial (multi-class) classifier (One vs. Rest)



- Split the training set into three separate binary classification problems
 - i.e. create a new fake training set
 - Triangle (1) vs crosses and squares (o) $h_{\theta}^1(x)$
 - $P(y=1 | x_1; \theta)$
 - Crosses (1) vs triangle and square (o) $h_{\theta}^2(x)$
 - $P(y=1 | x_2; \theta)$
 - Square (1) vs crosses and square (o) $h_{\theta}^3(x)$
 - $P(y=1 | x_3; \theta)$

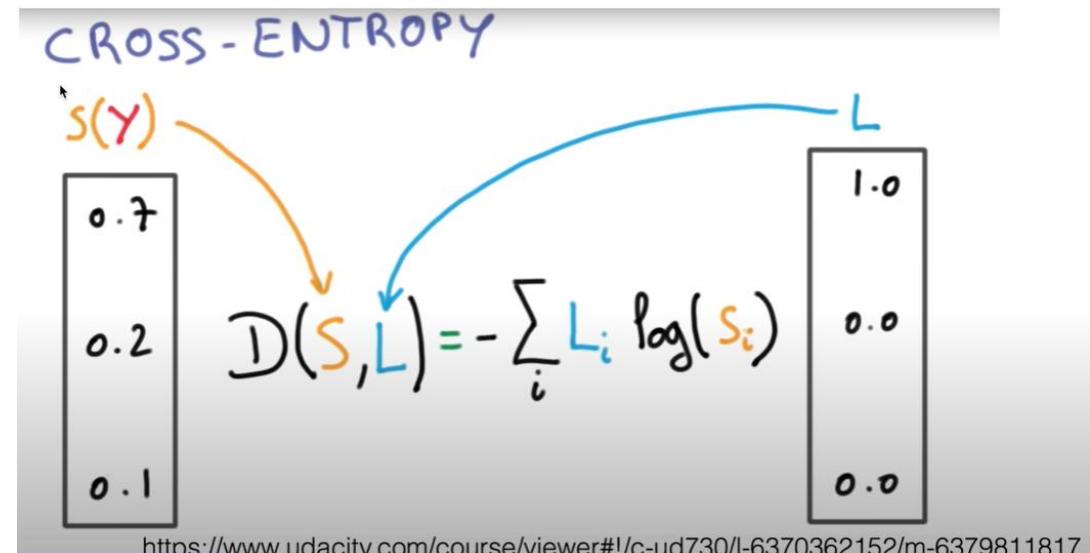
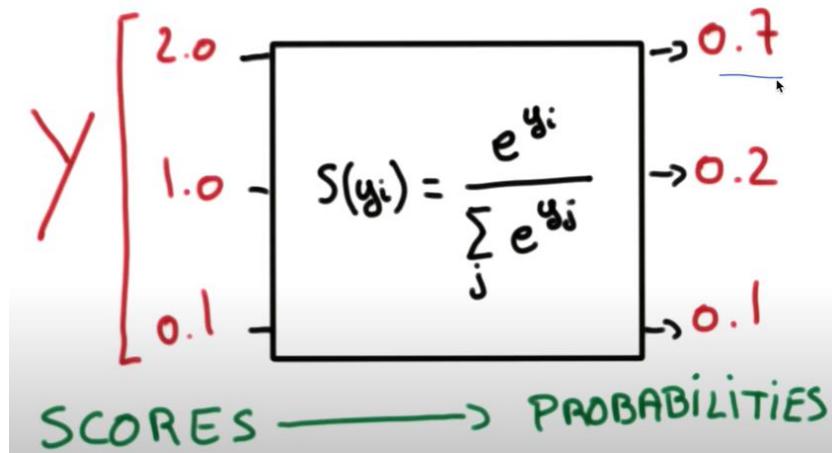
Overall

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

Linear Classification

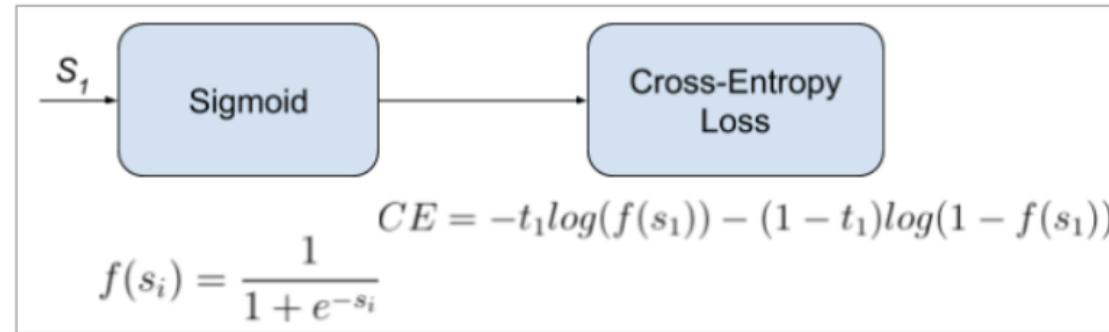
- **Softmax (regression) Classifier**

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

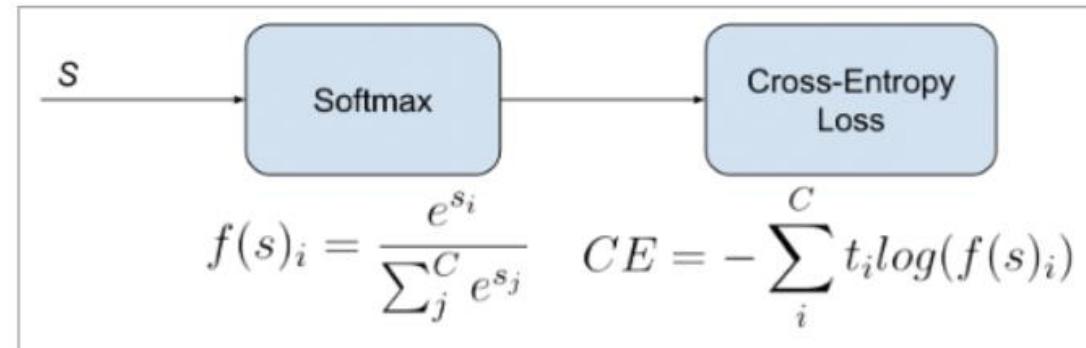


Binary and multi-class classification

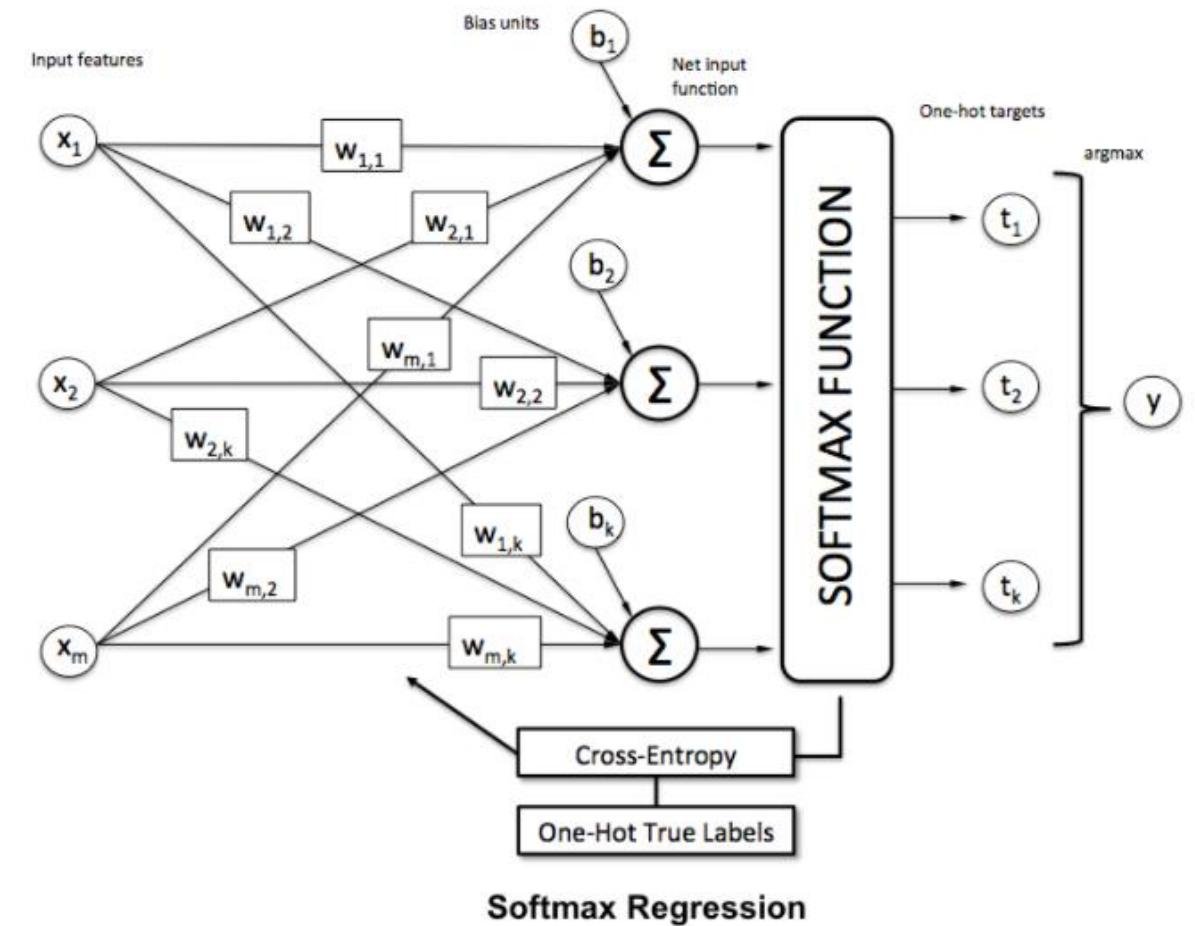
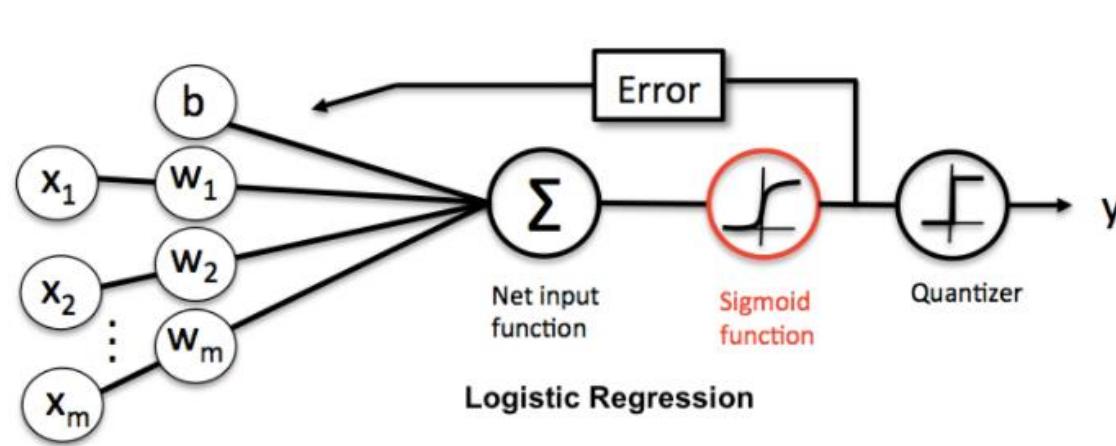
- Binary CE



- Categorical CE

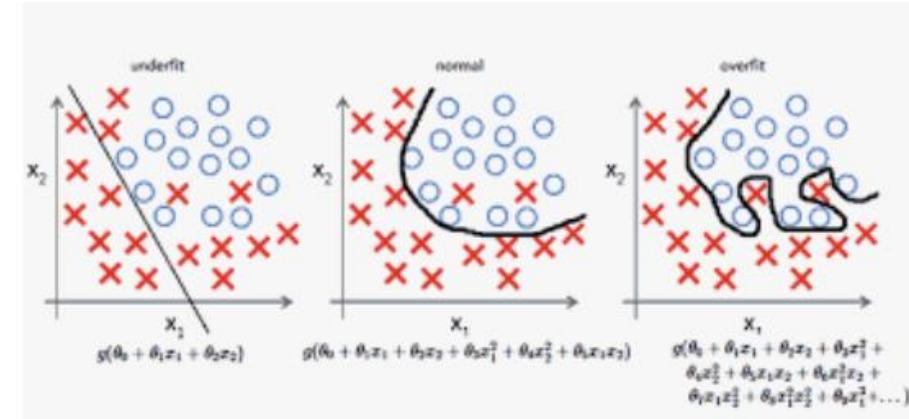
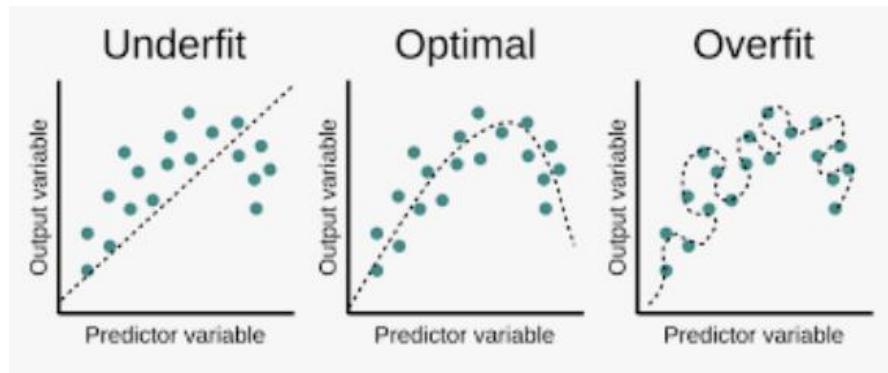


Logistic Regression and Softmax Regression



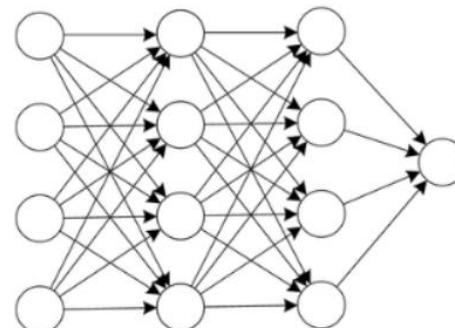
Overfitting and Underfitting

- Overfitting and Underfitting

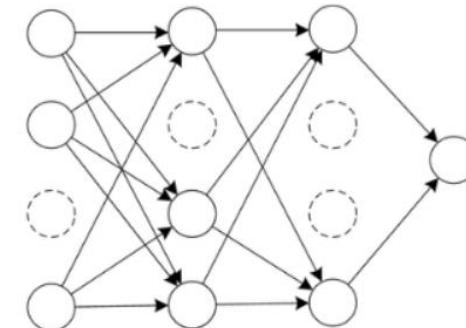


- How to reduce overfitting?

- More data
- Simplify the model
- Feature selection
- Data augmentation
- Regularization
- Early stopping
- Dropouts



(a) Standard Neural Network

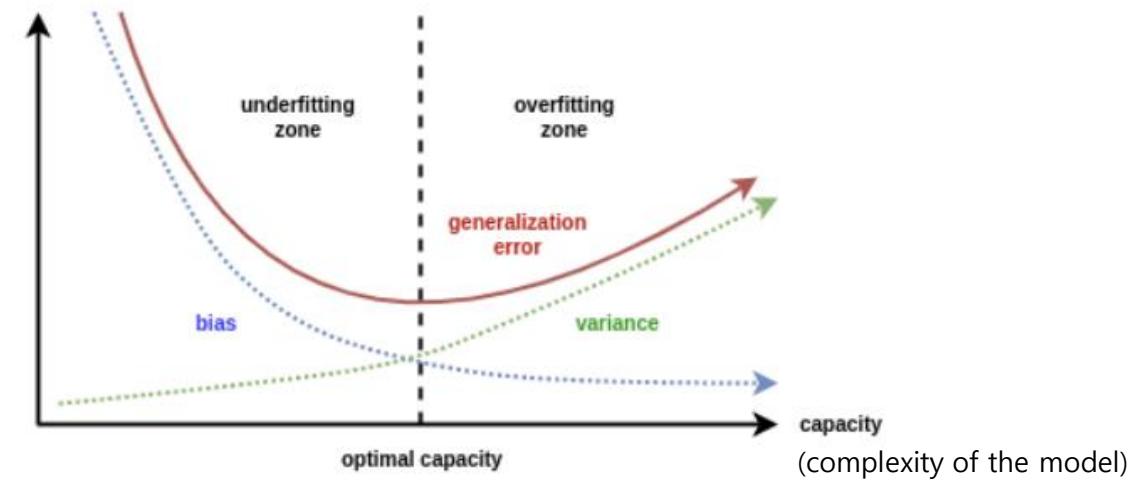
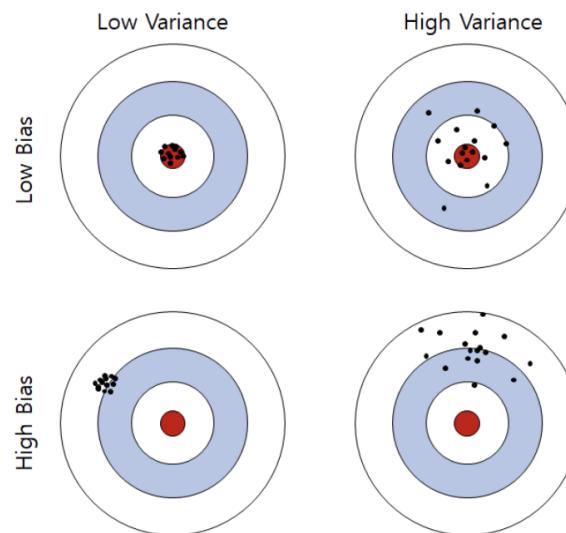


(b) Network after Dropout

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



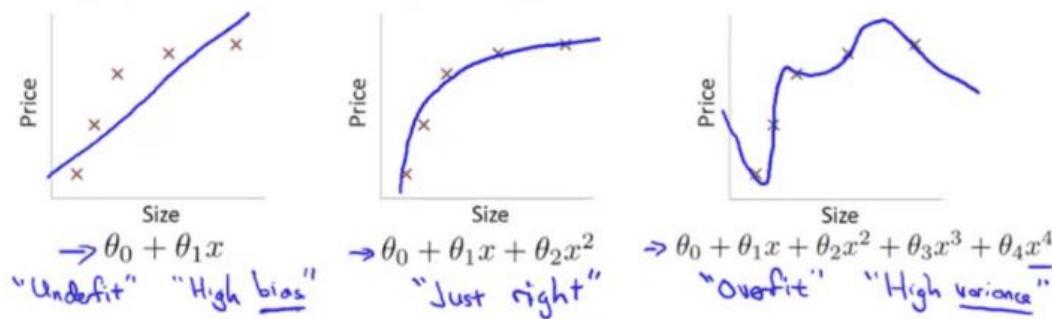
Bias-Variance tradeoff

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

Example: Linear regression (housing prices)



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

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.

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

- **R Squared (R^2)**

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

$$R^2 = 1 - \frac{\frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{\frac{1}{n} \sum_{i=1}^n (Y_i - \bar{Y})^2}$$

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:
$$\text{F1-score} = 2 * \text{Precision} * \text{Recall} / (\text{Precision} + \text{Recall})$$

Performance Metrics - classification

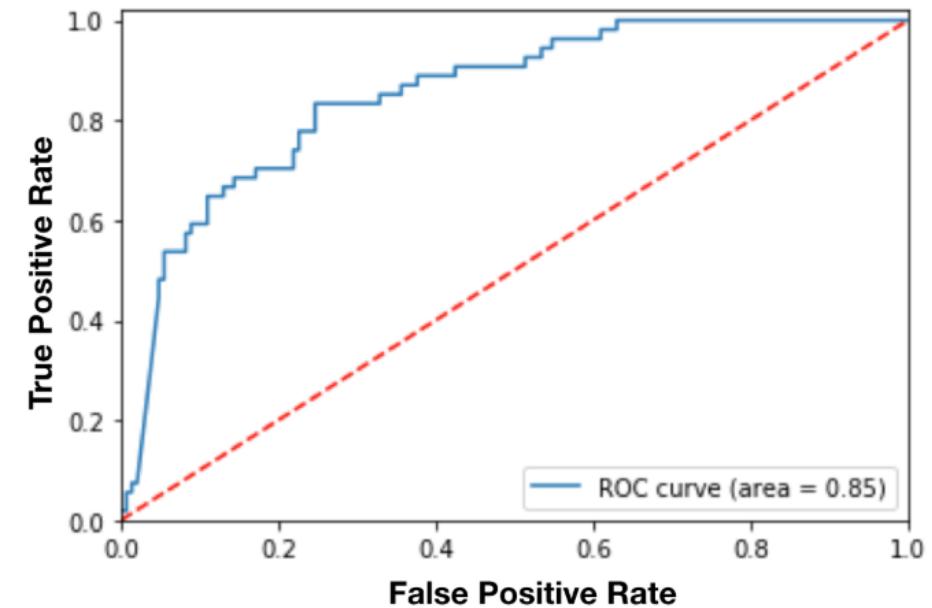
- **Dynamic: ROC Curve (Receiver Operating Characteristic curve)**
 - Shows the performance of a binary classifier as function of its cut-off threshold
 - It essentially shows the true positive rate(tpr) against the false positive rate(fpr) for various threshold values.
- **As an example,**
 - Suppose 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 |
| 3 | F | 0.77 | 10 | N | TN |
| 123 | F | 0.76 | 11 | N | FP |
| | | ... | | C | FN |
| 43 | F | 0.48 | 198 | N | TN |
| 93 | M | 0.42 | 199 | N | TN |
| 120 | F | 0.40 | 200 | N | TN |

↓
conservative

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

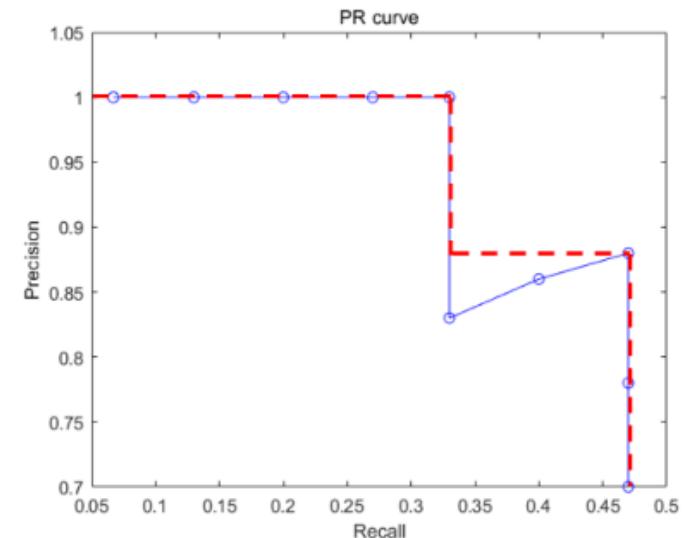
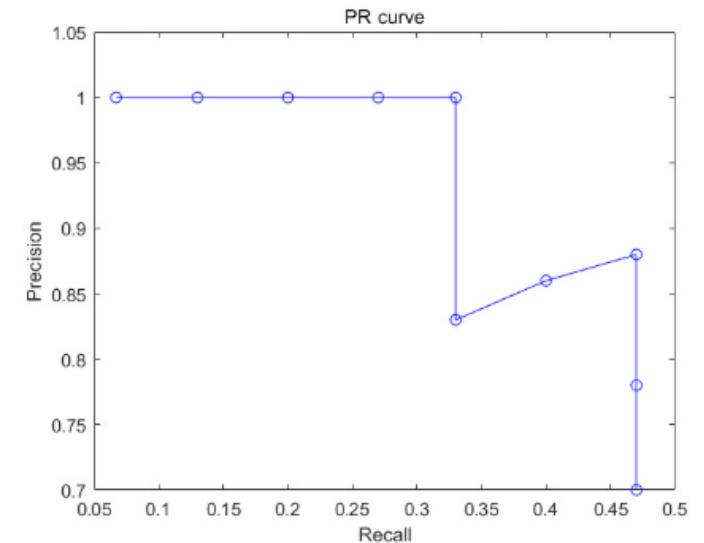


Performance Metrics (IoU and mAP)

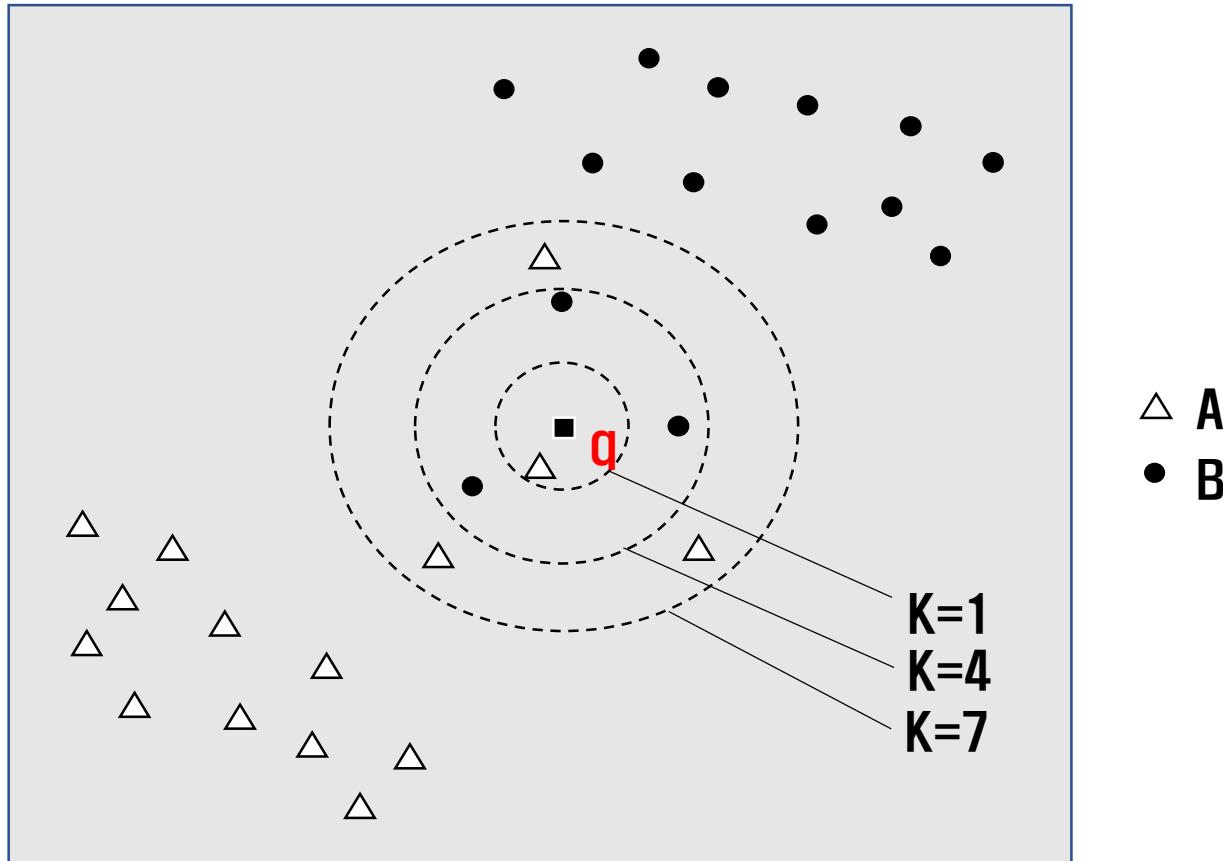
- **Object detection and Image Classification**

- 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

$$IoU = \frac{area(B_{gt} \cap B_p)}{area(B_{gt} \cup B_p)} = \frac{\text{Area of overlapping region}}{\text{Area of union region}}$$



Knn (K-Nearest Neighbor)



Knn (K-Nearest Neighbor)

- kNN의 장점
 - 훈련시간이 거의 없다
 - 알고리즘의 개념이 명확
 - 모델링에 필요한 하이퍼 파라미터 : 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 가까운지 새로 계산해야
 - 또한 새로운 샘플이 계속 추가될 때마다 가까운 이웃이 달라진다
 - Lazy 알고리즘
 - 나중에 계산량이 많은 알고리즘
- 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 $\begin{cases} G_{\text{left/right}} & \text{measures the impurity of the left/right subset,} \\ m_{\text{left/right}} & \text{is the number of instances in the left/right subset.} \end{cases}$

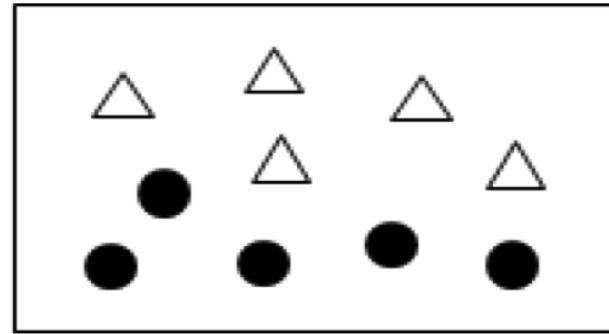
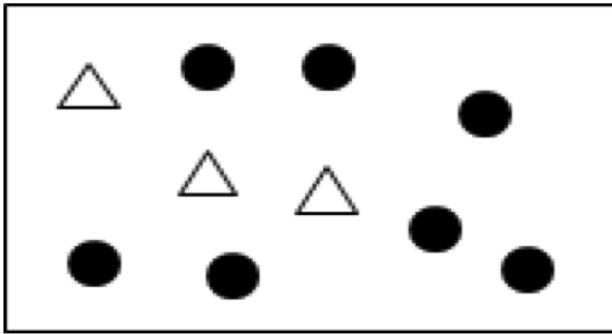
Decision Trees

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

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

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

Decision Trees

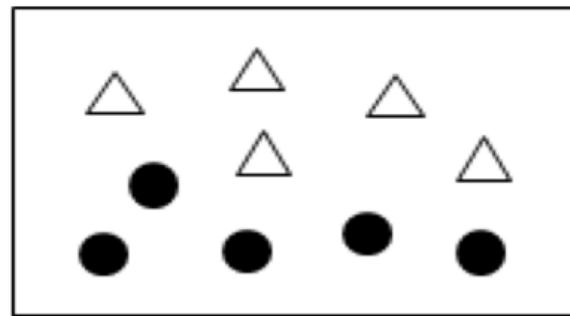
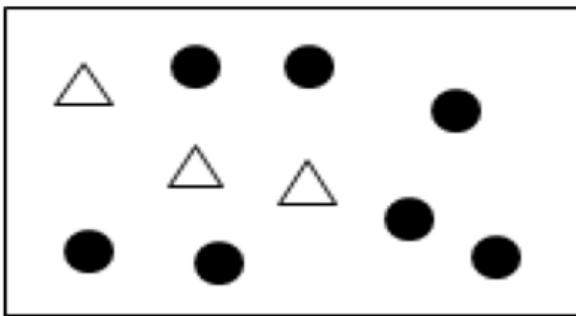


$$\text{좌측 박스: 지니}(7:3) = 1 - \left[\left(\frac{7}{10} \right)^2 + \left(\frac{3}{10} \right)^2 \right] = 1 - (0.49 + 0.09) = 0.42$$

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

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

Decision Trees

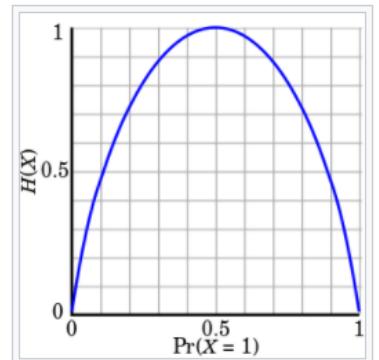


$$Entropy = - \sum_{k=1}^m p_k \log_2(p_k)$$

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

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

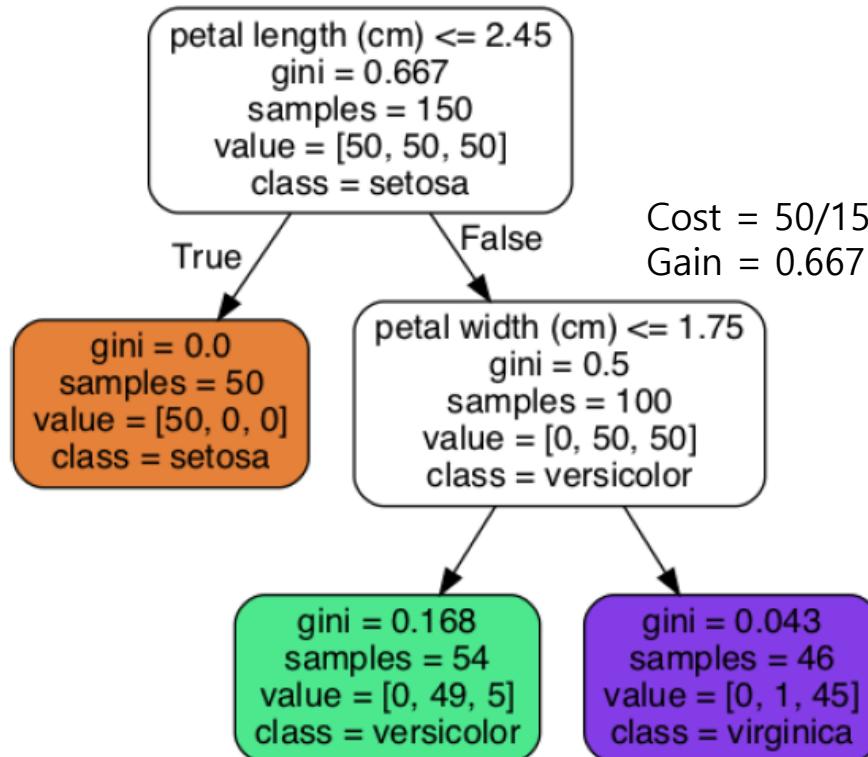
(*) worst: 1



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

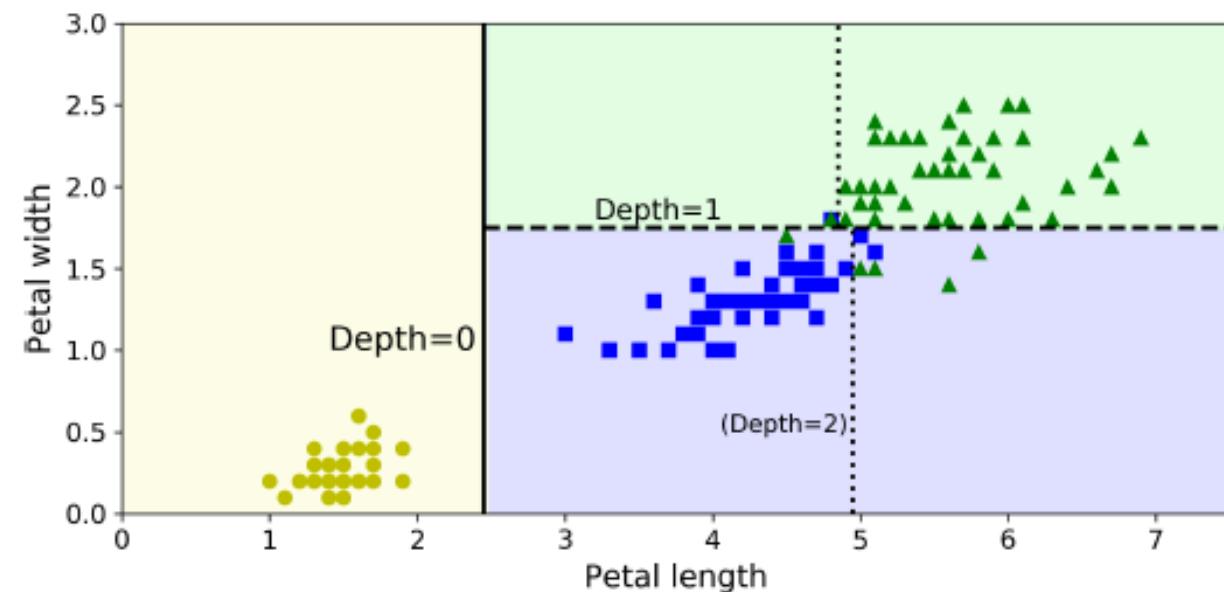
Decision Trees

$$\text{Gini} = 1 - [(1/3)^2 + (1/3)^2 + (1/3)^2] \\ = 0.667$$



$$\text{Cost} = 54/100 * 0.168 + 46/100 * 0.043 = 0.11 \\ \text{Gain} = 0.5 - 0.11 = 0.39$$

$$\text{Cost} = 50/150 * 0 + 100/150 * 0.5 = 0.333 \\ \text{Gain} = 0.667 - 0.333 = 0.334$$



Decision Trees

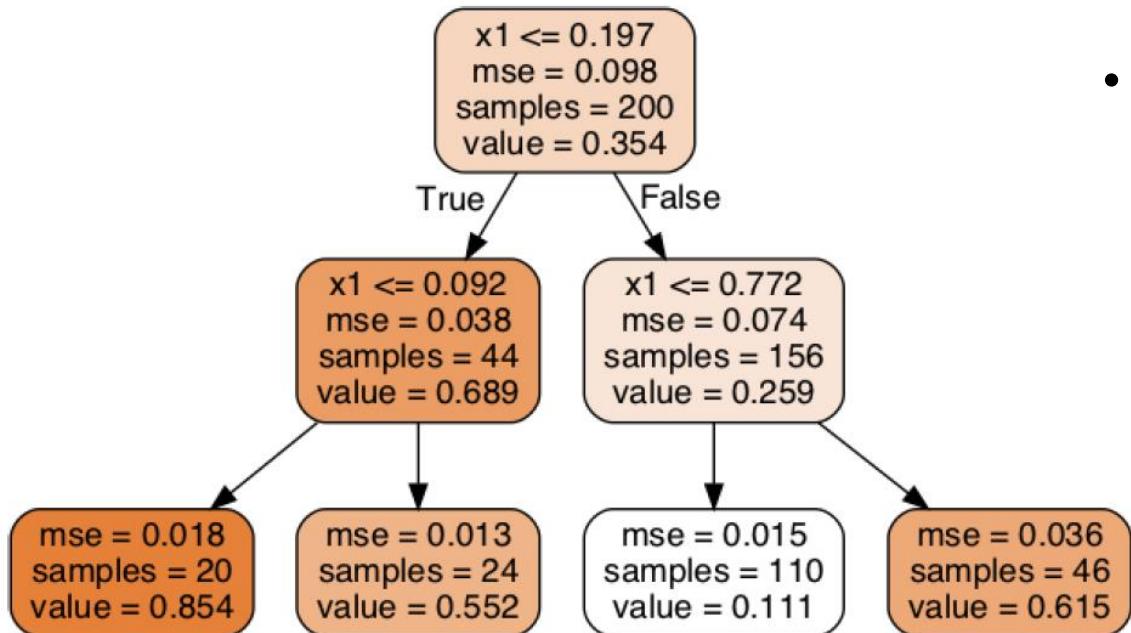
- **Hyper-Paramters**
 - `max_depth`: 트리의 최대 깊이 (이보다 깊은 트리를 만들지 않는다)
 - `max_leaf_nodes`: 리프 노드의 최대 수 (리프 노드를 이보다 많이 만들지 않는다)
 - `max_samples_split`: 분할하기 위한 최소 샘플수 (이보다 작으면 분할하지 않는다)
 - `min_samples_leaf`: 리프 노드에 포함될 최소 샘플수 (이보다 작은 노드는 만들지 않는다)
 - `max_features`: 최대 특성수 (분할할 때 이보다 적은 수의 특성만 사용한다)
- **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
 - 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 **Greedy algorithm**.

Decision Tree Regression

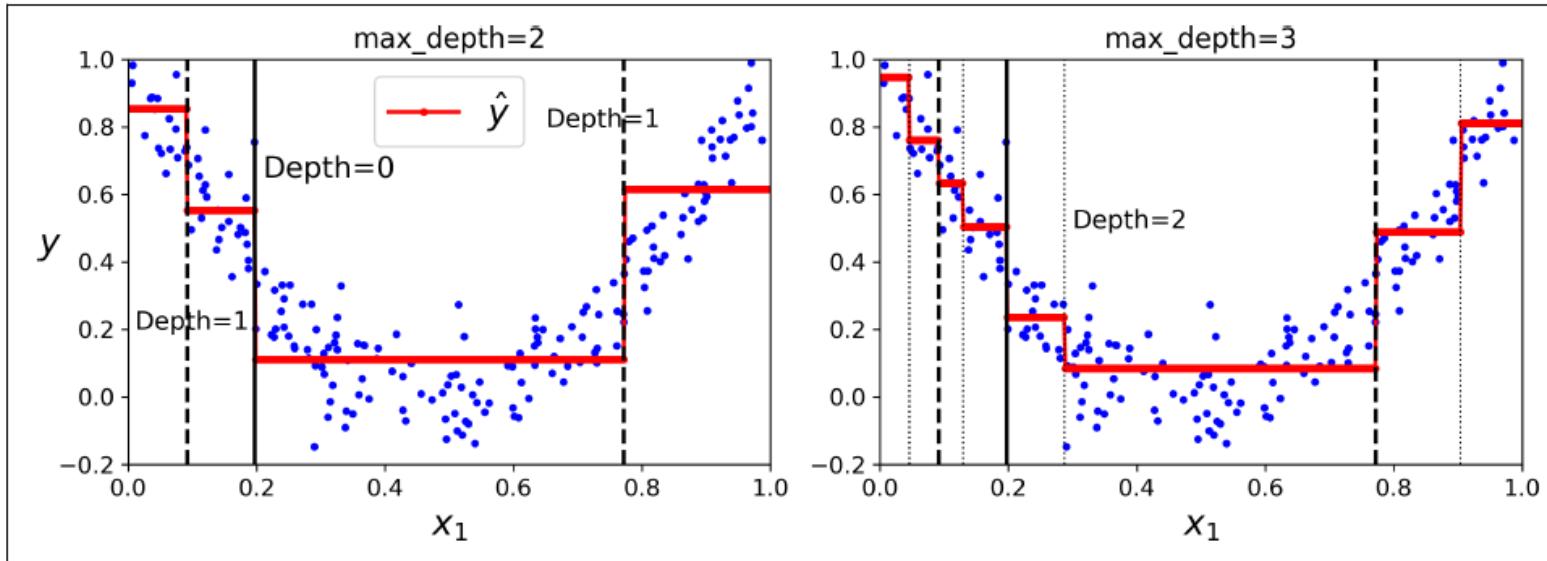


- It now tries to split the training set in a way that **minimizes the MSE**. (instead of minimizing impurity)

Equation 6-4. CART cost function for regression

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

Decision Tree Regression

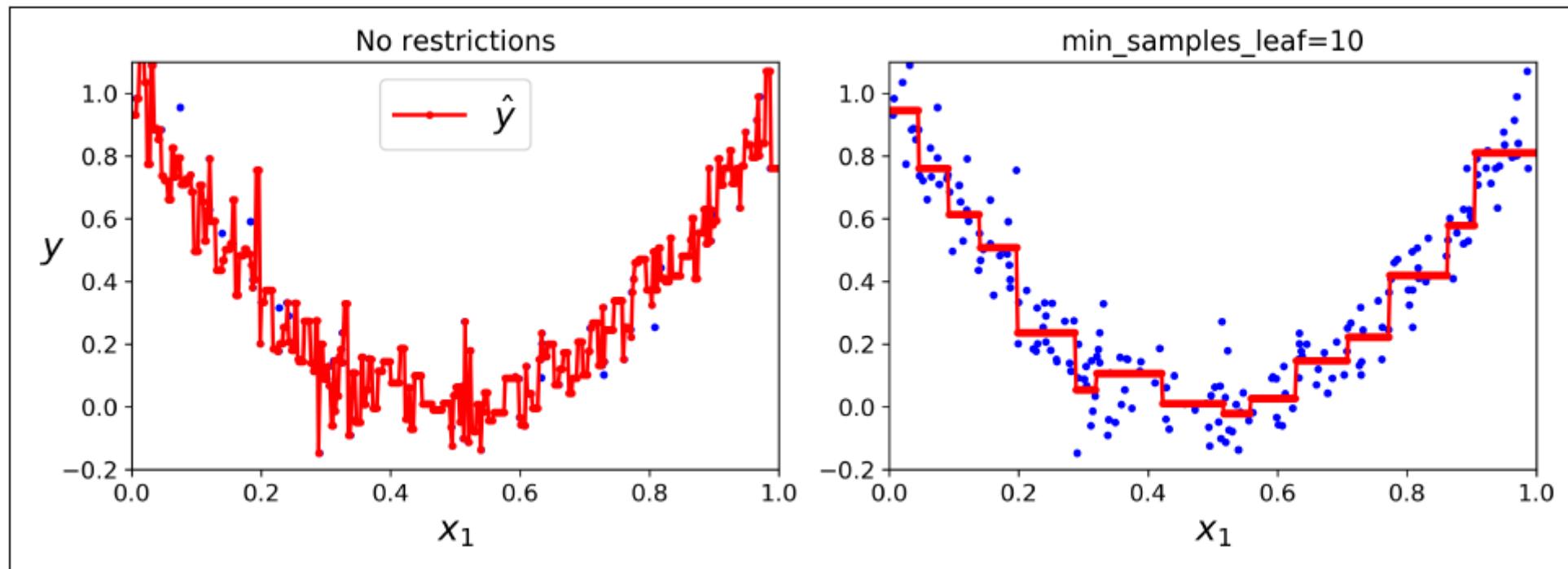


Equation 6-4. CART cost function for regression

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

Decision Tree Regression

- Regularizing the Model



Ensemble Models

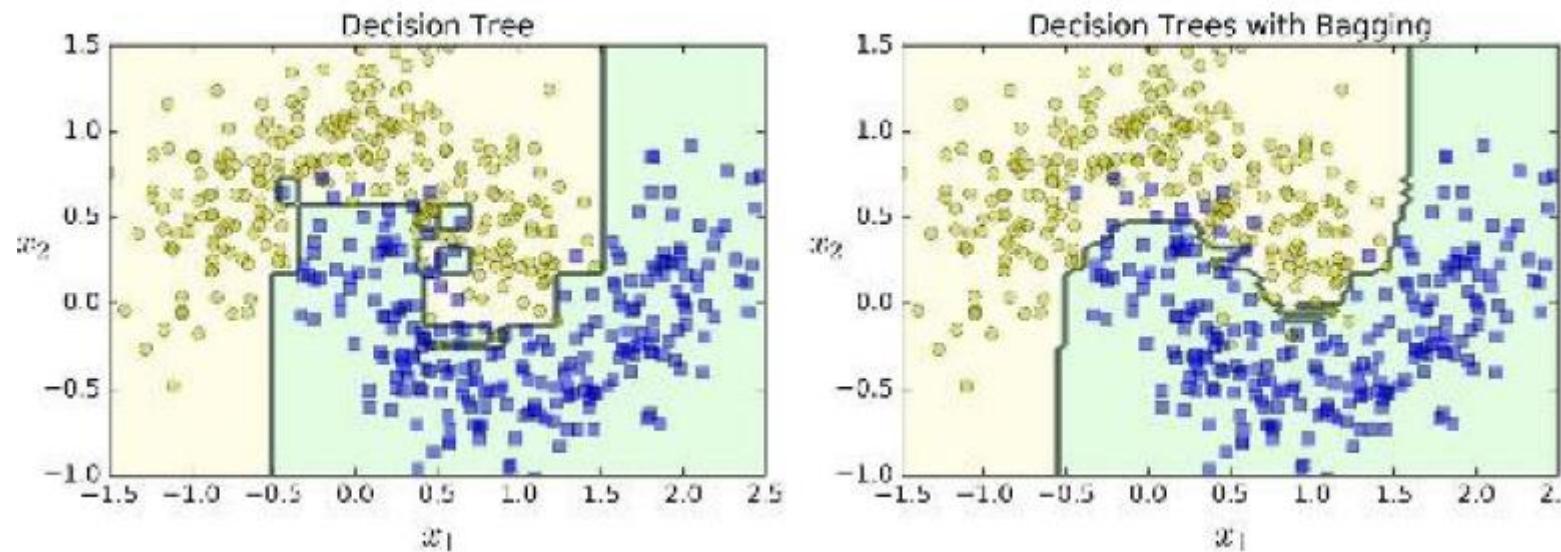
- **Ensemble method:**

- to aggregate the predictions of each classifier and predict the class that gets the most votes (**Hard Voting**: 직접투표)
- 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

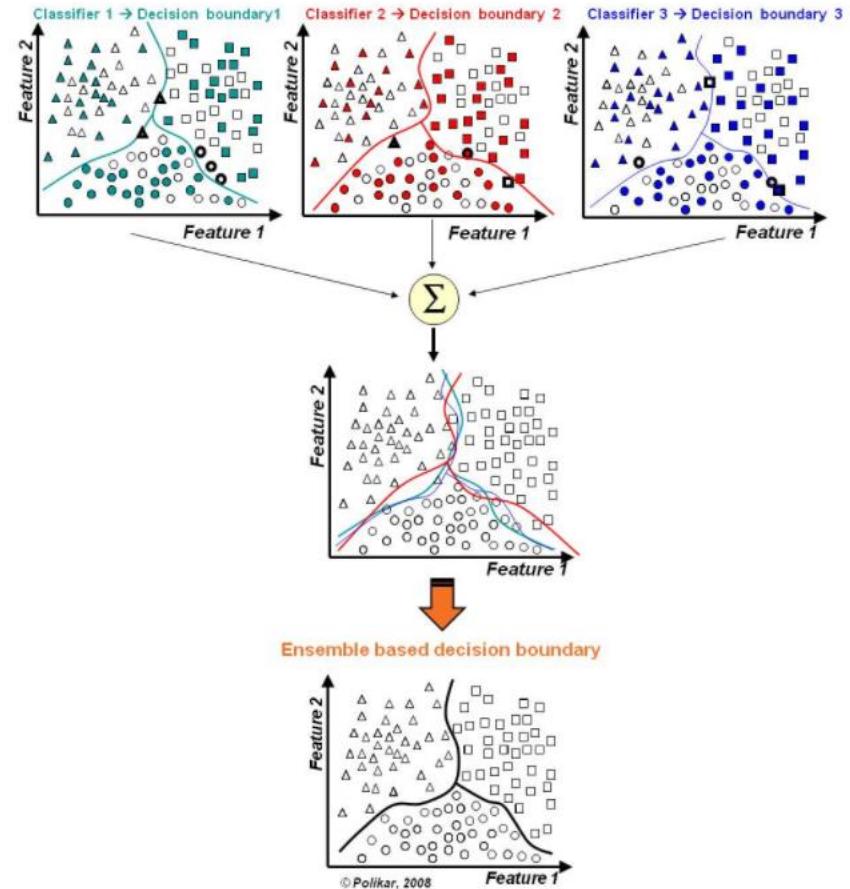
- **Decision Tree and Decision Tree with Bagging**
 - Moon dataset with 500 decision trees
 - The ensemble has a comparable bias, but a **smaller variance**. (roughly the same number of errors on the training set, but the decision boundary is less irregular)



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

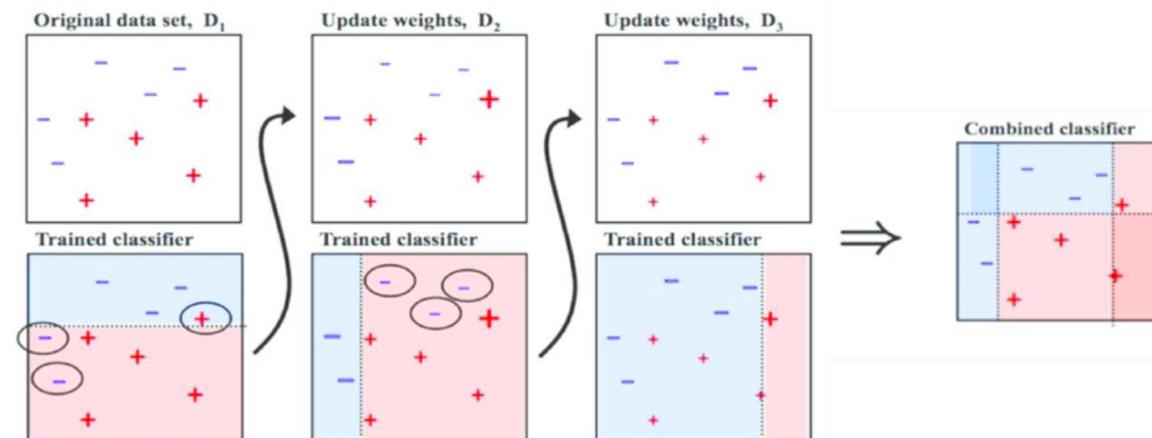


출처: <https://swalloow.github.io/bagging-boosting>

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 observation weights $w_i = 1/N$

2. For $m = 1, 2, \dots, M$

- Train $G_m(x)$

- Compute the weighted error $Err_m = \frac{\sum_{i=1}^N w_i \mathcal{I}(y^{(i)} \neq G_m(x^{(i)}))}{\sum_{i=1}^N w_i}$

- Compute coefficient $\alpha_m = \log\left(\frac{1-err_m}{err_m}\right)$

- Set data weights $w_i \leftarrow w_i \exp[\alpha_m \mathcal{I}(y^{(i)} \neq G_m(x^{(i)}))]$

3. Output $G(x) = \text{sign} \left[\sum_{m=1}^M \alpha_m G_m(x) \right]$

Weights on the error (loss)

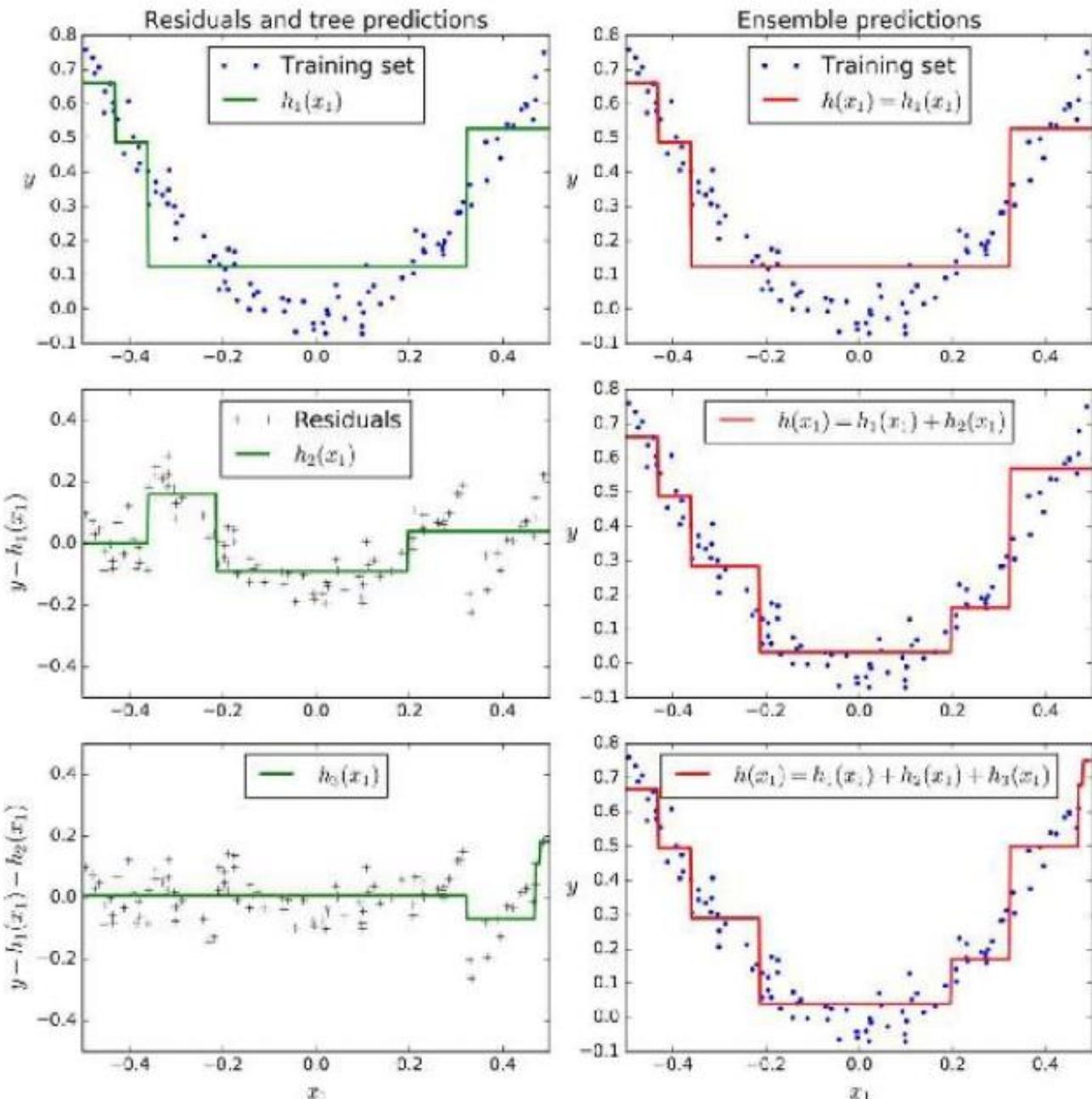
Contribution (weight) of each $G(x)$
(the more accurate, the higher influence)

Higher weight on misclassified

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 스트래핑**이라고도 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

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 $s(\text{similarity})$ 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)

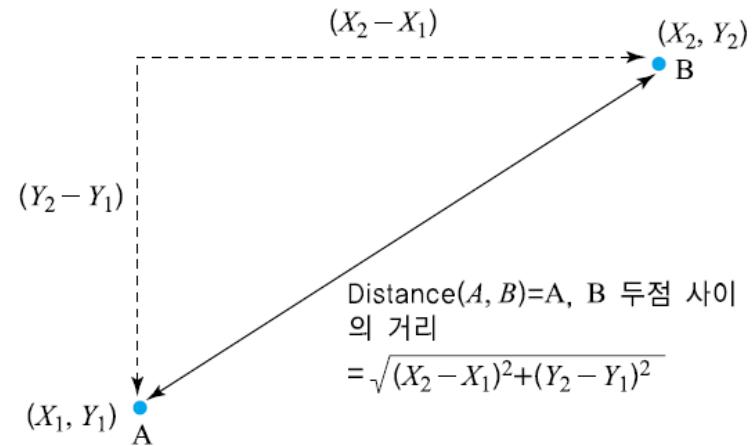
| 구분 | 키 | 몸무게 | 나이 |
|----|-------|------|-----|
| A | 174cm | 70kg | 21세 |
| B | 170cm | 61kg | 27세 |
| C | 162cm | 73kg | 29세 |

Clustering

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

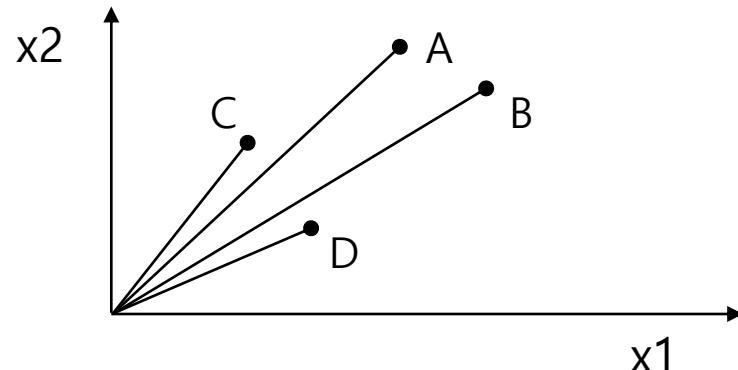
N-차원

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



- Cosine distance – 방향성, 주향

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



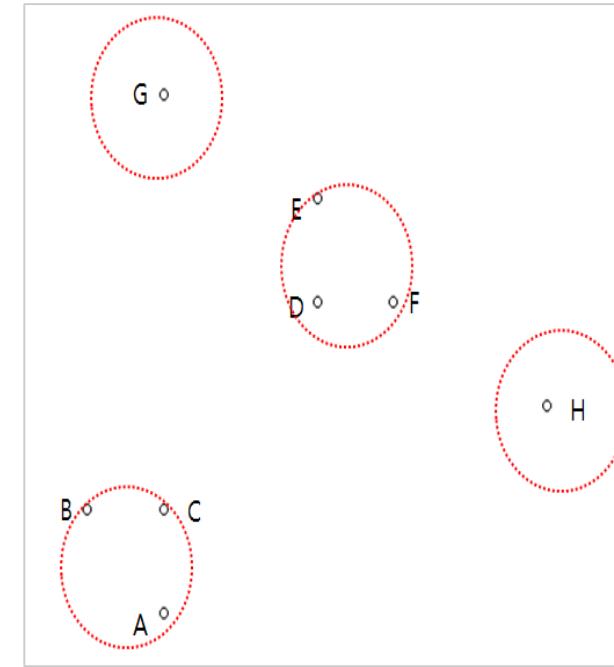
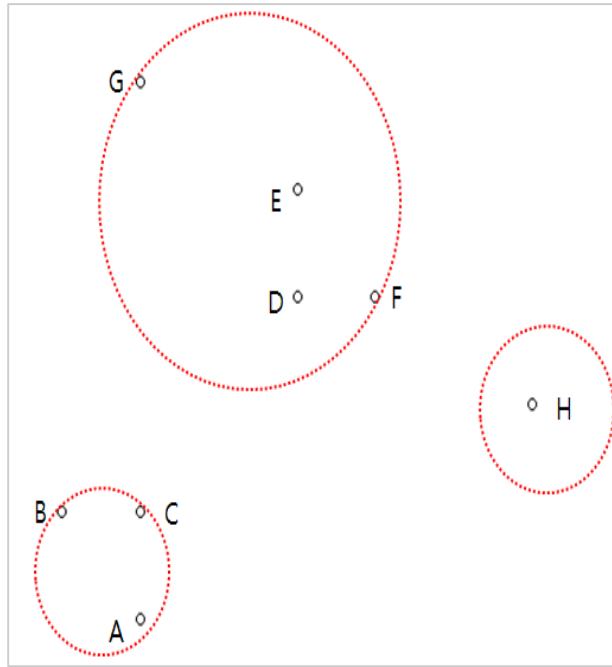
Clustering

- Jaccard similarity (자카드 유사도)
 - 비슷한 취향의 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, $0.01 < 0.02$ 이므로 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, $0.076 > 0.047$ 이므로 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

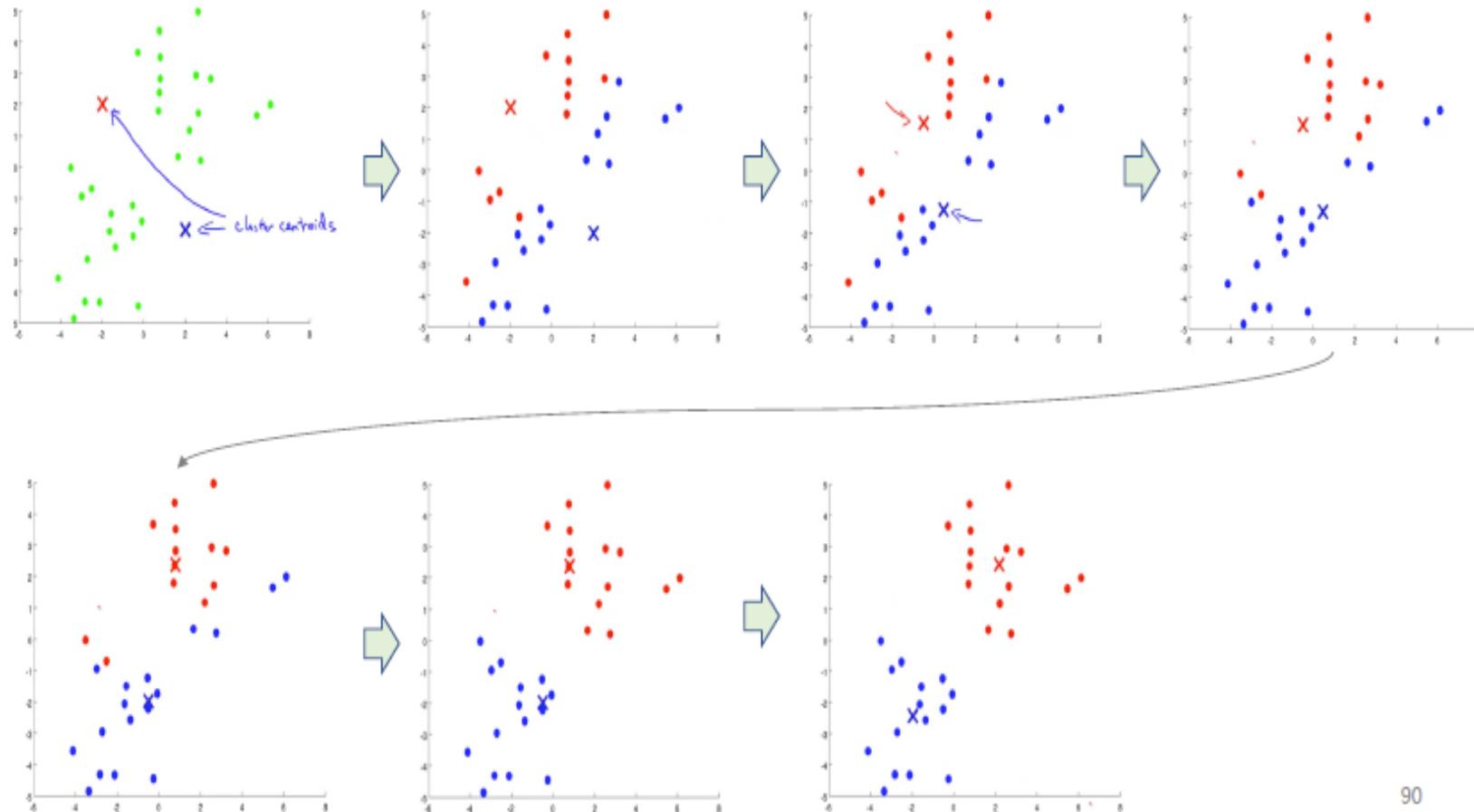


Clustering (군집화)

- K-means()
 - 공간상에 임의의 k 개의 임의의 초기 지점을 클러스터 중심점으로(cluster center) 정함
 - 클러스터 중심점을 중심으로 거리가 가까운 항목을 선택하여 클러스터 공간을 나눔
 - 각 클러스터에 포함된 항목들의 평균 위치를 구해 이를 새로운 클러스터 중심점 (centroid)으로 변경
 - 새로 설정된 센트로이드를 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

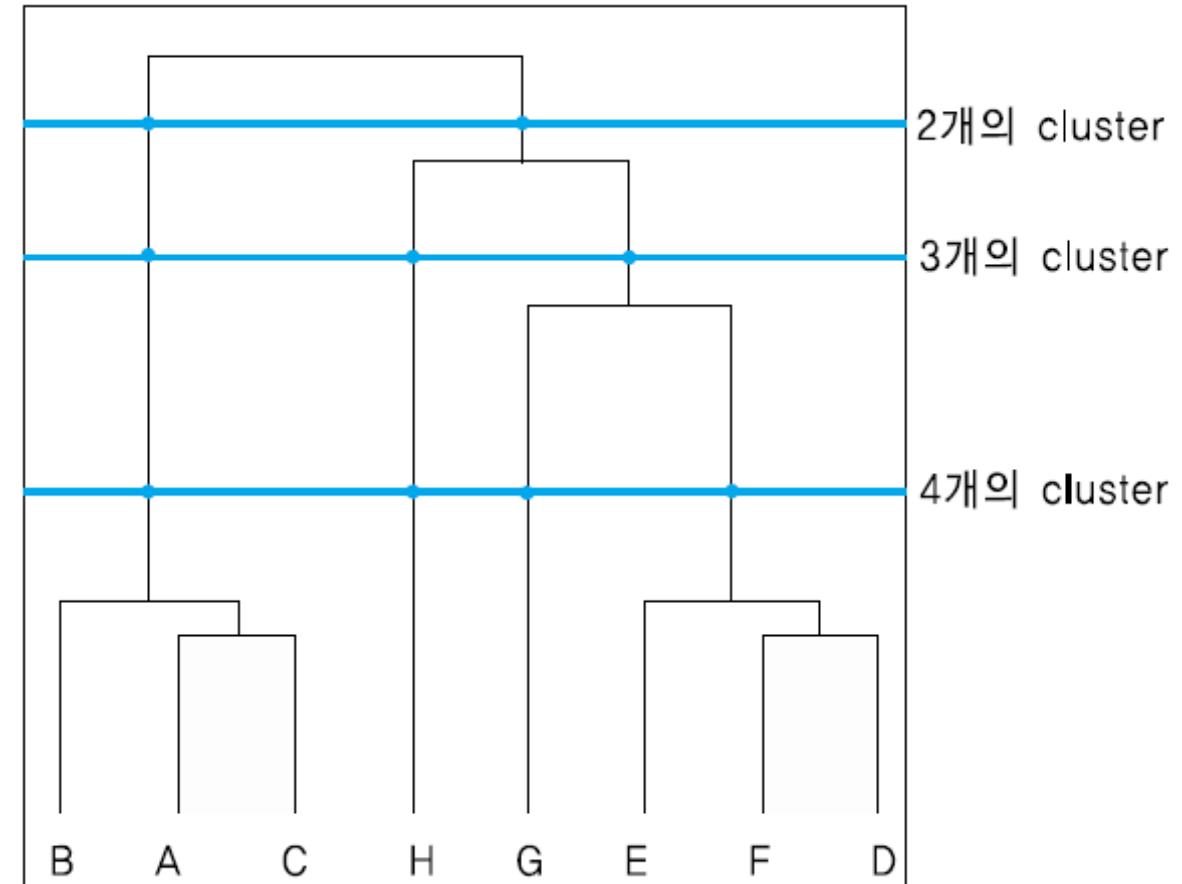
Clustering (군집화)

K-Means 클러스터링이 진행되는 과정



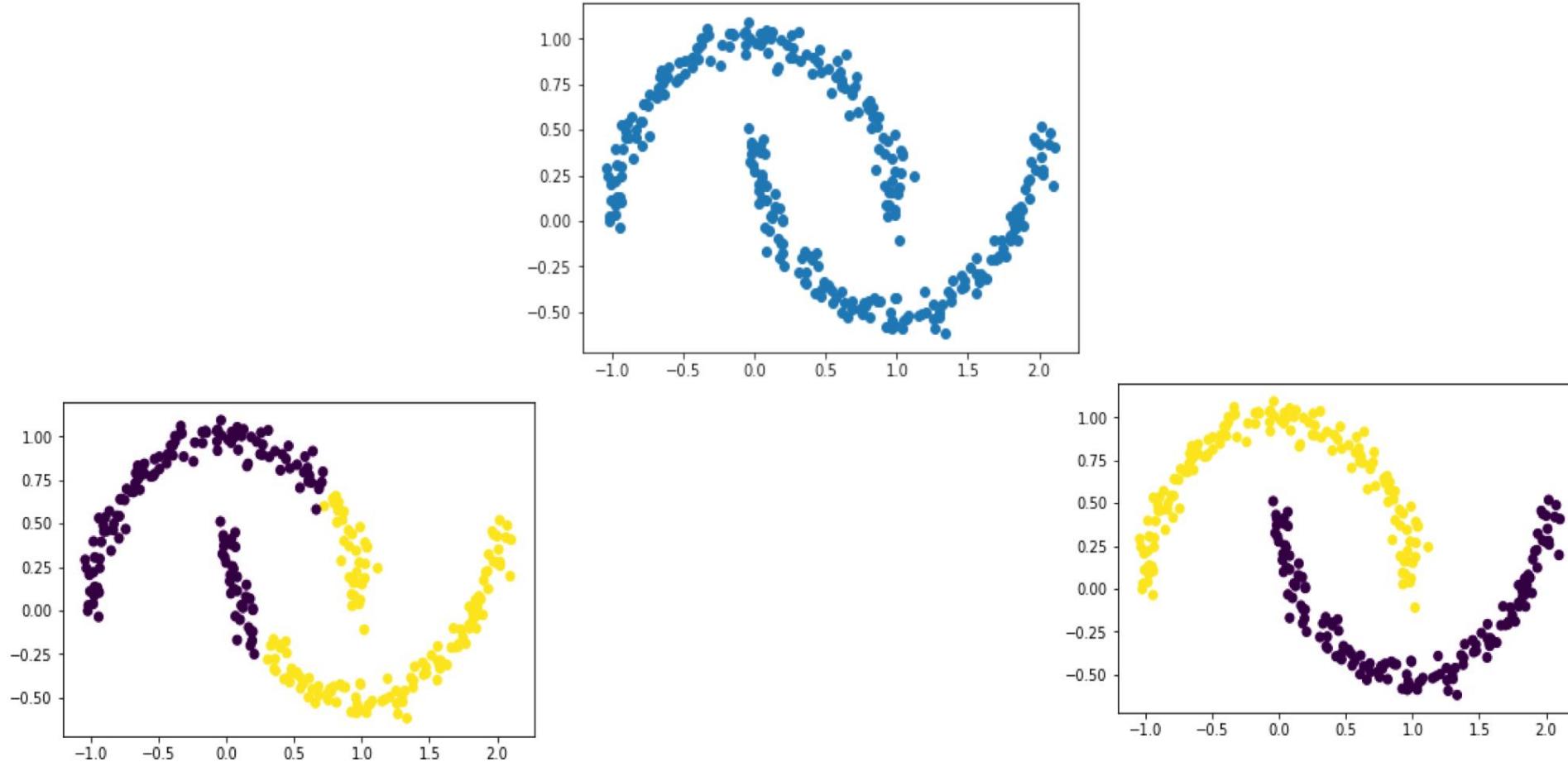
Clustering (군집화)

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



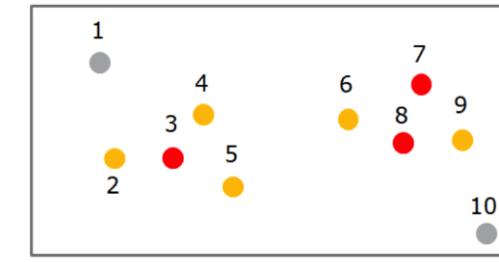
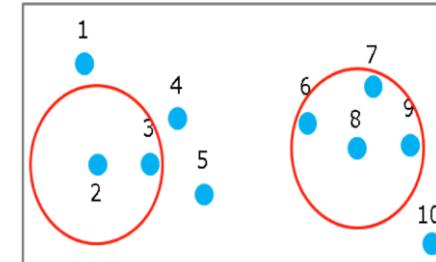
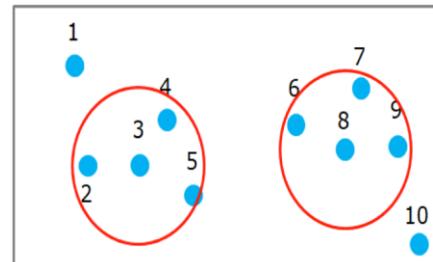
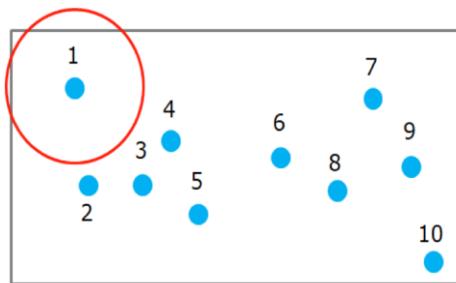
Clustering (군집화)

- Two Moon dataset



Clustering (군집화)

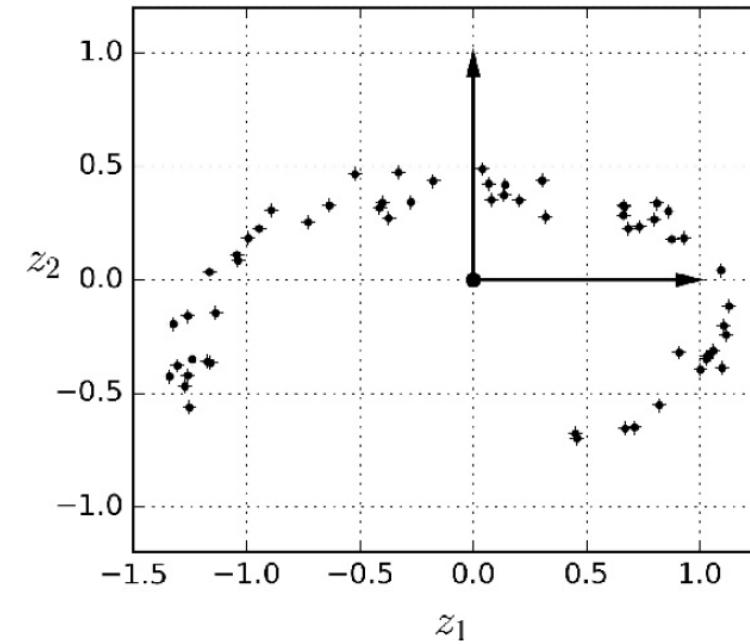
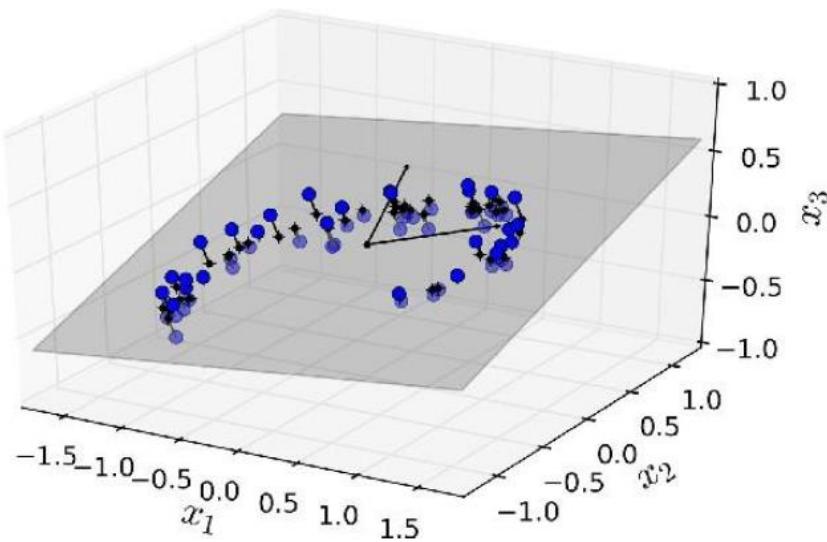
- DBSCAN(Density Based Spatial Clustering of Applications with Noise)
 - One of the most common clustering algorithm
 - Density-based (밀도기반): “가까이 있는 샘플들은 같은 군집에 속한다” 는 원칙
 - **Core point**: 거리 e (epsilon) 내에 m (minPts) 개의 점이 있을 때 – 스스로 Cluster 형성
 - **Border point**: Core point 는 아니지만 Core point 의 군집에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



● 노이즈 데이터 ● 경계 데이터 ● 코어 데이터

Dimension Reduction

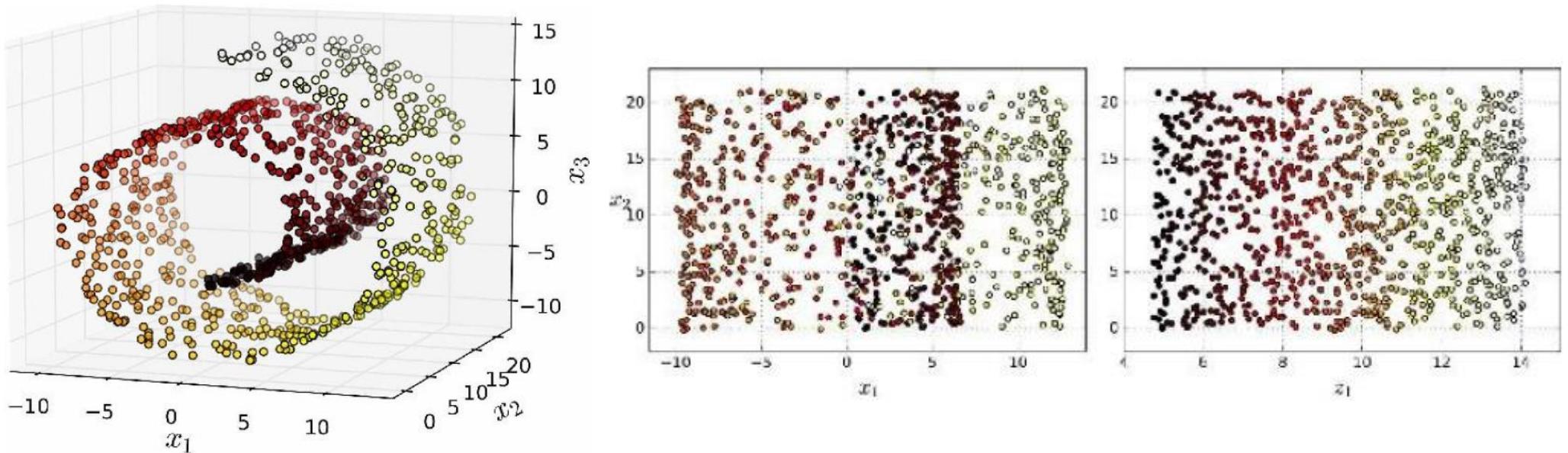
- Dimension Reduction approach
 - Projection
 - Manifold Learning



A 3D dataset lying close to a 2D subspace

Dimension Reduction

- Dimension Reduction approach
 - Projection
 - Manifold Learning

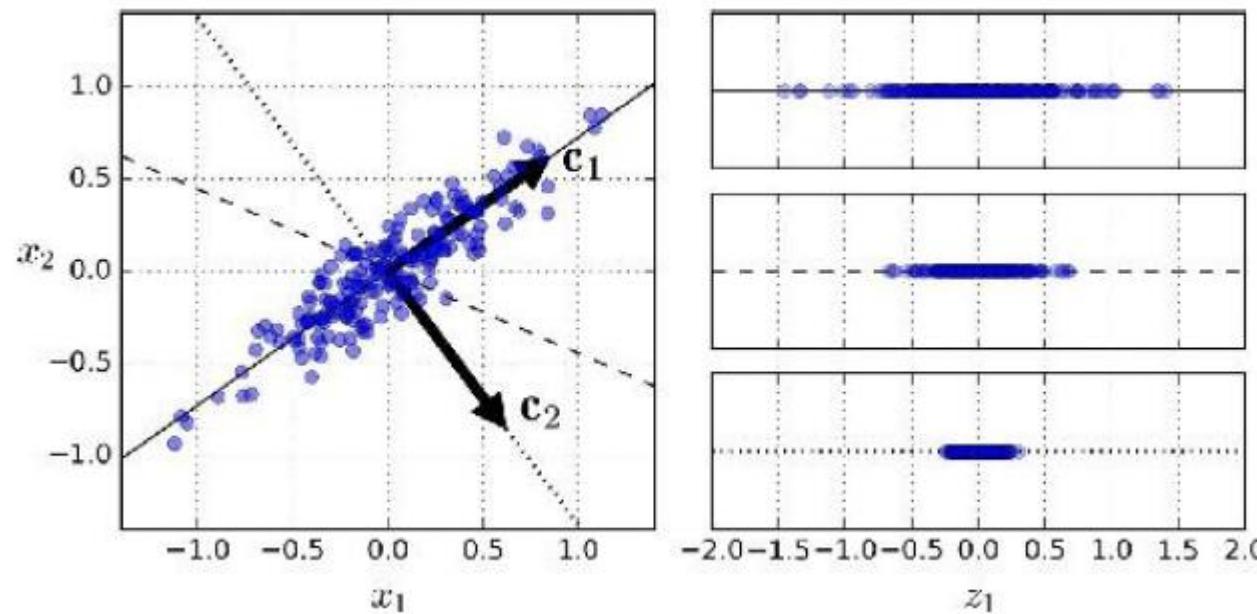


Swiss roll: Projection is not always Good. – Projection and Unrolling.

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.



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 ($n \times p \rightarrow n \times k$, where $k \ll p$)
 - Data analysis and visualization
 - Can be implemented using **SVD** or **Eigenvalue Decomposition**

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 $i \in \{1, \dots, r\}$, where as usual $r = \text{rank}(A)$.

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

Dimension Reduction

- PCA calculation

Step 1. 데이터 정규화 (mean centering)

Step 2. 기존 변수의 covariance (correlation) matrix 계산

Step 3. Covariance (correlation) matrix로부터 eigenvalue 및 이에 해당되는 eigenvector를 계산

Step 4. Eigenvalue 및 해당되는 eigenvectors를 순서대로 나열

$$\lambda(1) > \lambda(2) > \lambda(3) > \lambda(4) > \lambda(5)$$

$e(1) > e(2) > e(3) > e(4) > e(5)$, $e(i)$, $i=1,\dots,5$ is a vector

Step 5. 정렬된 eigenvector를 토대로 기존 변수를 변환

$$Z_1 = e(1)\mathbf{X} = e_{11} \cdot X_1 + e_{12} \cdot X_2 + \dots + e_{15} \cdot X_5$$

$$Z_2 = e(2)\mathbf{X} = e_{21} \cdot X_1 + e_{22} \cdot X_2 + \dots + e_{25} \cdot X_5$$

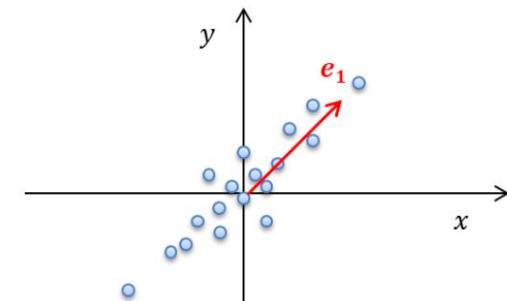
...

...

$$Z_5 = e(5)\mathbf{X} = e_{51} \cdot X_1 + e_{52} \cdot X_2 + \dots + e_{55} \cdot X_5$$

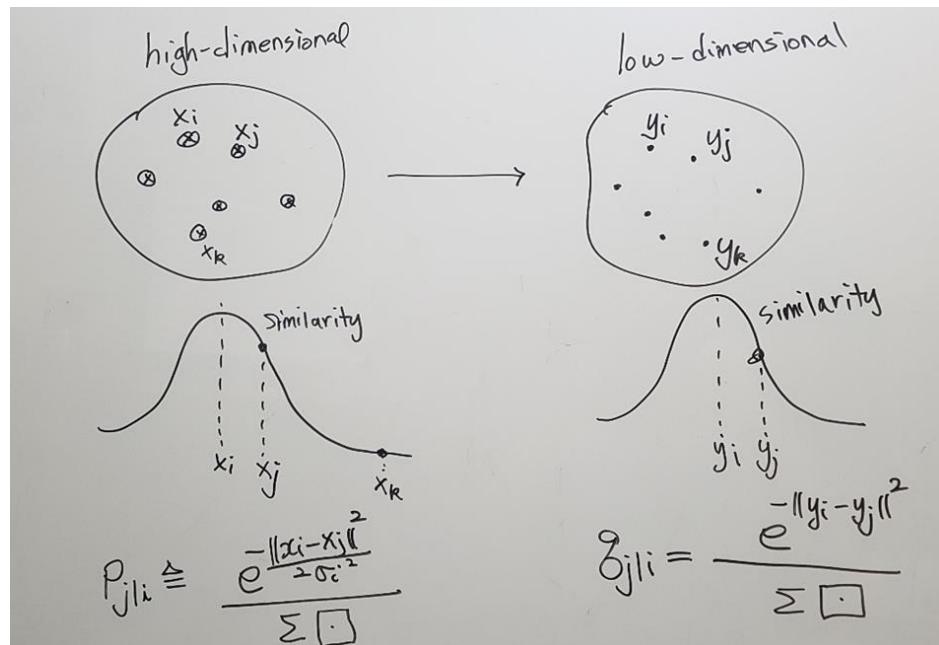
$$\text{Cov}(x,y) = \frac{\sum (x_i - \bar{x}) * (y_i - \bar{y})}{N}$$

Eigen vector of $\text{Cov}(x,y)$: 분산의 방향
Eigen value: 분산의 크기



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)



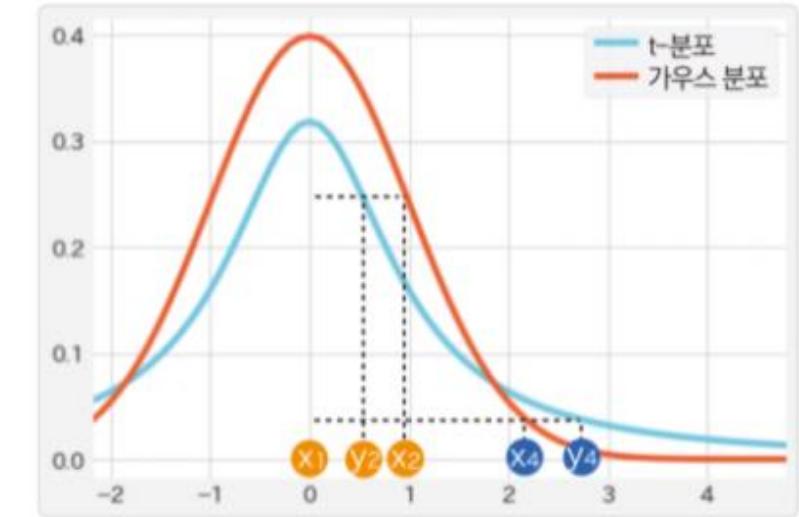
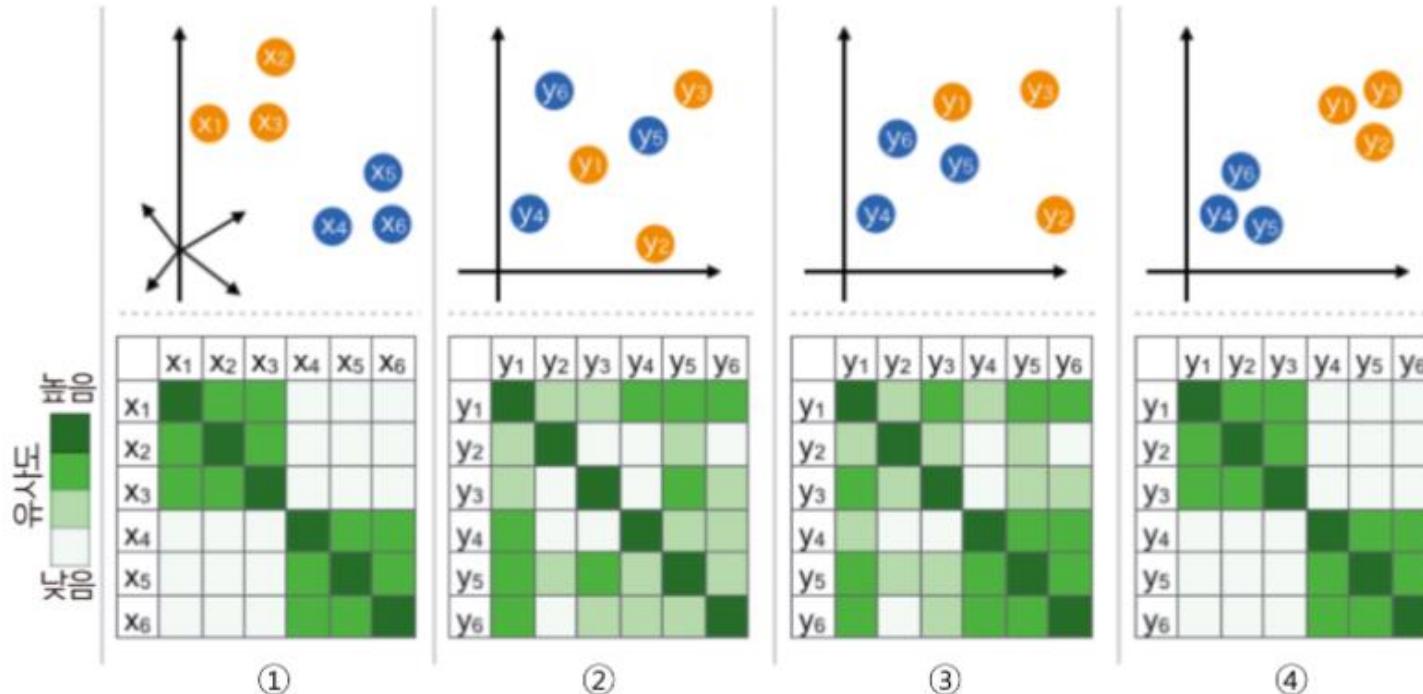
- Hyper-parameter '**perplexity**' controls σ_i , normally $5 \sim 50$
- We want to make $q_{j|i} \rightarrow p_{j|i}$, the cost function C is

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

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

Dimension Reduction

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



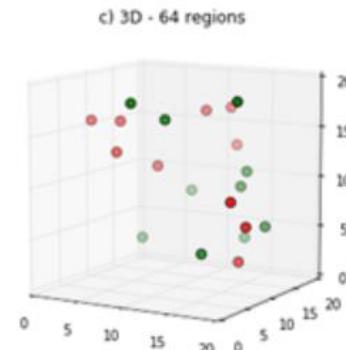
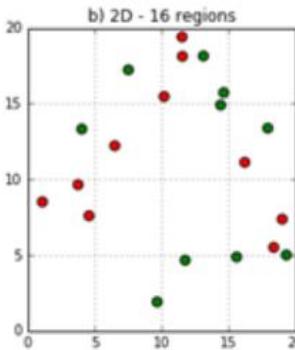
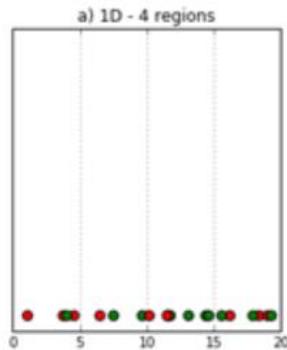
(low dimensional space상에서)
high similarity 는 더 가깝게, low similarity 는 더 멀게 배치

Practical issues in machine learning

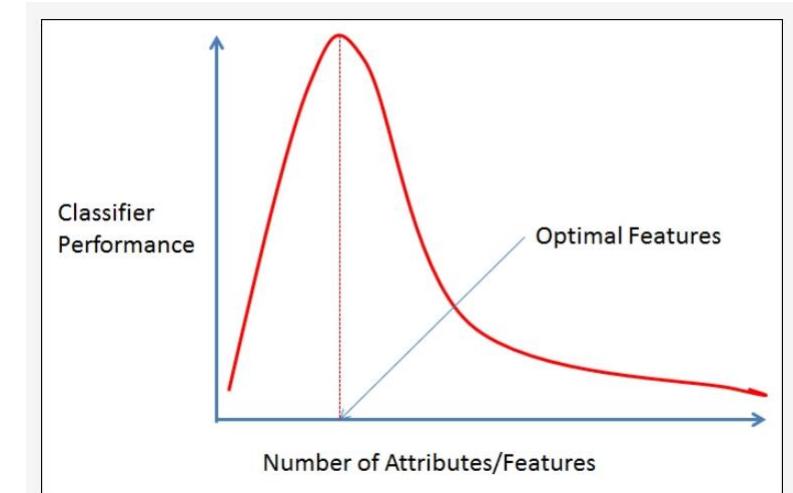
| issue | result | method |
|---|--|---|
| Data volume, velocity, and scalability | <ul style="list-style-type: none">May be infeasible due to constraints in algorithms and hardware | <ul style="list-style-type: none">Data sampling (stratified sampling, varying sample sizes) |
| Data quality and noise (missing values, duplicate values, incorrect values, Incorrect formatting) | <ul style="list-style-type: none">Incorrect or incomplete model | <ul style="list-style-type: none">data cleaning |
| Imbalanced data | <ul style="list-style-type: none">affects the choice of learning, the process of selecting algorithms, model evaluation and verificationMay suffer large biases | <ul style="list-style-type: none">cost-sensitive learning, ensemble learning, outlier detection |
| Overfitting | <ul style="list-style-type: none">Poor performance (to unseen data) | <ul style="list-style-type: none">More data, simple model, regularization, early stopping, dropout |
| Curse of dimensionality (too many features) | <ul style="list-style-type: none">Introduce sparsity (fewer data points on average per unit volume of feature space), hence poor performance (in distance-based models) | <ul style="list-style-type: none">Dimension reductionFeature selectionFeature engineering |

Practical issues in machine learning

- **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

How to deploy ML model?

- Deploy your machine learning model into production
- Some free deployment platforms:
 - Algorithmia: create code snippets and you can call your code as an API
 - PythonAnywhere: easy to run Python in cloud (do not support GPU)
 - Heroku: flexible and easy to use
 - GCP(Google Could Platform): offers AI platform, App engine, Could functions
 - Microsoft Azure Functions: serverless cloud service as a FaaS (Functions-as-a-service)
 - AWS Lambda from Amazon: serverless computing service as part of Amazon Web Services
 - Use the **mc2gen** Python library: convert the model into 14 different programming languages
 - More commercial platforms
 - See <https://www.freecodecamp.org/news/deploy-your-machine-learning-models-for-free/>

More on Machine Learning

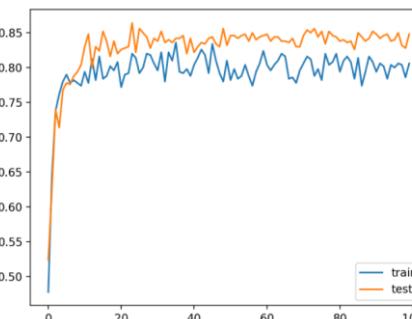
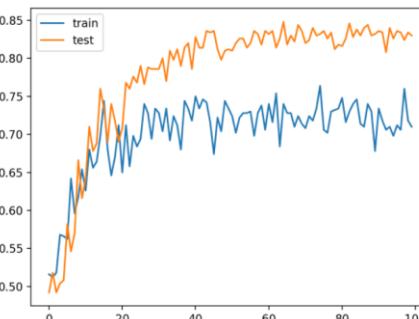
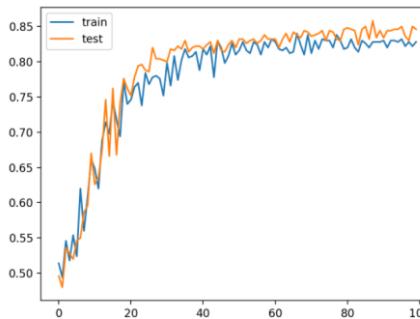
- **Batch normalization**

- To reduce gradient vanishing and exploding problem
- Automatically standardize the inputs to layers in Deep Learning network (over mini-batch)
- Dramatically **accelerating** the training process, and in some cases **improves** the performance
- Can be used **before** or **after** the activation function (in ANN, CNN, RNN)

```
2 model = Sequential  
3 model.add(Dense(32))  
4 model.add(BatchNormalization())  
5 model.add(Activation('relu'))
```

```
1 ...  
2 model = Sequential  
3 model.add(Dense(32, activation='relu'))  
4 model.add(BatchNormalization())
```

- (example) a simple 2-layer MLP classification (<https://machinelearningmastery.com/>)



In practice, run the model a few times and compare the average outcome !

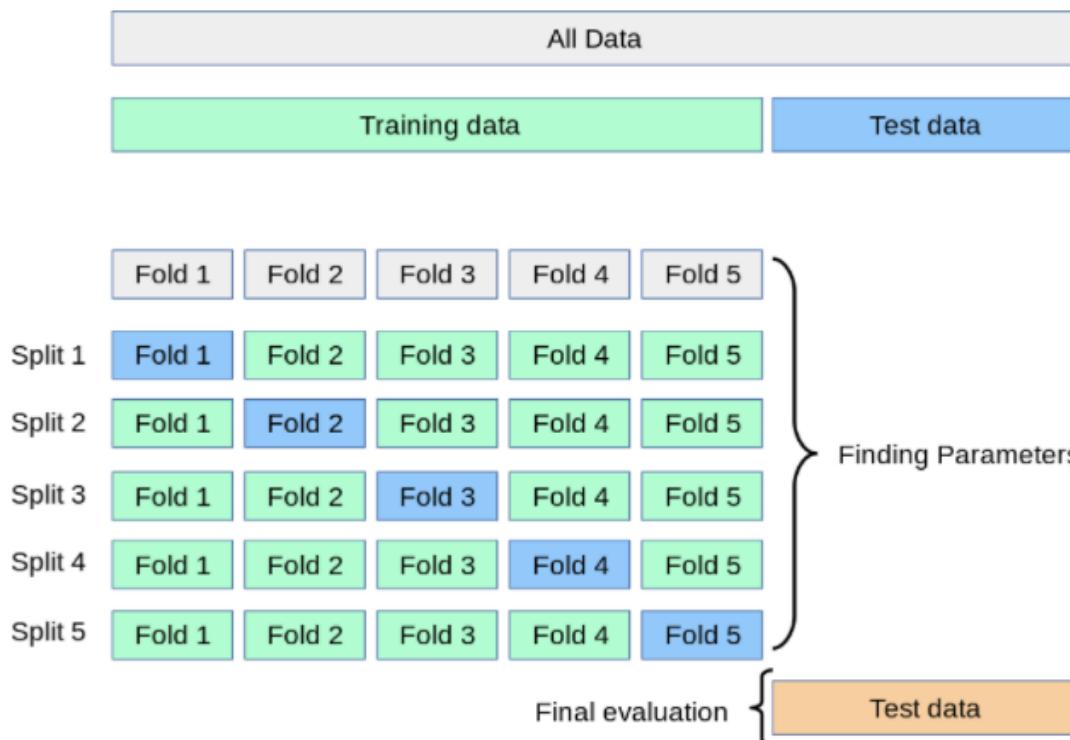
More on Machine Learning

- **Initialization of neural networks**
 - Initialization is critical to performance, and any constant initialization will perform poorly.
 - Too small or too large initial weights will lead slow learning and divergence.
 - visual demo at <https://www.deeplearning.ai/ai-notes/initialization/>
- **How to find appropriate values (rule of thumb)**
 - The **mean** of the activations should be zero
 - The **variance** of activations should stay the same across every layer
- **Xavier** and **He** initialization,
 - For every layer:
 - Weights are initialized with: $\text{mean}=0$, $\text{variance} = 1 / (\text{fan_in} + \text{fan_out})$ or $2 / (\text{fan_in})$
 - Biases are initialized with zeros
 - **Xavier** works better for layers with sigmoid activation, and **He** initialization works better for layers with ReLu.
- Keras supports both.

More on Machine Learning

- **(stratified) K-Fold Cross Validation**

- Helps to generalize the model (average)
- Can see how the model is robust, and data is reliable

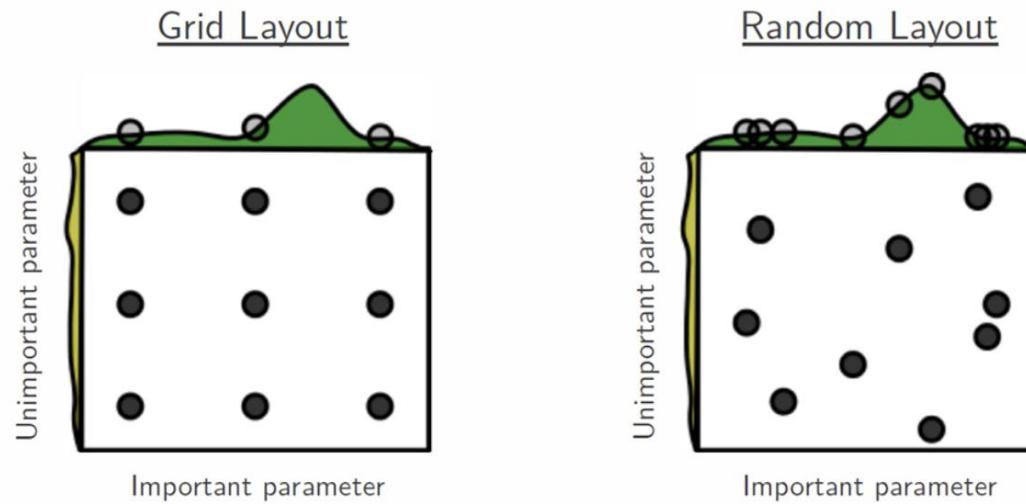


```
>>> from sklearn.model_selection import cross_val_score
>>> clf = svm.SVC(kernel='linear', C=1, random_state=42)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores
array([0.96..., 1. , 0.96..., 0.96..., 1. ])
```

More on Machine Learning

- **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



More on Machine Learning

- **Class imbalance problem**

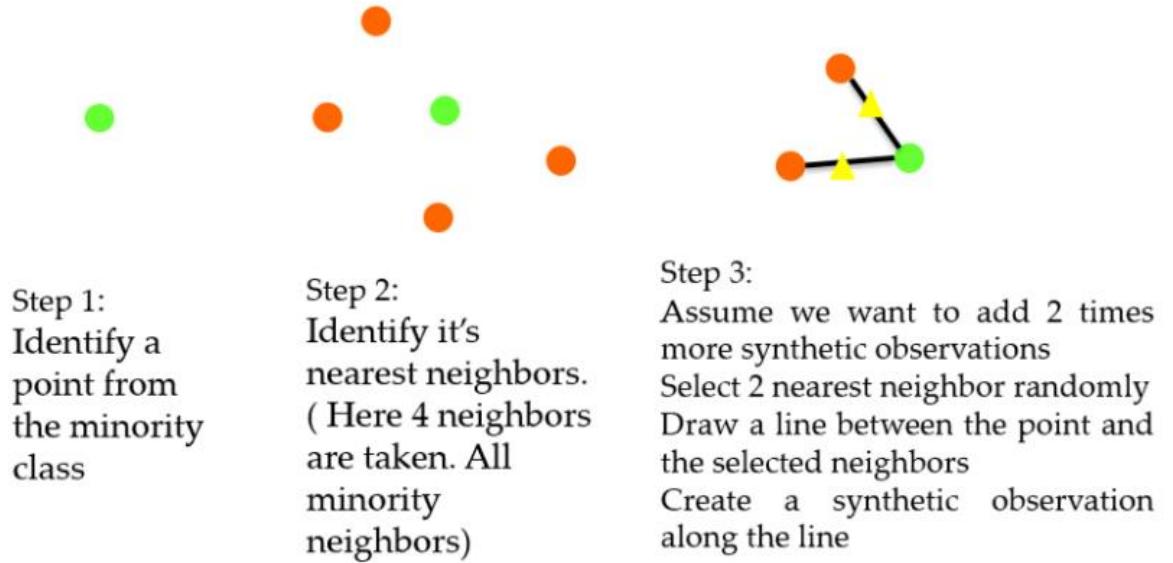
- Class distributions are highly imbalanced in the training dataset
- Tend to have low prediction accuracy for the infrequent (minority) class
- Exists in many real word classification problems, such as fraud detection, spam detection, threat-object detection, anomaly detection, etc.
- Causes: properties of the domain, biased sampling, measurement error

- **How to reduce the imbalance problem?**

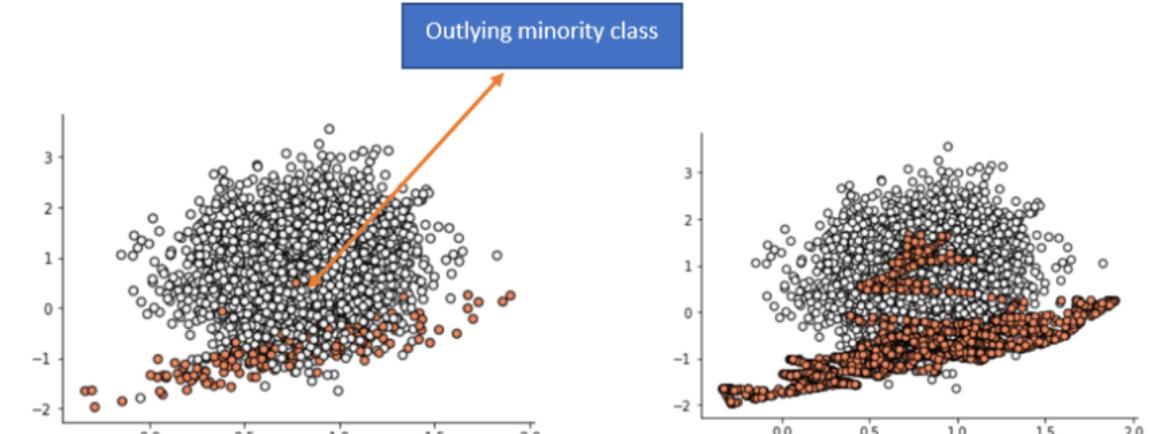
- Artificial resampling: over-sampling (replicating minority class), under-sampling of majority class
- **SMOTE**(Synthetic Minority Oversampling TEchnique): make synthetic data points by finding the nearest neighbors to each minority sample
- **Augmentation** or Use generative model for synthetic data
- 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)



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



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

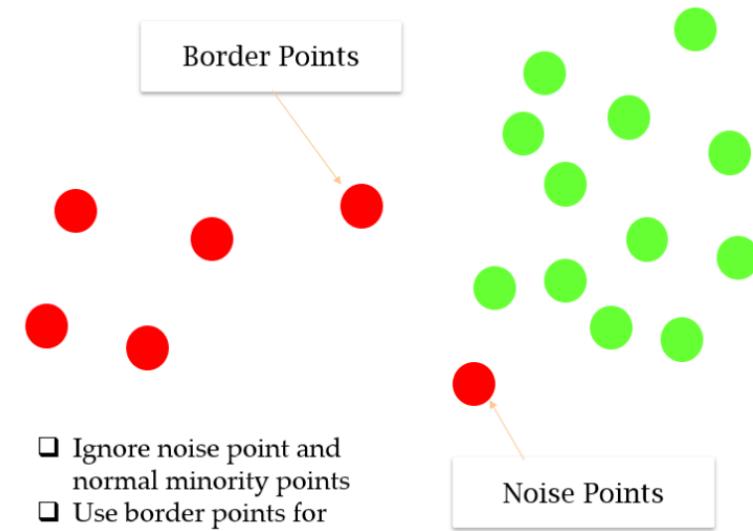
- If there are outlying minority classes and appear in the majority class, it creates a line bridge with the majority class. (problem!)

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.**

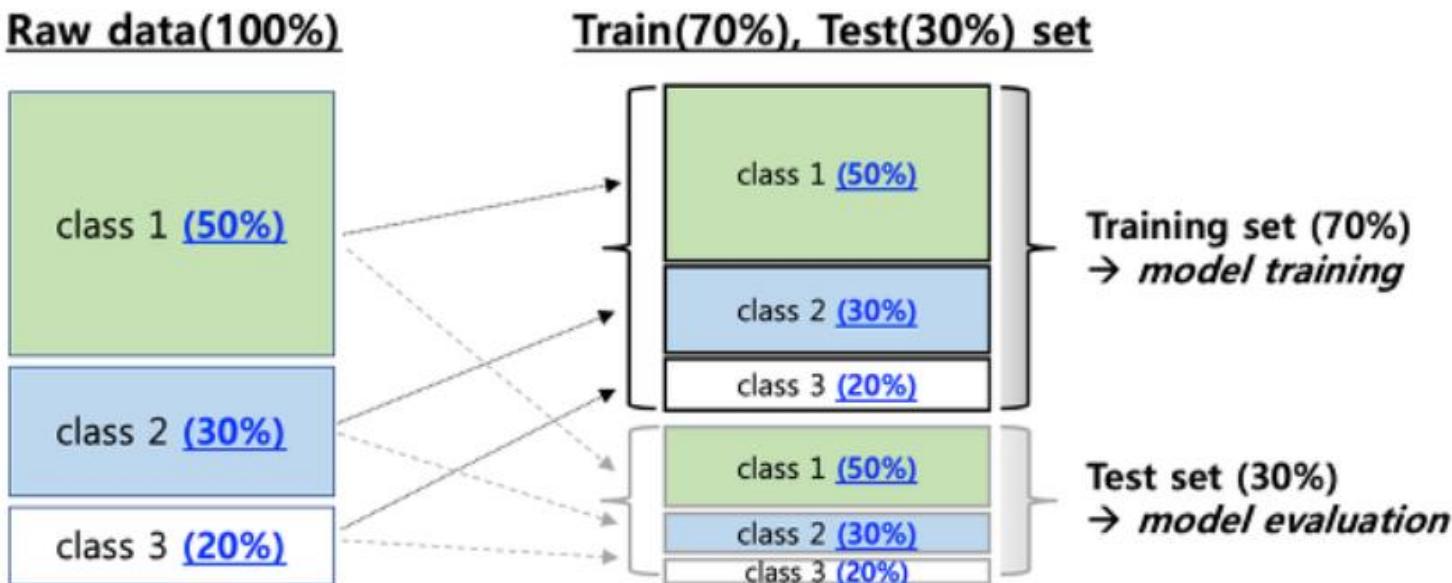
- More variants
 - ADASYN
 - and more ...



Border Line SMOTE : (Image Source Author)

Imbalance Problem

- Splitting dataset for Training and Testing



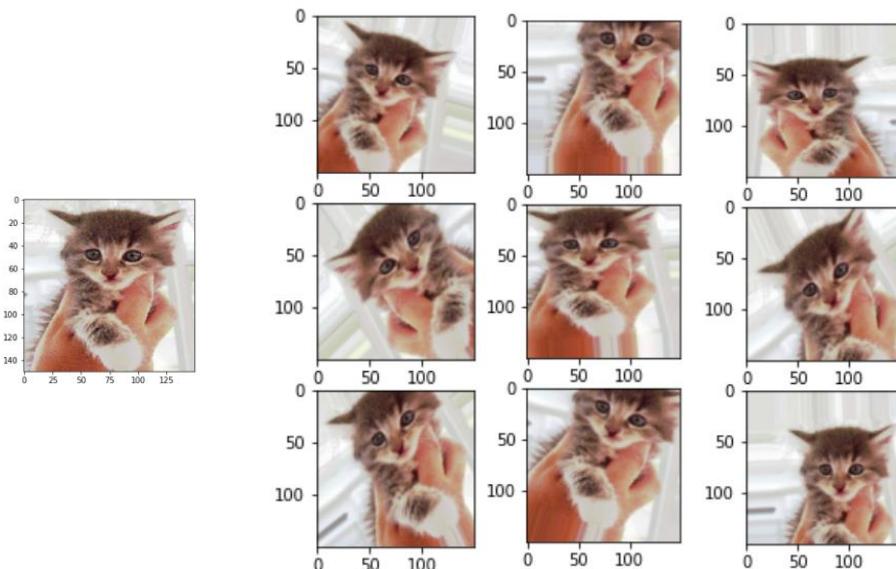
`sklearn.model_selection.train_test_split(X, y, test_size=0.3, stratify=stratum_col)`
→ returns $X_{train}, X_{test}, y_{train}, y_{test}$ set

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

More on Machine Learning

- **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

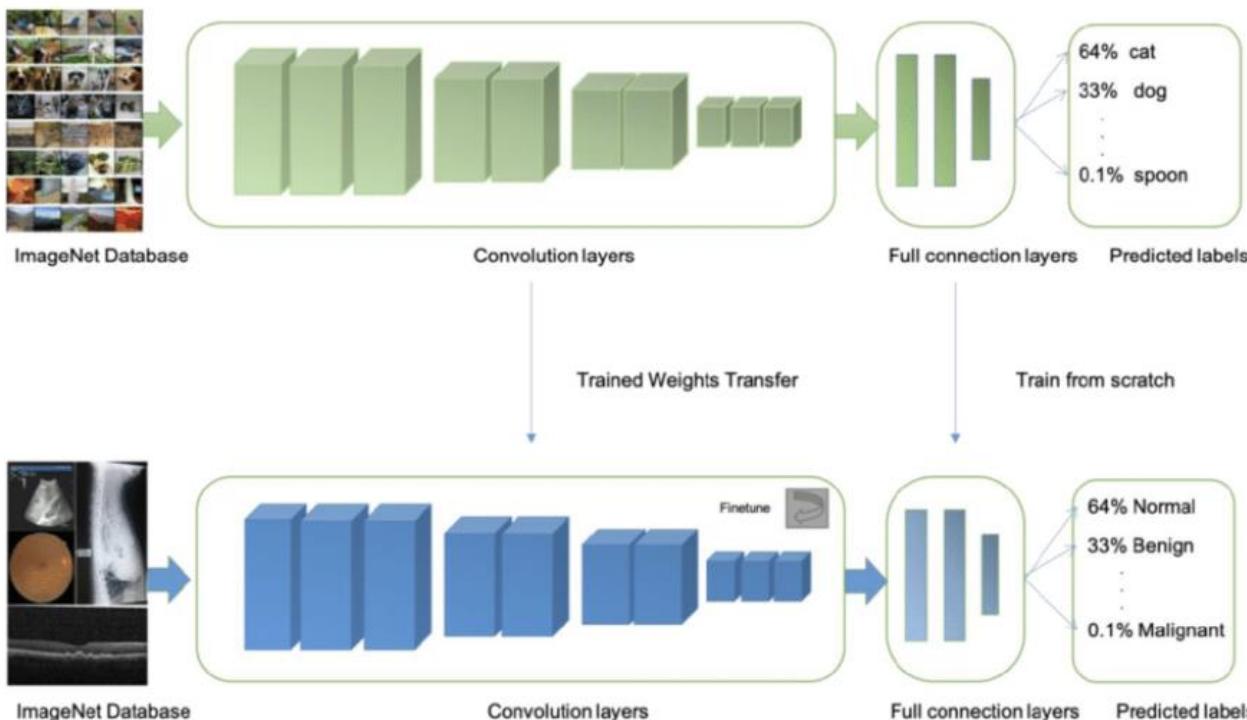


```
1 train_datagen = ImageDataGenerator(  
2     rescale= 1./255,  
3     rotation_range = 40,  
4     width_shift_range = 0.2,  
5     height_shift_range = 0.2,  
6     shear_range=0.2,  
7     zoom_range=0.2,  
8     horizontal_flip = True)
```

More on Machine 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



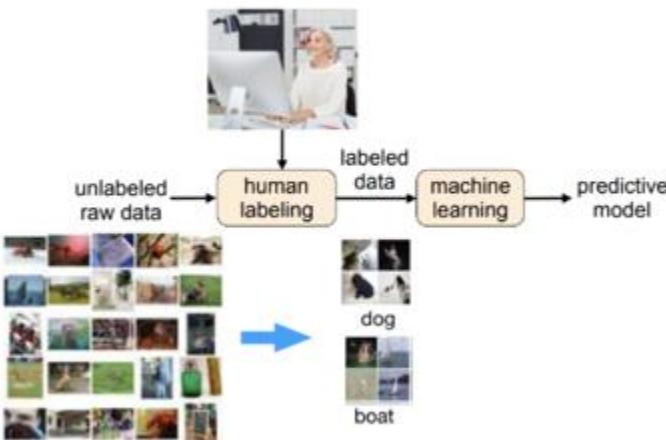
[ref: <https://www.researchgate.net/figure/>]

More on Machine Learning

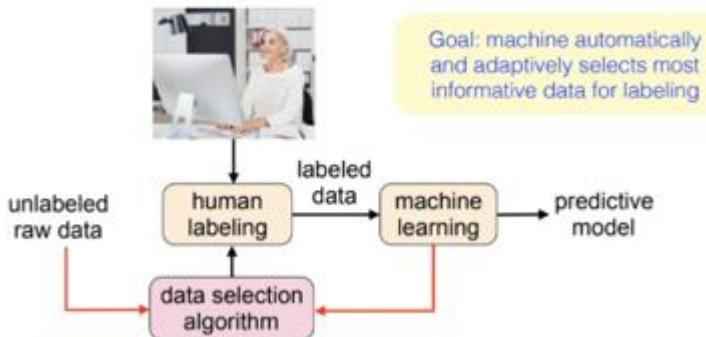
- **Active learning**

- 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

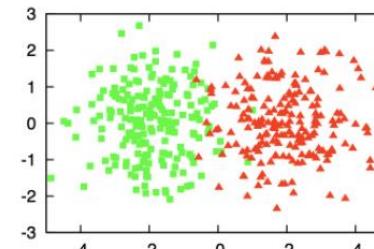
Conventional (Passive) Machine Learning



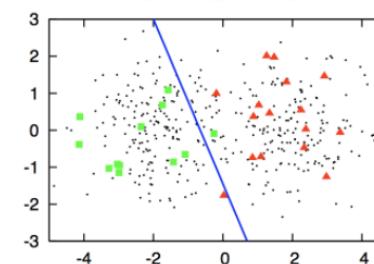
Active Machine Learning



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



poor selection



better selection

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**

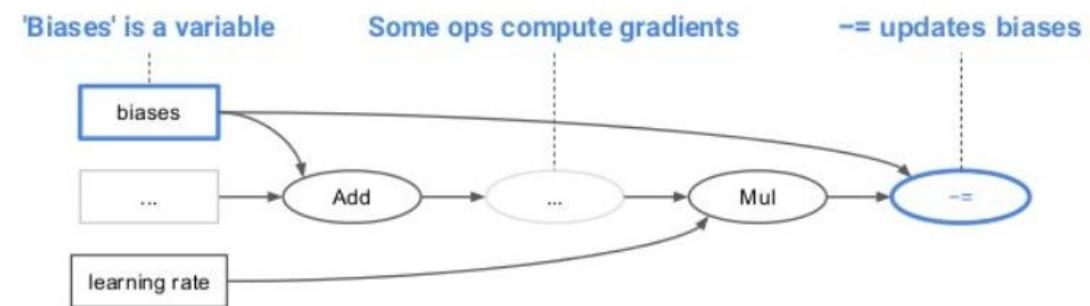
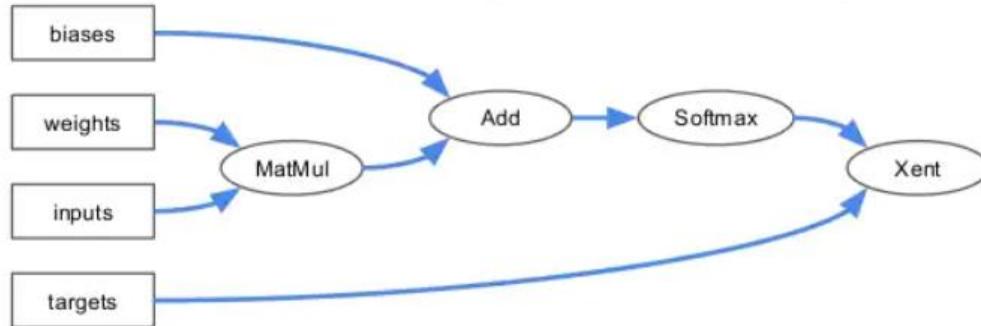
- Provides reasonable default values for most parameters

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:

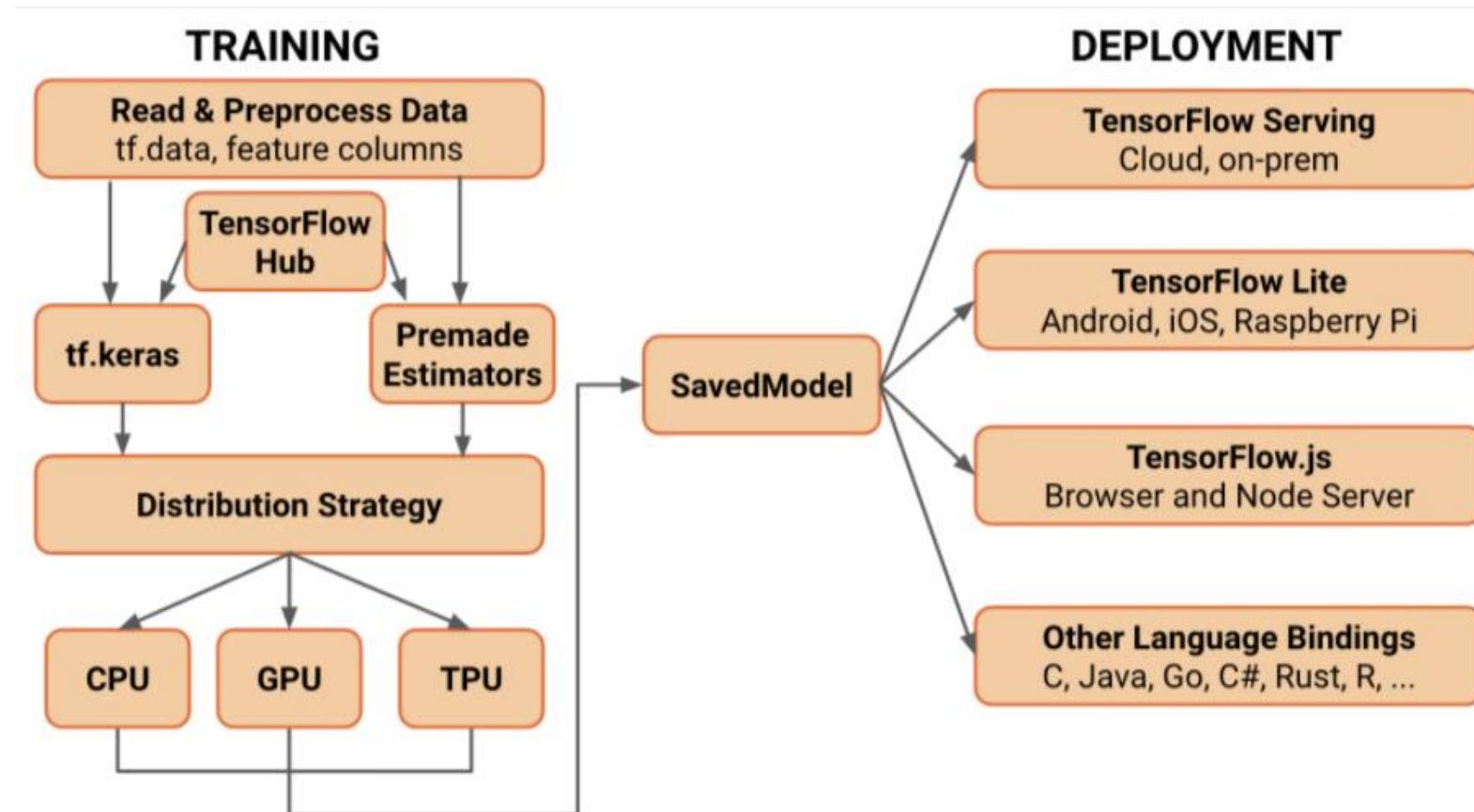
- Backward graph and update are added automatically to graph

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)

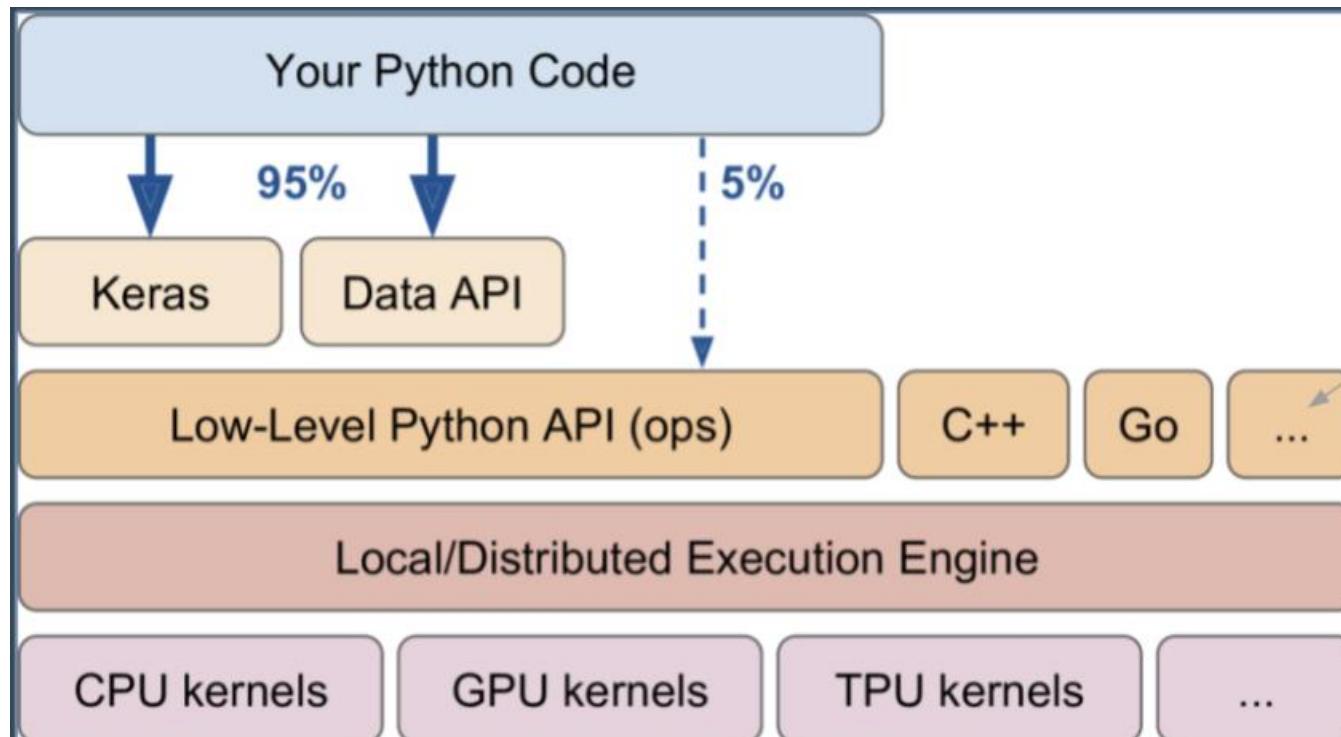
Tensorflow 2.0

- 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()
```