Lecture 7-3: Ensemble Learning
Random Forests

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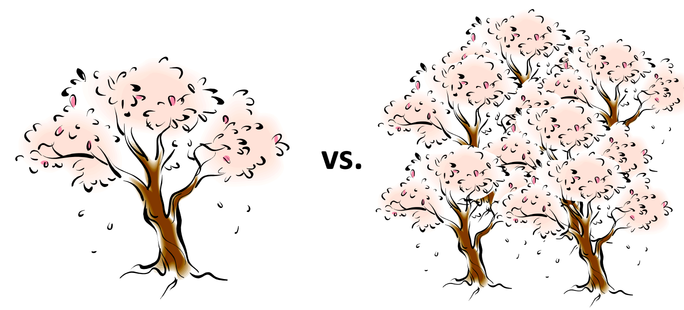
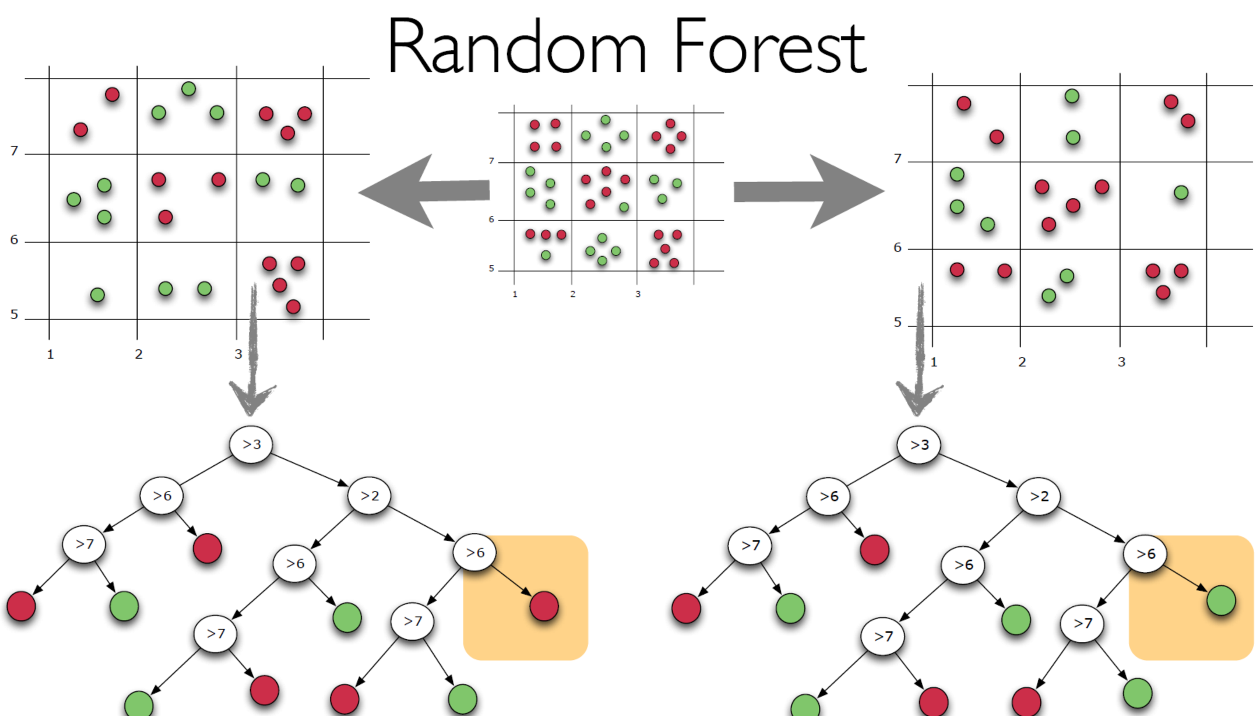
Random Forests

- A specialized bagging for decision tree algorithms
- Two ways to increase the diversity of ensemble
    - ✓ Bagging
    - ✓ Randomly chosen predictor variables





Random Forests

- Random Forests: Algorithm

1. For $b = 1$ to B:

   (a) Draw a $\boxed{\text{bootstrap sample}}$ $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select $\boxed{m \text{ variables at random}}$ from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

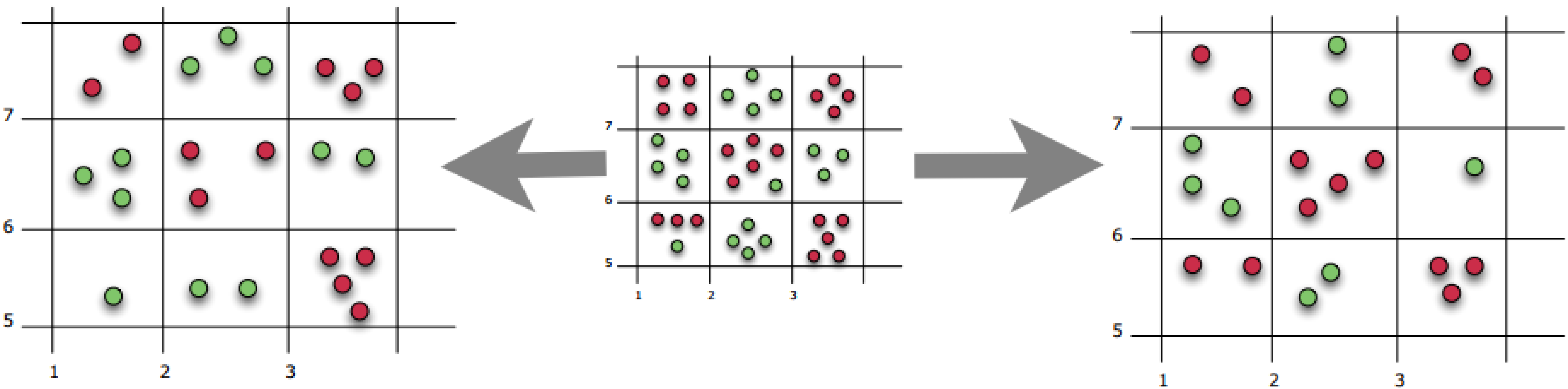
Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote } \{\hat{C}_b(x)\}_1^B$.

https://stat.ethz.ch/education/semesters/ss2012/ams/slides/v10.2.pdf

Random Forests

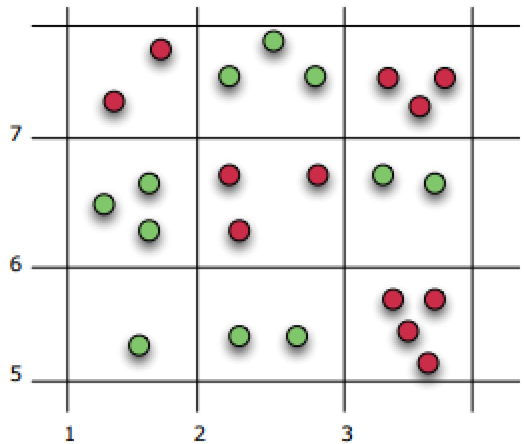
- Bagging
  - ✓ Sampling with replacement



Random Forests

- Bagging
  - ✓ Randomly selected variable

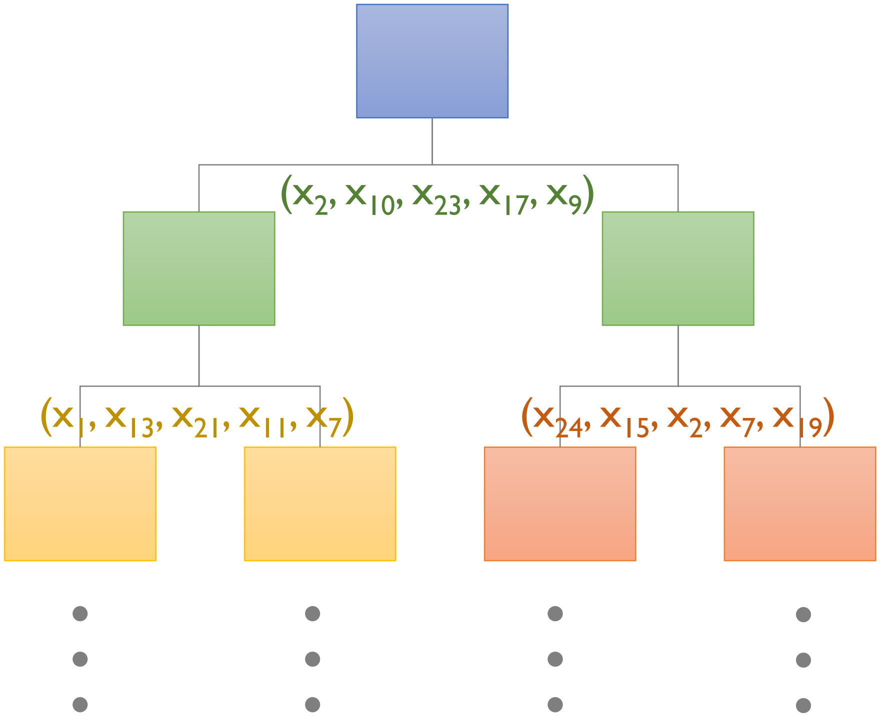
Bootstrap i (X in R^{25})



$(x_2, x_{10}, x_{23}, x_{17}, x_9)$

$(x_1, x_{13}, x_{21}, x_{11}, x_7)$

$(x_{24}, x_{15}, x_2, x_7, x_{19})$



Random Forests

- Generalization Error

  ✓ Each tree in random forests may over-fit the data because pruning is not conducted.

  ✓ If the population size is large enough, then the generalization error of random forests bounded by

  $$Generalization\ Error\ \leq \frac{\bar{\rho}(1-s^2)}{s^2}$$

    - $\bar{\rho}$ is the mean value of the correlation coefficients between individual trees
    - s^2 is the margin function (for binary classification, it is simply the average difference proportions between the correct and incorrect trees over all training data.

  ✓ The more accurate the individual classifiers, the larger the s^2 and the lower the generalization error

  ✓ The less correlated among the classifiers, the lower the generalization error.

Random Forests

- Variable Importance
  - ✓ Step 1: Compute the OOB error for the original dataset (e_i)
  - ✓ Step 2: Compute the OOB error for the dataset in which the variable x_i is permuted (p_i)
  - ✓ Step 3: Compute the variable importance based on the mean and standard deviation of (p_i-e_i) over all trees in the population

Random Forests

Original OOB Data

ID	X1	...	**Xi**	...	Xd	Y
1			**0.1**			
2			**0.5**			
3			**1.1**			
4			**1.2**			
5			**0.4**			
6			**0.2**			
7			**0.7**			
8			**0.8**			
9			**1.4**			
10			**1.6**			

변수 i가 Tree를 split하는데
한번도 사용되지 않았다면

i번째 변수에 대한 random permutation이 수행된 OOB Data

ID	X1	...	**Xi**	...	Xd	Y
1			**1.1**			
2			**0.2**			
3			**0.1**			
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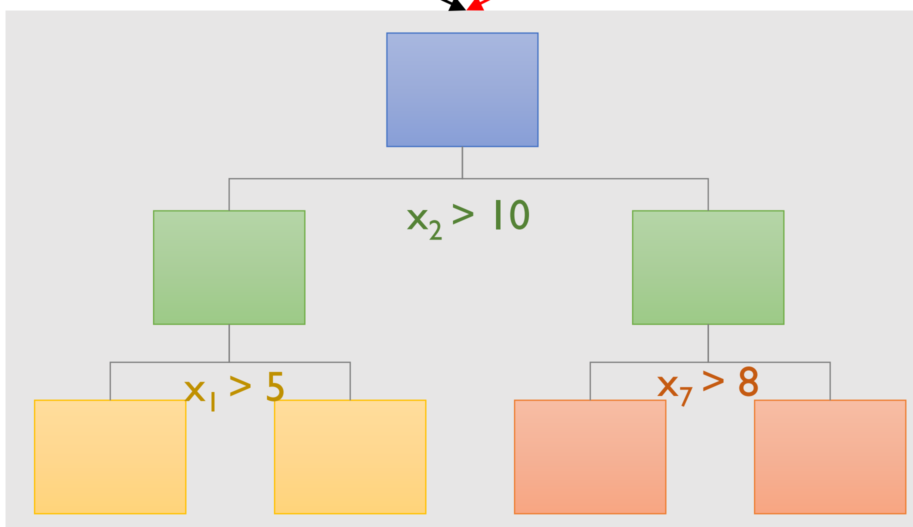

OOB Error of the Original Data e_i = OOB Error of the Permuted Data p_i

Random Forests

Original OOB Data

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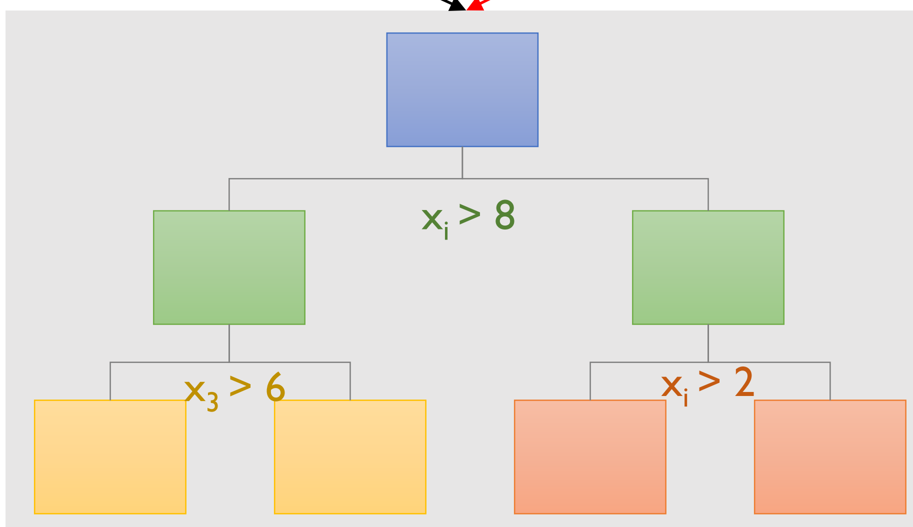
변수 i가 Tree를 split하는데
중요하게 사용되었다면



OOB Error of the Original Data e_i < OOB Error of the Permuted Data p_i

Random Forests

- 변수의 중요도
  - ✓ 랜덤 포레스트에서 변수의 중요도가 높다면
    - 1) Random permutation 전-후의 OOB Error 차이가 크게 나타나야 하며,
    - 2) 그 차이의 편차가 적어야 함

    - m번째 tree에서 변수 i에 대한 Random permutation 전후 OOB error의 차이

$$d_i^m = p_i^m - e_i^m$$

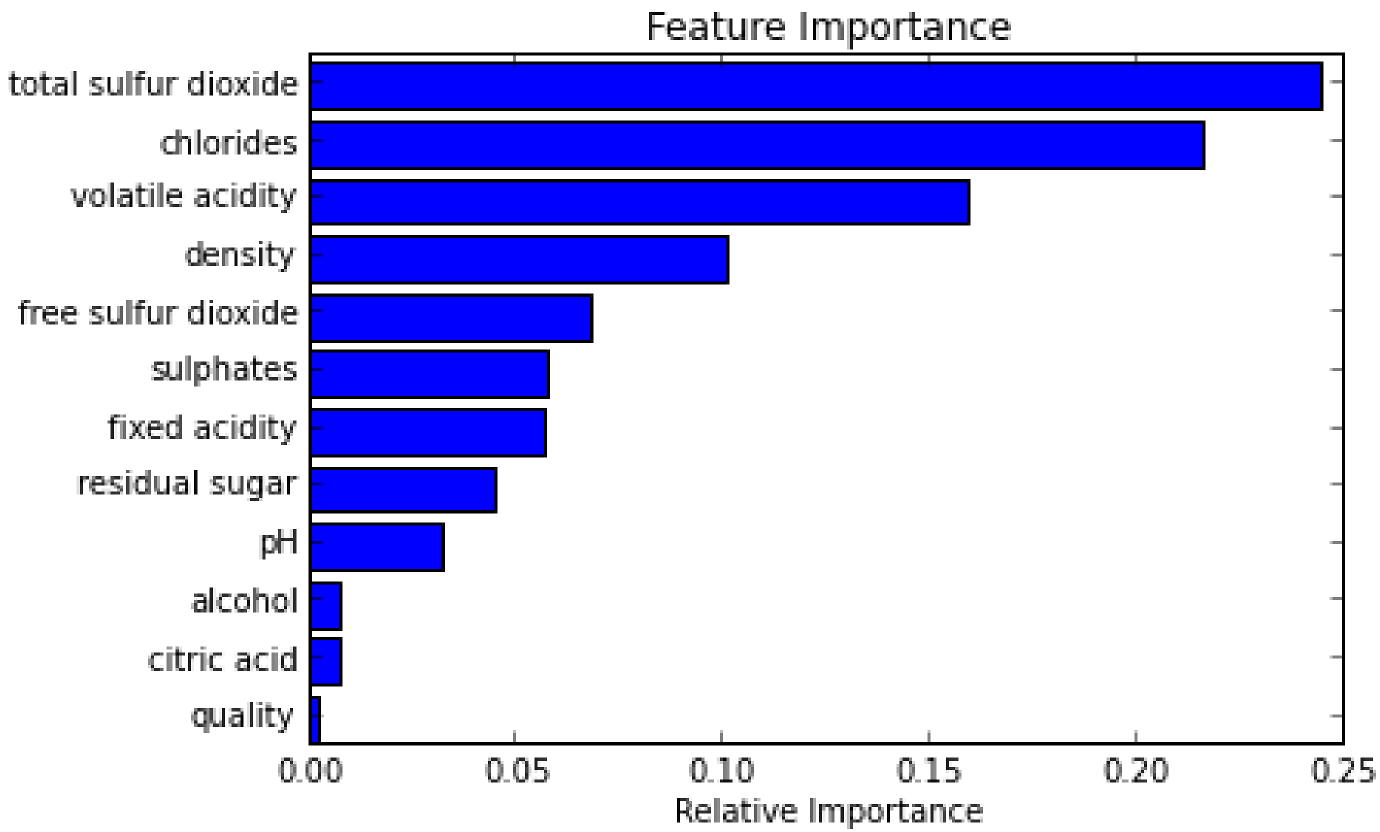
    - 전체 Tree들에 대한 OOB error 차이의 평균 및 분산

$$\overline{d}_i = \frac{1}{m}\sum_{i=1}^{m} d_i^m, \quad s_i^2 = \frac{1}{m-1}\sum_{i=1}^{m}(d_i^m - \overline{d}_i)^2$$

    - i번째 변수의 중요도: $v_i = \dfrac{\overline{d}_i}{s_i}$

Random Forests

- 변수 중요도 산출 결과




Q & A