Bagging and Random Forest

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Bagging: Motivation

❖ Averaging reduces variance:

$$\mathrm{Var}(\bar{X}) = \frac{\mathrm{Var}(X)}{N}$$

- Average models to reduce model variance
- One problem: We have only one training set.

  ➔ Where do multiple models come from?

Bagging

❖ Solution

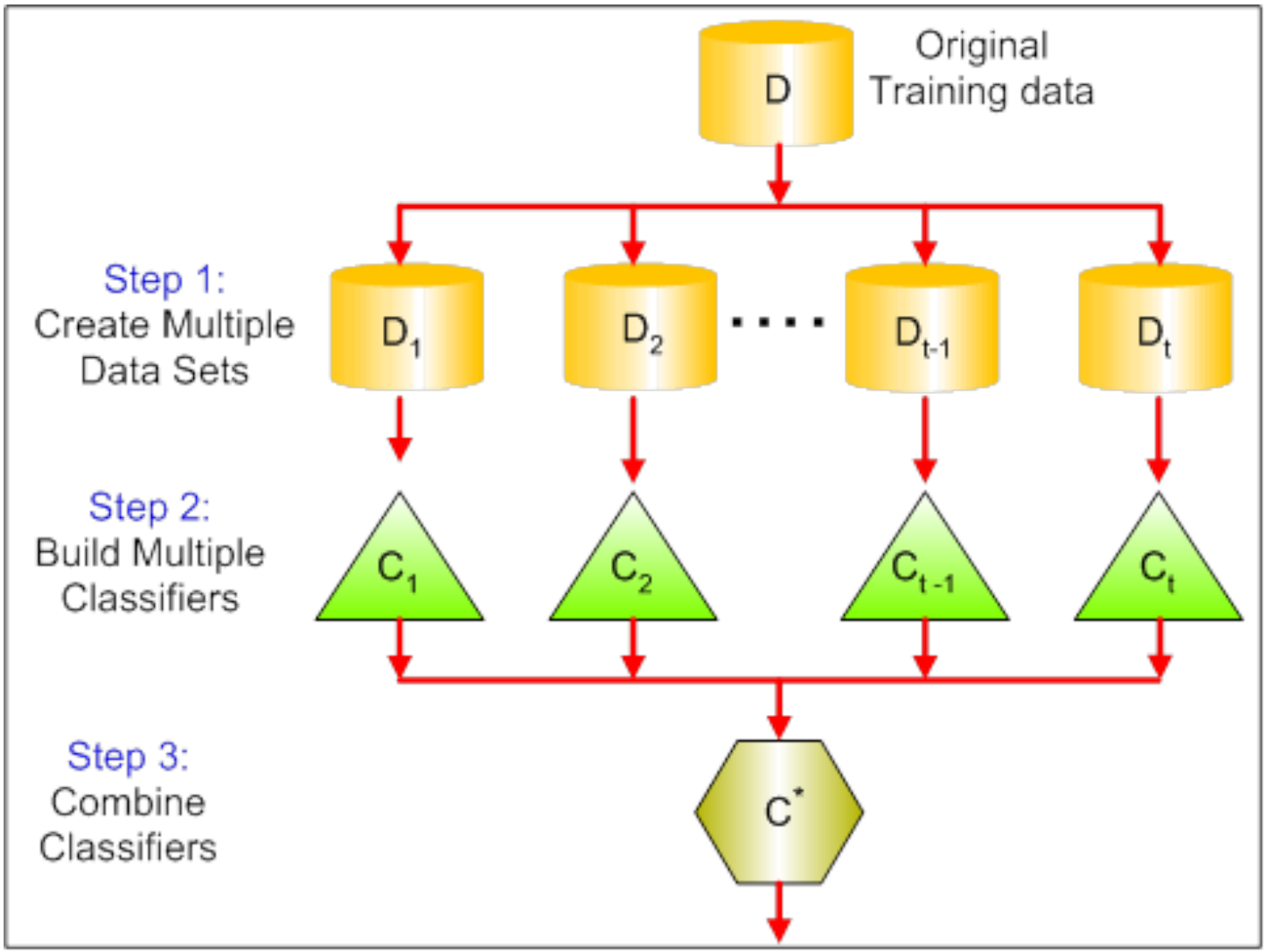
- Take repeated bootstrap samples from training set D.
- *Bootstrap sampling*: Given set D containing *N* training points, create D' by drawing *n* (*N* > *n*) points at random with replacement from D (복원추출)

❖ Bagging (Bootstrap Aggregation)

(proposed by Leo Breiman (1994), who proposed CART algorithm)

- Create *k* bootstrap samples $D_1, D_2, \ldots, D_k$.
- Train distinct classifier on each D_i.
- Classify new instance by majority vote or average.

Bagging



출처: https://www.analyticsvidhya.com/blog/2015/09/questions-ensemble-modeling/

Bagging

❖ The bagging method is similar to expert system.

- 하나의 의안을 해결하기 위해 여러 분야의 전문가에게 도움을 구함

❖ What algorithms can be used?

- (이론상으로는) 모든 알고리즘이 사용 가능함
  - 가급적 다양한 알고리즘을 사용하는 것이 중요! ➔ **Model diversity**
- 그러나 decision tree가 자연스럽게 많이 이용되기 시작
  - Full-grown tree는 bias를 매우 낮고, variance가 매우 높기 때문에 여러 개의 full-grown tree를 이용하여 variance를 낮추자.
  - 그렇다면 어떻게 model diversity를 확보할 것인가?

Random forest: Motivation

- **Decision tree (especially CART algorithm)**
  - Advantages
    - Extracting decision rules (If A, then B)
    - Selecting important predictors automatically
  - Limitation
    - not great for nonlinear decision boundary
- **Bagging trees can be a solution to overcome aforementioned limitation.**
  - However, in the bagging structure, same classifiers may be correlated highly so that generalization performance of bagging is degraded.

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Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?

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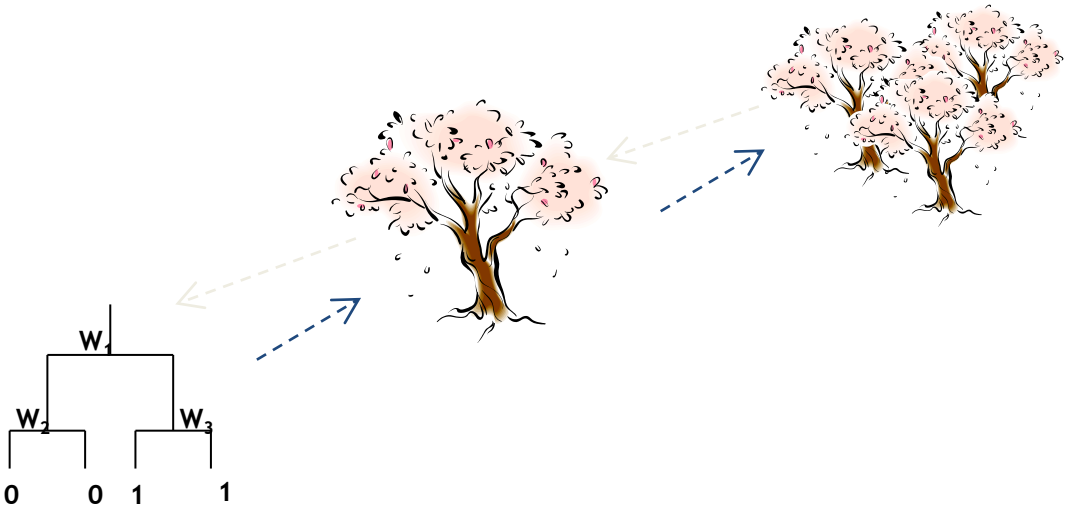
Abstract

We evaluate **179 classifiers** arising from **17 families** (discriminant analysis, Bayesian, neural networks, support vector machines, decision trees, rule-based classifiers, boosting, bagging, stacking, random forests and other ensembles, generalized linear models, nearest-neighbors, partial least squares and principal component regression, logistic and multinomial regression, multiple adaptive regression splines and other methods), implemented in Weka, R (with and without the caret package), C and Matlab, including all the relevant classifiers available today. We use **121 data sets**, which represent **the whole UCI** data base (excluding the large-scale problems) and other own real problems, in order to achieve significant conclusions about the classifier behavior, not dependent on the data set collection. **The classifiers most likely to be the bests are the random forest** (RF) versions, the best of which (implemented in R and accessed via caret) achieves 94.1% of the maximum accuracy overcoming 90% in the 84.3% of the data sets. However, the dif-

Random forest

- Developed by Leo Breiman(father of CART and bagging) at University of California, Berkeley (1996, 1999)
- Special case of the “model averaging” approach
- Attempt to reduce bias of single tree



Random forest: 2 randomization

❖ Why RF?

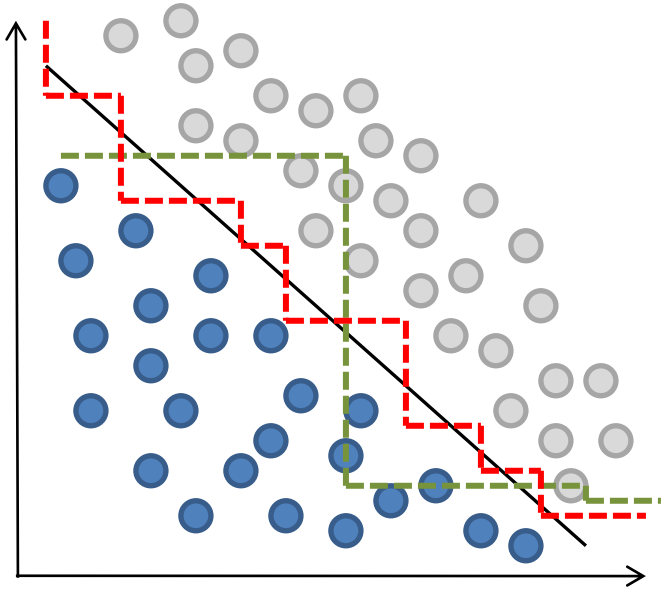
- To maintain some advantage(Selecting important predictors) of a single tree model while reducing bias, 2 randomization are applied to the RF model.
- 1st randomization: **Bagging**
- 2nd randomization: **Predictor subsets chosen randomly**
  - Sub-classifiers in bagging structure are trained by same algorithm, CART. However, by this randomization, each sub-classifier's training set has different characteristics from others.

⇨ **Bootstrapping training set + Bootstrapping features**

Random forest: 2 randomization

- **Randomization through "bagging"**
  - Parallel combination of learners, independently trained on distinct bootstrap samples
  - Final prediction is the mean prediction (regression) or class with maximum votes (classification)

- **Bagging methods reduce variance**
  - **Black line** : Actual decision boundary
  - Green line : Single tree's decision boundary
  - Red line : Random Forest's decision boundary



Sketch for a random tree and a random forest

$$X = \begin{pmatrix} 1 & 5 & 0 & -1 & 2 \\ 0 & 3 & 9 & 1 & -3 \\ 2 & 8 & 9 & 0 & 3 \\ 3 & -1 & 0 & -2 & 3 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

$$X^{(1)} = \begin{pmatrix} 1 & 0 & 2 \\ 2 & 9 & 3 \\ 3 & 0 & 3 \end{pmatrix} \qquad Y^{(1)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$X^{(2)} = \begin{pmatrix} 5 & -1 & 2 \\ 3 & 1 & -3 \\ 8 & 0 & 3 \end{pmatrix} \qquad Y^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

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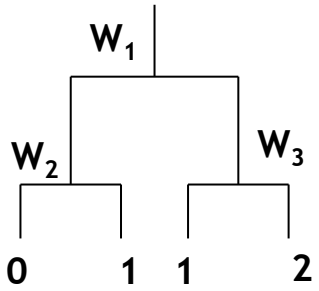
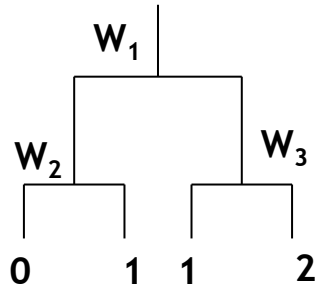




Random forest: 2 randomization

- **Randomization through "predictor subsets"**
  - If each single tree in forest uses all predictors, it is just a "simple" bagging method
  - Random Forests algorithm chooses predictor subsets randomly, and constructs a single tree by training each predictor subset.
  - The number of predictors of each tree = m_{try}
    - Generally, in a classification problem, $m_{try} = \sqrt{p}$ (*p*: number of all predictors)
    - Generally, in a regression problem, $m_{try} = \mathrm{p}/3$

[Example] Predictor set = {X_1, X_2, X_3, …, X12}

➔ Regression tree 1's predictor subset = {X1, X4, X5, X9}

➔ Regression tree 2's predictor subset = {X1, X2, X10, X11}

➔ Regression tree 3's predictor subset = {X7, X8, X10, X12}

…

➔ Regression tree *n*'s predictor subset = {X1, X2, X6, X12}

Random forest: Training

- **By 2 randomization, construct a bootstrap sample from training set.**
- **Train a tree using above bootstrap sample.**
  - Each tree is fully-grown until the impurity of each terminal node is zero.
  - As RF combines full-grown tree, we can expect that RF does not overfit. (Breiman, 2001) ➔ Core point of *Bagging approach*
  - Parameters: number of predictors in each tree, number of trees

Random forest: Inference

Same inference to bagging method

❖ For classification

- Majority vote: 각 single tree의 classification 결과를 보고 다수가 예측한 클래스로 최종 예측
- Probability prediction: 전체 single tree에서 각 클래스로 예측한 tree의 비율을 이용. Cut-off를 이용하여 분류할 때 사용

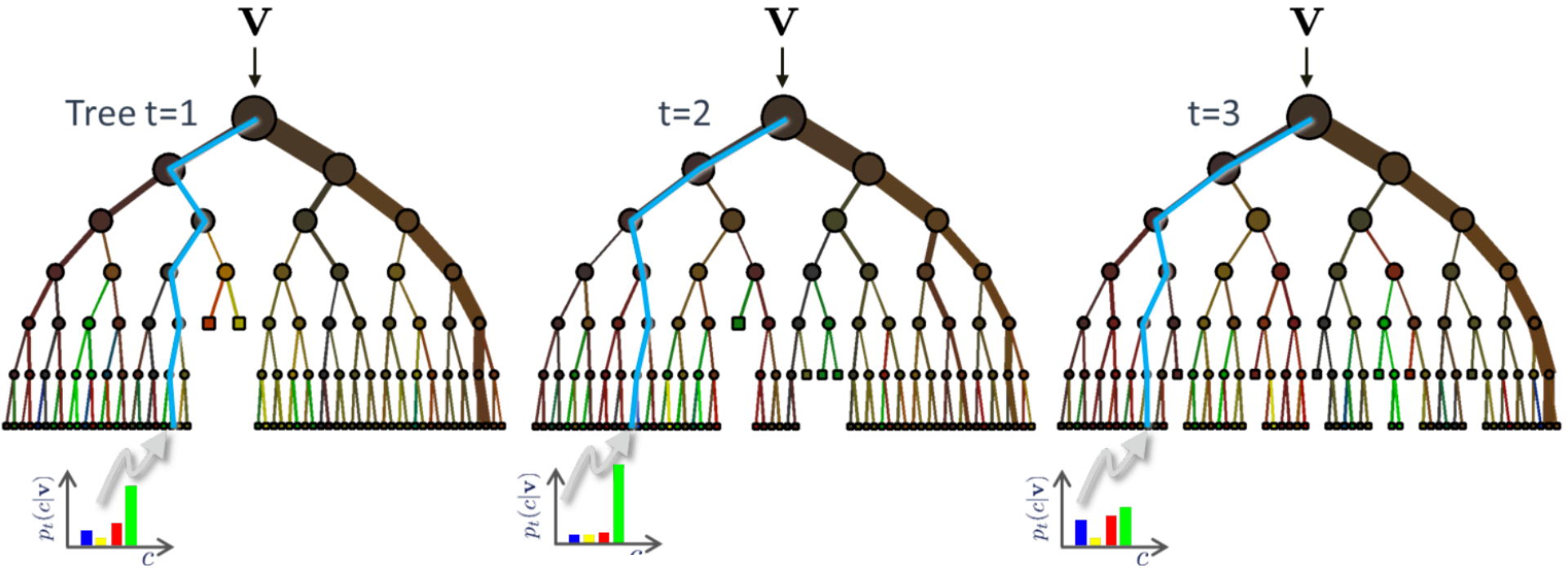
❖ For regression

- Average: 각 single tree가 예측한 값의 평균으로 최종 예측

Random forest

❖ Random forest: Testing

- A new data point $\mathbf{v}$ is pushed through each component tree.



$$p(c|\mathbf{v}) = \frac{1}{T}\sum_{t}^{T} p_t(c|\mathbf{v})$$

(Criminisi et al., 2011)

Random forest: Feature importance

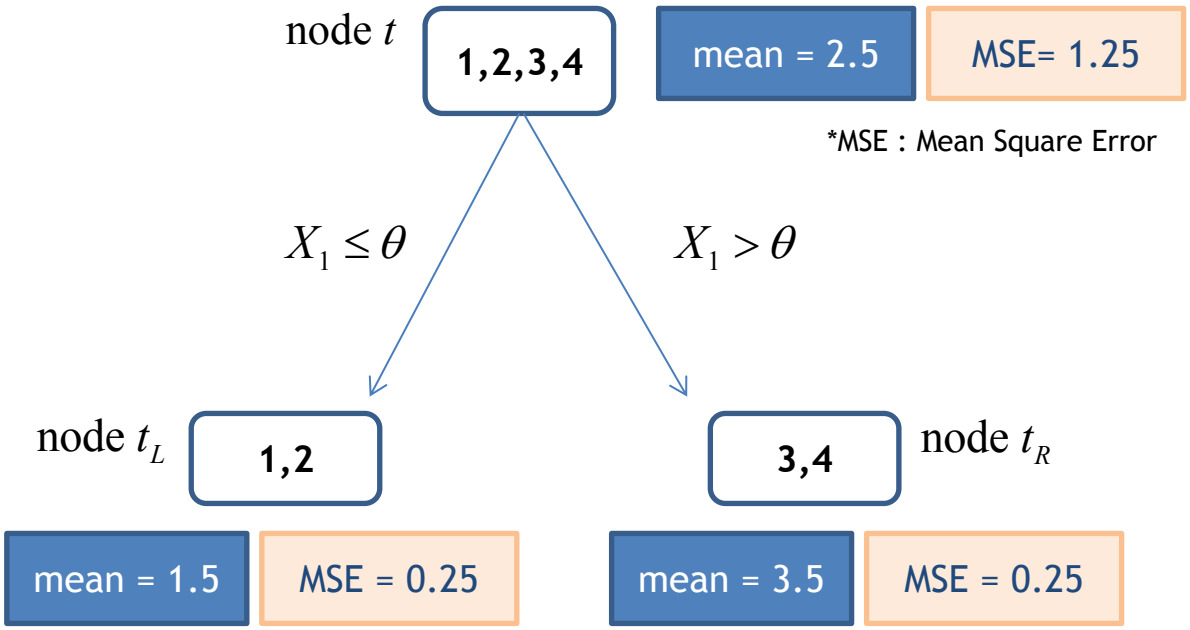
❖ Feature importance in random forest

- Each single tree selects important predictors automatically.
- Random forest can evaluate each predictor by combining all single tree's opinion.
- 2 ways
  - Mean decrease impurity
  - Mean decrease accuracy

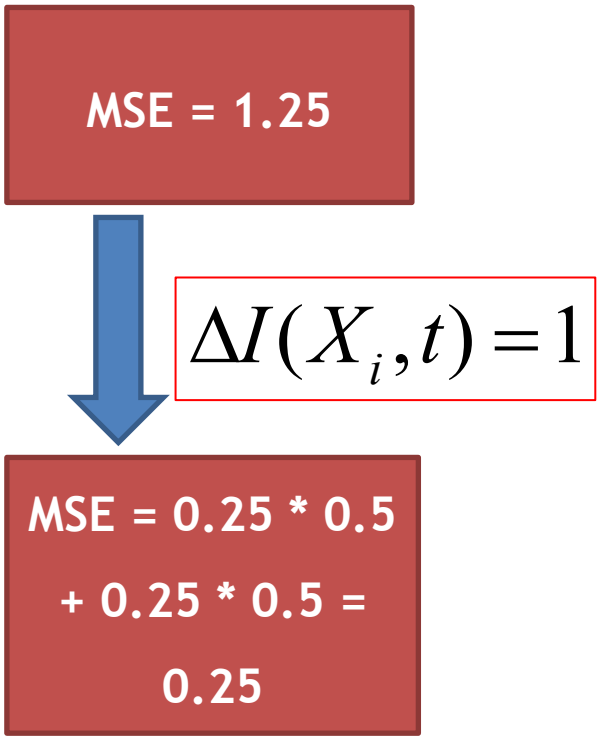
Random forest: Feature importance

❖ Mean decrease impurity

- In a single tree,



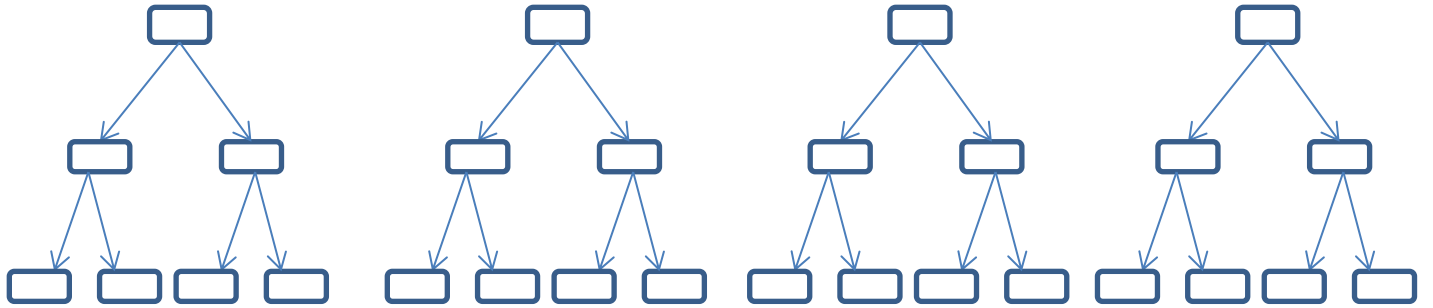
$$\Delta I(X_i, t) = I(t) - p_L I(t_L) - p_R I(t_R)$$



Random forest: Feature importance

❖ Mean decrease impurity

- Consider a forest of 4 trees.



$\Delta I(X_1, T_1) = 1$ $\Delta I(X_1, T_2) = 1.2$ $\Delta I(X_1, T_3) = 3.2$ $\Delta I(X_1, T_4) = 0.75$

$$\text{Importance}(X_1) = \frac{1}{M}\sum_{m=1}^{M}\Delta I(X_1, T_m) = \frac{1+1.2+3.2+0.75}{4} = 1.5375$$

Random forest: Feature importance

❖ Mean decrease accuracy

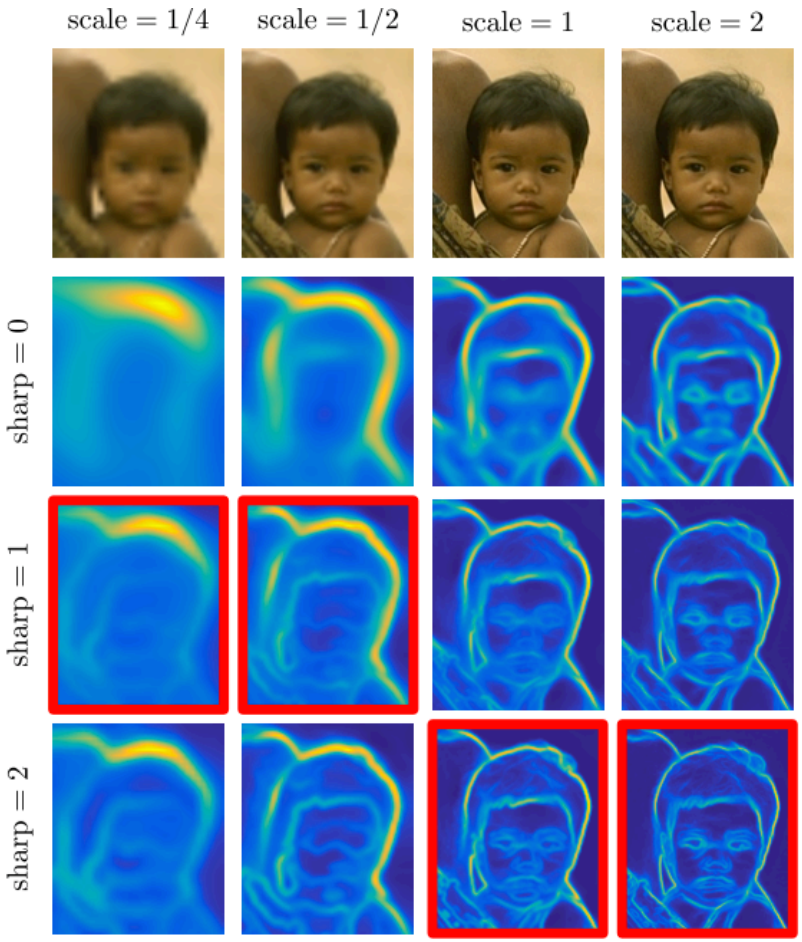
- 1. Train a random forest.
- 2. Calculate test error ($test\_error\_base$).
- 3. Permute variable X_i.
  - Rearrange the values of X_i or change them randomly.
- 4. Re-calculate test error ($test\_error\_changed$).
- 5. Importance of $X_i = test\_error\_changed - test\_error\_base$

If the variable is not important, then permuting that variable will not degrade prediction accuracy.

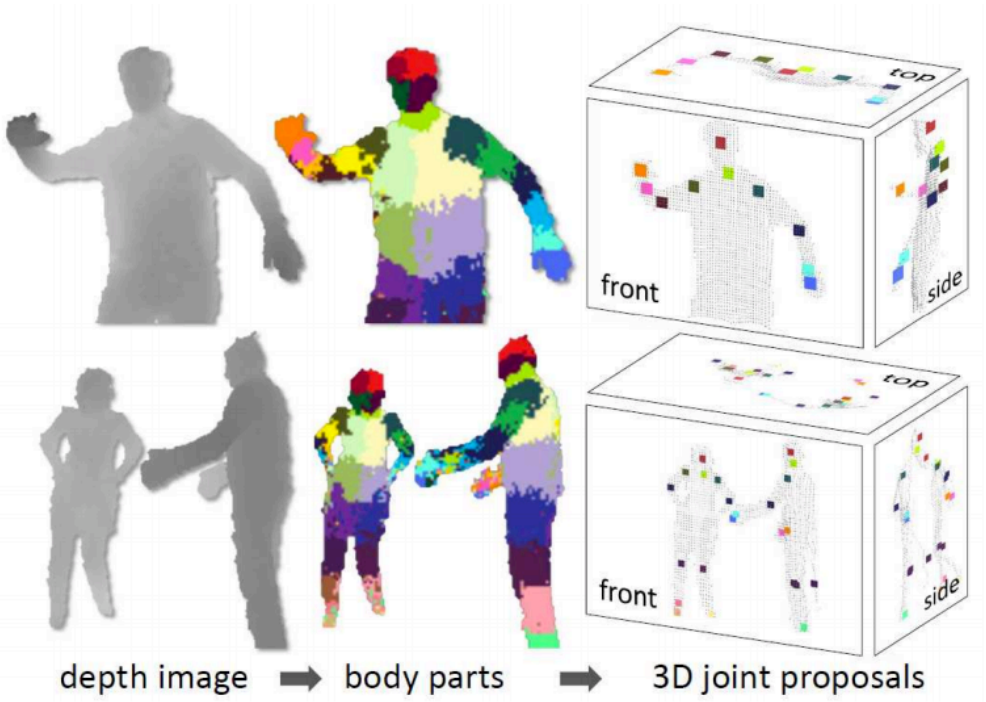
Random forest: Applications

Random forest is widely used for various purpose in the field of computer vision.

➔ Object / edge detection, Object tracking, Image classification, etc.



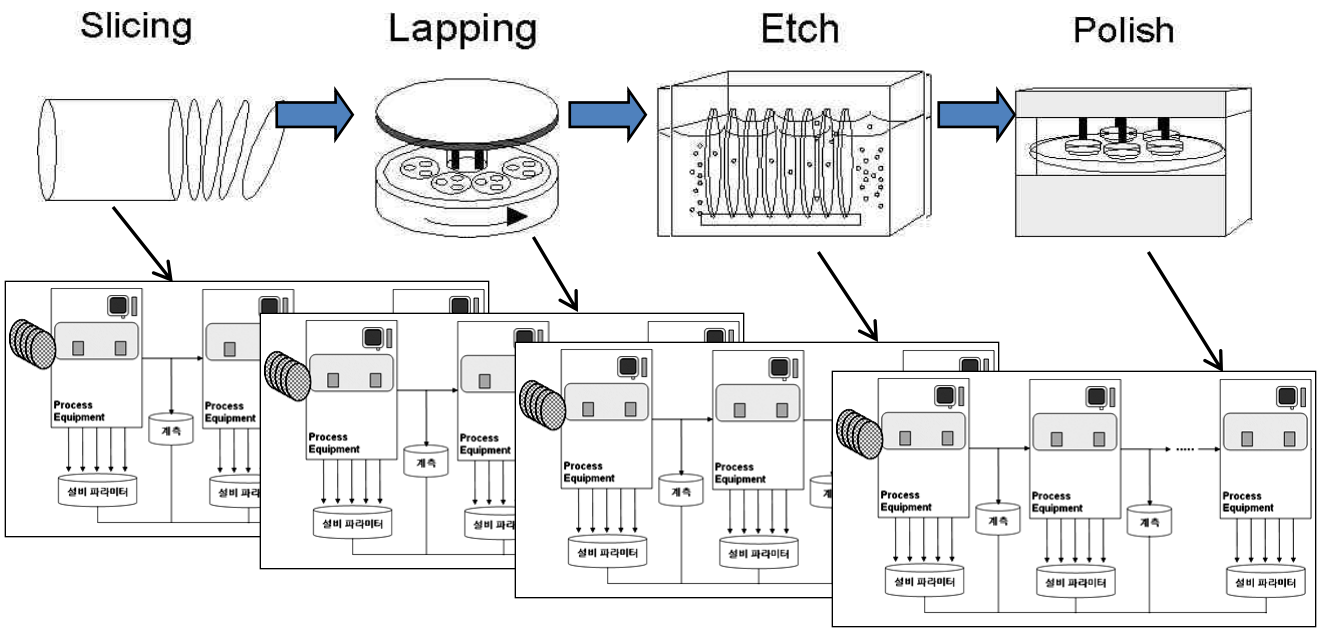
(Hallman & Fowlkes, 2015)



(Newcombe et al., 2011)

Random forest: Applications

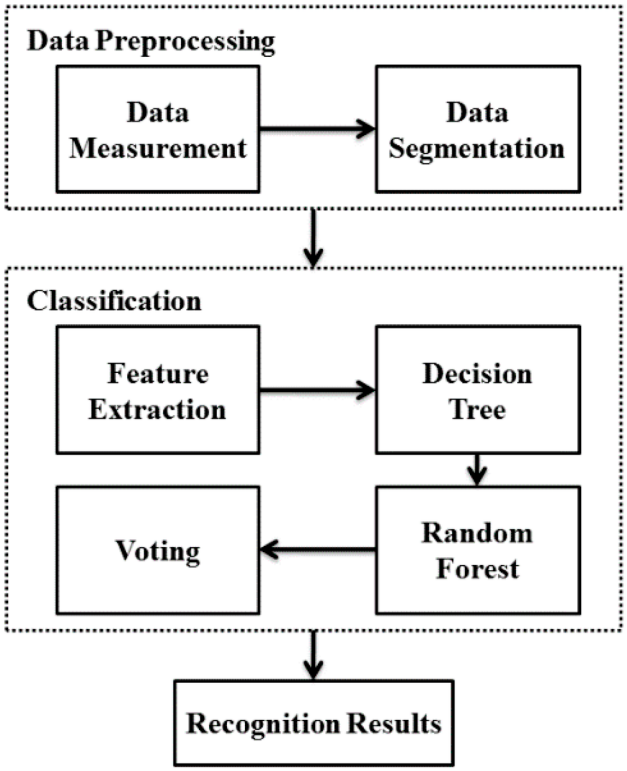
- **Semiconductor process and wafer yield**
  - The semiconductor process consists of hundreds of processes.
  - Yield: Measured by the number of semiconductors operating normally among the semiconductor in a wafer
  - It is very important to predict the yield and to see the influence of the process sensor on it.



(Ko et al., 2010)

Random forest: Applications

Random forest shows good prediction performance even for fat data with a large number of predictors.



Random forest can extract importance values of all predictors.

Period	Y	Best Model	RMSE	R^2
2	1	GA-LR	0.1646	0.9820
	2	GA-LR	0.5073	0.9175
	3	GA-LR	0.1616	0.9570
5	1	GA-LR	0.3250	0.6570
	2	GA-LR	0.3323	0.7994
	3	GA-LR	0.3253	0.7780
6	1	GA-LR	0.5406	0.8780
	2	GA-LR	1.0010	0.6288
	3	GA-LR	0.6110	0.7829
8	1	Stepwise-LR	1.6608	0.8849
	2	GA-LR	1.1897	0.9685
	3	GA-LR	1.1967	0.9113
All	**1**	**Random Forests**	**1.4944**	**0.7448**
	2	**Random Forests**	**2.1527**	**0.7516**
	3	**Random Forests**	**1.4253**	**0.7540**

(Ko et al., 2010)