Artificial Intelligence III:
Artificial Intelligence and Deep Learning

Lecture 5

Ensemble

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Agenda

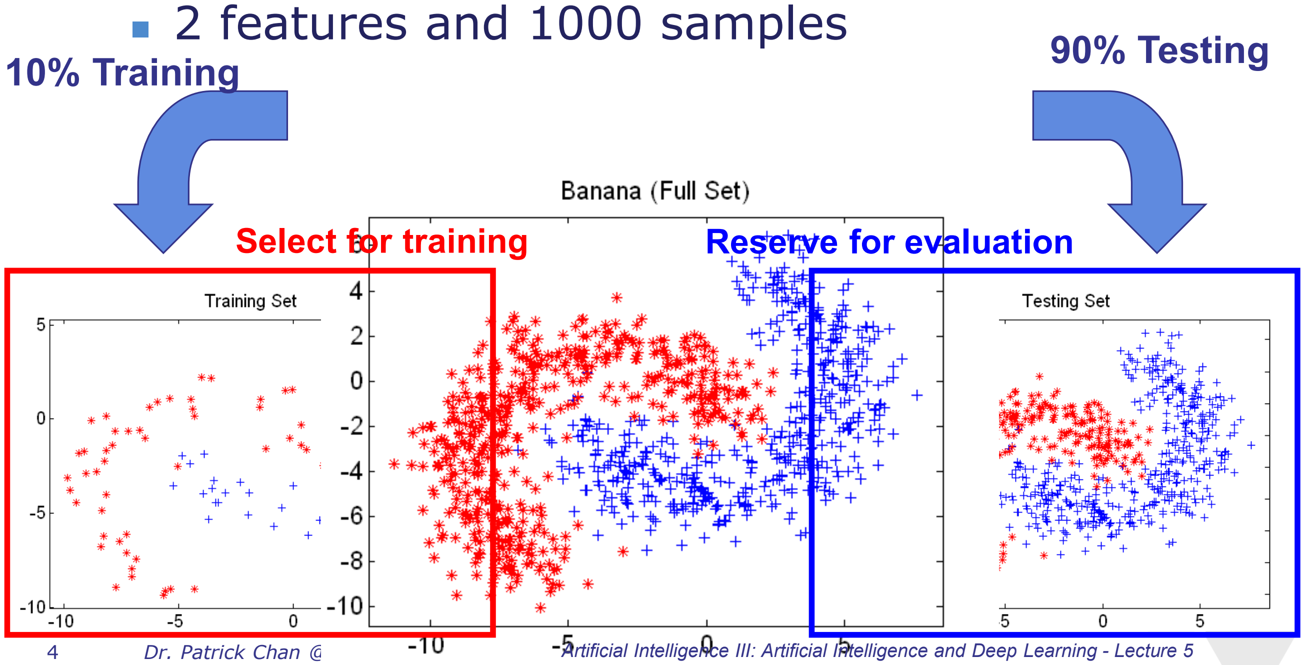
- Why Ensemble
- Fusion
- Diversity
- Construction Method

Why Ensemble?

- How to choose the best model for a classification problem?
  - Trial and Error
  - Train many classifiers with different settings
  - Evaluate how good they are

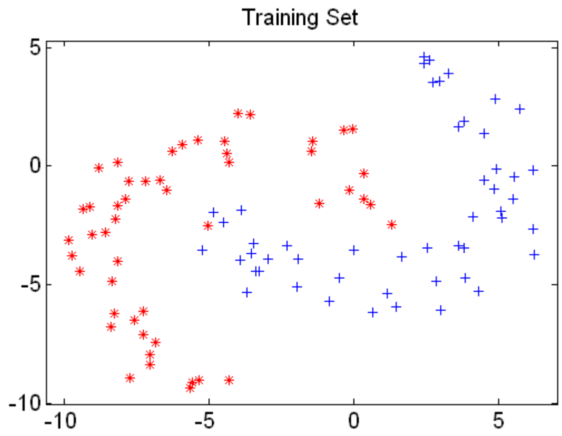
Why Ensemble?

- Banana Artificial Dataset
  - 2 class problem
  - 2 features and 1000 samples

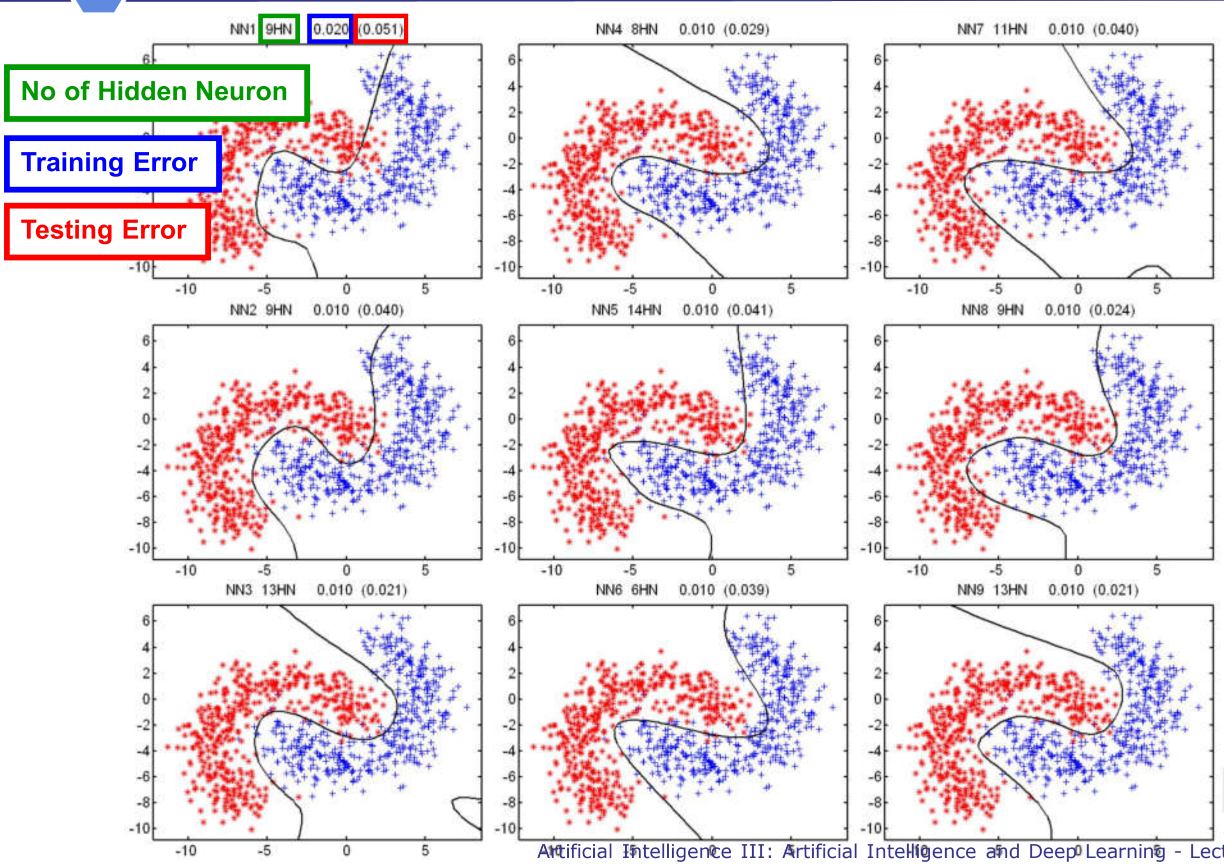


Why Ensemble?

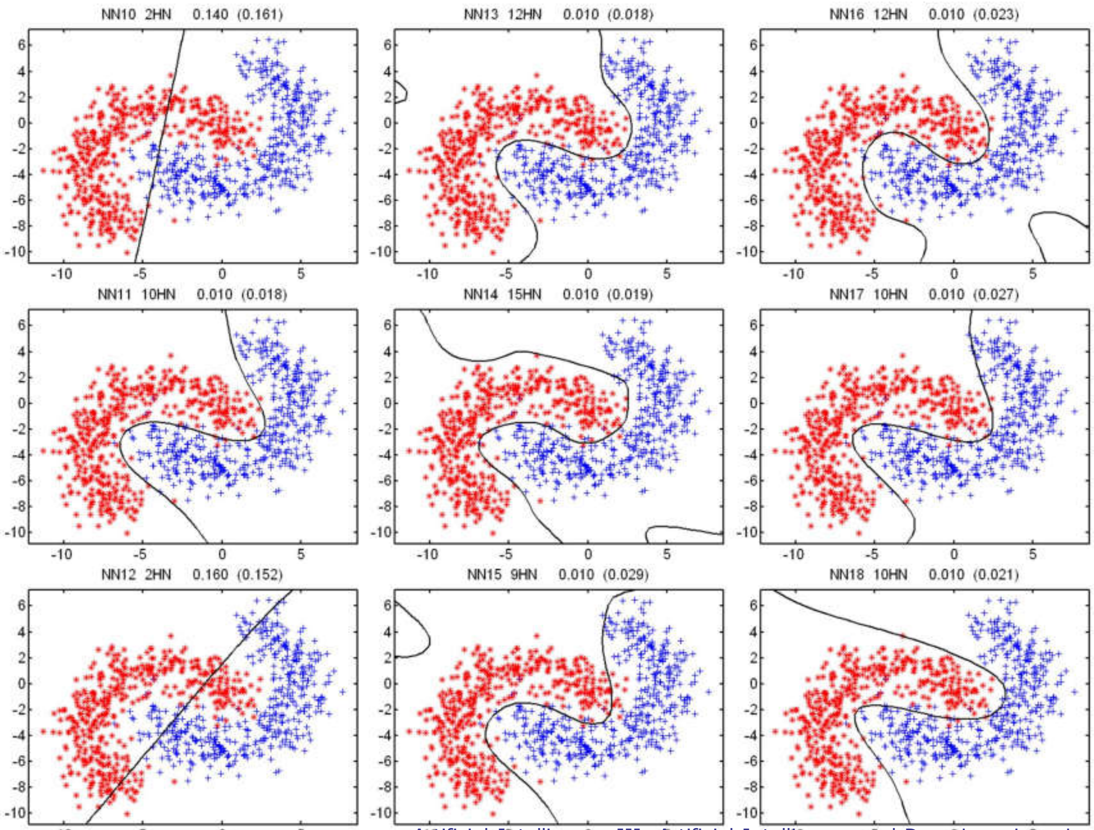
- Assume a simple MLPNN with one hidden layer is used
- No idea how many hidden neurons should be used
- Many 3-layer MLPNNs with different settings are trained



Why Ensemble?



Why Ensemble?



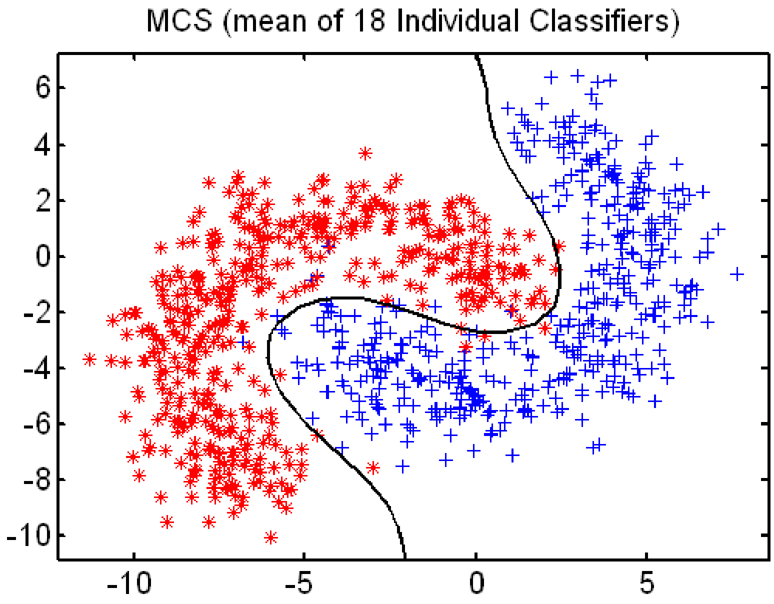
Why Ensemble?

- How to choose the best classifier?
  - Selection Criteria
    - Training Accuracy
      - Many choices
      - #2, #3..
    - Training Accuracy+Complexity
      - Classifier with smallest number of hidden neurons and lowest training accuracy?
      - #6?
  - Which criterion is the best?

	#	HN	Training Error	Test Error
	1	9	0.020	0.051
	2	9	0.010	0.040
	3	13	0.010	0.021
	4	8	0.010	0.029
	5	14	0.010	0.041
Worst	6	6	0.010	0.039
	7	11	0.010	0.040
	8	9	0.010	0.024
	9	13	0.010	0.021
	10	2	0.140	0.161
Best	11	10	0.010	0.018
	12	2	0.160	0.152
	13	12	0.010	0.018
	14	15	0.010	0.019
	15	9	0.010	0.029
	16	12	0.010	0.023
	17	10	0.010	0.027
	18	10	0.010	0.021

Why Ensemble?

- How about combine all of them?



Training Error = 0.0100

Testing Error = 0.0167

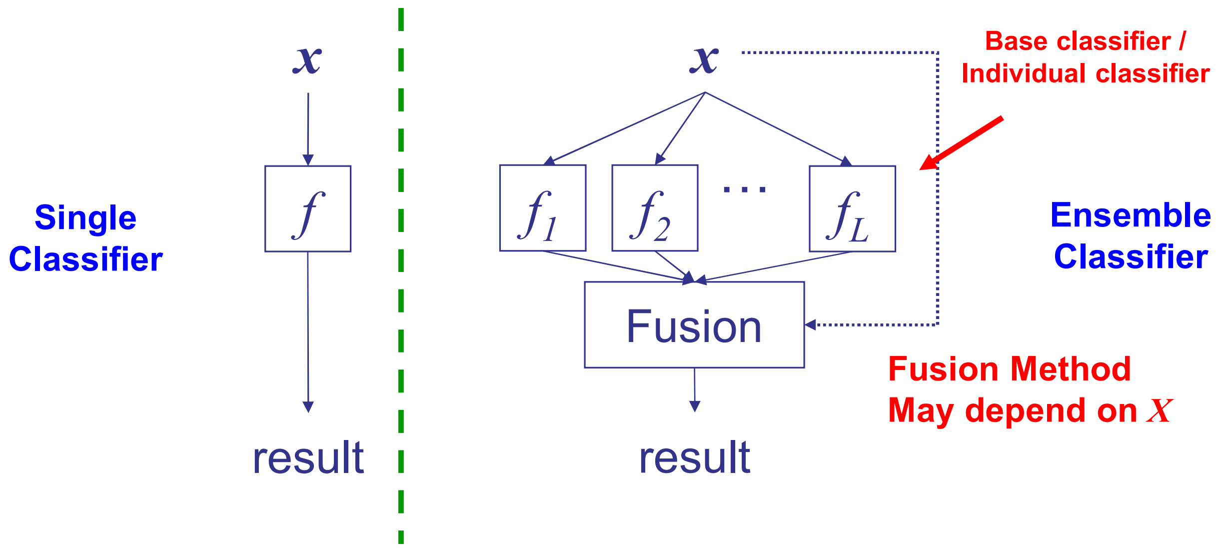
Its performance is better than the best individual classifier (0.018)

But no guarantee!

Why Ensemble?

- Drawbacks of selecting the BEST
  - Selecting a wrong one definitely leads to erroneous result
  - The "best" classifier is not necessarily the ideal choice
    - Different classifiers may contain different valuable information
    - Potentially valuable information may be lost by discarding results of less-successful classifiers
  - A single classifier may not be adequate to handle today's increasingly complex problems

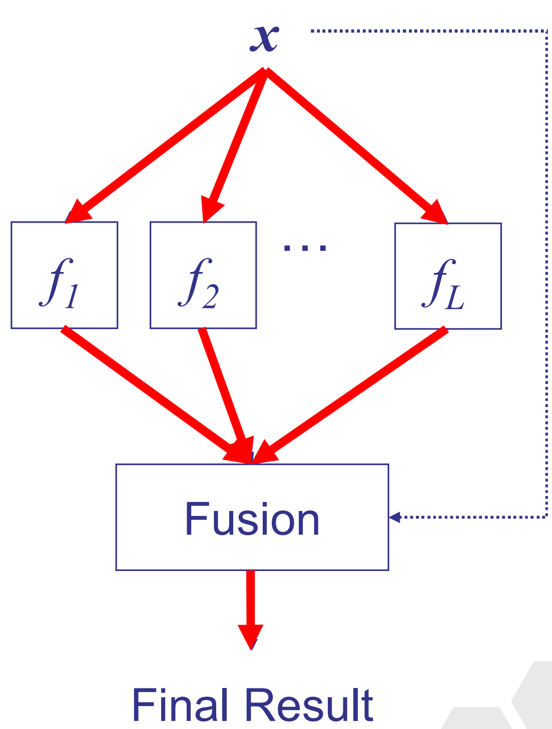
Ensemble



- Sometimes called Multiple Classifier System (MCS)
- Consists of a set of individual classifiers united by a fusion method

Ensemble

1. Sample x is fed into each base classifier
2. Each base classifier makes it's own decision
3. Final decision is made by combining all individual decisions



Ensemble

- Ensemble must be better than Single?
  - All cases: NO!
  - But practically,
    yes for many cases

Ensemble

- Three factors affecting the performance (accuracy) of ensemble:
  - Accuracy of base classifiers
    - How good are the base classifiers?
  - Fusion Method
    - How to combine classifiers?
  - Diversity among base classifiers
    - How different are the decisions reached by the classifiers?

Three Key Factors

Accuracy of Base Classifiers

- Performance of a base classifier is affected by
  - Training Dataset (sample and feature)
  - Learning Model (type of classifier)
  - Parameters (e.g. neuron and layer # in a NN)
- If base classifiers are poor, ensemble cannot be good
  - But we still can hope it will be better than base classifiers

Three Key Factors

Fusion Method

- A method to arrive at a group decision
- Two categories based on classifier output:
  - Label output
    - Output is a class ID
    - E.g. [1 0 0]
      x is Class 1

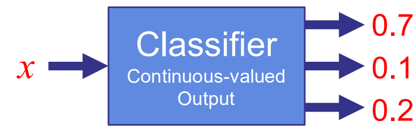
	y1	y2	y3
Classifier 1	1	0	0
Classifier 2	0	1	0
Classifier 3	1	0	0
Classifier 4	0	0	1

$$\begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,c} \\ y_{2,1} & y_{2,2} & & y_{2,c} \\ \vdots & & \ddots & \vdots \\ y_{L,1} & y_{L,2} & \cdots & y_{L,c} \end{bmatrix} = D(x)$$

Three Key Factors

Fusion Method

- A method to arrive at a group decision
- Two categories based on classifier output:
  - Continuous-valued output
    - Output a real value (probability) for each class
    - E.g. [0.7 0.1 0.2]
      x is Class 1 is 0.7,
      Class 2 is 0.1,
      Class 3 is 0.2



	y1	y2	y3
Classifier 1	0.7	0.1	0.2
Classifier 2	0.2	0.3	0.5
Classifier 3	0.8	0.1	0.1
Classifier 4	0.7	0.3	0.0

$$\Rightarrow \begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,c} \\ y_{2,1} & y_{2,2} & & y_{2,c} \\ \vdots & & \ddots & \vdots \\ y_{L,1} & y_{L,2} & \cdots & y_{L,c} \end{bmatrix} = D(x)$$

Three Key Factors: Fusion Method

Decision Profile

- Decision Profile (D) of a number of base classifier f_i ($i = 1 \ldots L$)

Row: Outputs of a base classifier on all classes

$$D(x) = \begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,c} \\ y_{2,1} & y_{2,2} & & y_{2,c} \\ \vdots & & \ddots & \vdots \\ y_{L,1} & y_{L,2} & \cdots & y_{L,c} \end{bmatrix}$$

Column: Outputs of all base classifier on a class

  - c : the number of classes
  - L : the number of base classifiers
  - $y_{i,j}$: the output of ith classifier on jth class

Label Output

- Label output of a base classifier can be represented by one-hot
  - 1 indicate the class x belongs to
  - Other classes are 0

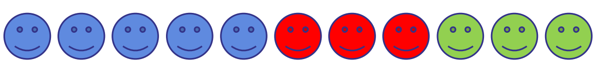
- For Example:
  - 3-class problem
  - 4 base classifiers and their decisions are class 2, class 3, class 1 and class 2

Row: a classifier
Column: a class

$$D(x) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Label Output

- Majority Vote



  - Also called the Plurality
  - The class with the most votes $\max\limits_{j=1\ldots c} \sum_{i=1}^{L} d_{i,j}$
  - For example:

$$\begin{array}{c} \begin{array}{ccc} y_1 & y_2 & y_3 \end{array} \\ D(x) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \\ \begin{array}{ccc} 1 & 2 & 1 \end{array} \end{array}$$

Row: a classifier
Column: a class

Class 2 is the majority

Three Key Factors: Fusion Method
Label Output

- **Simple Majority** 
  - A class has 50% + 1 votes ($\max_{j=1\ldots c} \sum_{i=1}^{L} d_{i,j} > L/2$)
  - More strictive than Majority Vote
  - Many unknown cases

$$D(x) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

No decision

- **Unanimity** 
  - All base classifiers have the same decision
  - $\max_{j=1\ldots c} \sum_{i=1}^{L} d_{i,j} = L$
  - Many unknown cases

$$D(x) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

No decision

Three Key Factors: Fusion Method
Label Output

- Voting method assumes each base classifier has same classification ability
- However, in most cases, this is not true
- **Weighted Majority Vote**
  - Assign a weight (w_i) to the ith base classifier based on its ability
    - A large w indicates more accurate
    - E.g. Evaluated by accuracy on Training Set
  - The class is y_k if $\sum_{i=1}^{L} w_i d_{i,k} = \max_{j=1\ldots c} \sum_{i=1}^{L} w_i d_{i,j}$

Three Key Factors: Fusion Method

Label Output

- Example: 3 classes, 5 base classifiers

$$D(x) = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{matrix} 3 & 1 & 1 \end{matrix}$$

Unanimity **?** (all votes)

Simple Majority y_1 (votes > 50%)

Majority Vote y_1 (most votes)

Weighted Majority Vote y_2

$$w = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.2 \\ 0.5 \\ 0.1 \end{bmatrix}$$

Class 1 $0.1 \times 1 + 0.1 \times 1 + 0.2 \times 1 + 0.5 \times 0 + 0.1 \times 0 = 0.4$

Class 2 $0.1 \times 0 + 0.1 \times 0 + 0.2 \times 0 + 0.5 \times 1 + 0.1 \times 0 = 0.5$

Class 3 $0.1 \times 0 + 0.1 \times 0 + 0.2 \times 0 + 0.5 \times 0 + 0.1 \times 1 = 0.1$

Three Key Factors: Fusion Method

Continuous-valued Output

- Base classifier outputs a real value (not a label) for each class
- The values in D are a real number
- For Example:
  - 3-class problem
  - 4 base classifiers

Row: a classifier
Column: a class

$$D(x) = \begin{bmatrix} 0.1 & 0.7 & 0.2 \\ 0.0 & 0.2 & 0.8 \\ 0.9 & 0.1 & 0.0 \\ 0.1 & 0.8 & 0.1 \end{bmatrix}$$

- Based on D, fusion of Continuous-valued Output calculated a real value for each class ($\mu_j, j = 1..c$)

Continuous-valued Output

- Statistical Operator
  - Product
    $$\mu_j(x) = \prod_{i=1}^{L} d_{i,j}(x)$$
  - Median
    $$\mu_j(x) = \operatorname*{median}_i\{d_{i,j}(x)\}$$
  - Minimum
    $$\mu_j(x) = \min_i\{d_{i,j}(x)\}$$
  - Maximum
    $$\mu_j(x) = \max_i\{d_{i,j}(x)\}$$
  - Simple Mean
    $$\mu_j(x) = \frac{1}{L}\sum_{i=1}^{L} d_{i,j}(x)$$
  - Trimmed Mean
    - Values are sorted and K percent of the values are dropped on each side
    - Find the mean of remaining values

Continuous-valued Output

- Weighted Average
  - L Weights
    - One weight per base classifier

    $$\mu_j(x) = \sum_{i=1}^{L} w_i d_{i,j}(x)$$
  - $c \times L$ Weights
    - Weights are specific for each class per base classifier

    $$\mu_j(x) = \sum_{i=1}^{L} w_{ij} d_{i,j}(x)$$

Continuous-valued Output

- Example:
  - 3 classes
  - 5 base classifiers

$$D(x)=\begin{bmatrix}0.6 & 0.4 & 0.1\\ 0.7 & 0.2 & 0.7\\ 0.5 & 0.2 & 0.1\\ 0.5 & 0.7 & 0.6\\ 0.5 & 0.8 & 0.6\end{bmatrix}$$

Product	0.05	0.01	0.00	y_1
Median	0.5	0.4	0.6	y_3
Maximum	0.7	0.8	0.7	y_2
Minimum	0.5	0.2	0.1	y_1
Average	0.56	0.46	0.42	y_1
Trim 20% Average	0.53	0.43	0.43	y_1

Continuous-valued Output

- Example:
  - 3 classes
  - 5 base classifiers

$$D(x)=\begin{bmatrix}0.6 & 0.4 & 0.1\\ 0.7 & 0.2 & 0.7\\ 0.5 & 0.2 & 0.1\\ 0.5 & 0.7 & 0.6\\ 0.5 & 0.8 & 0.6\end{bmatrix}$$

Weight Average

L Weight

$$w=\begin{bmatrix}0.4\\ 0.2\\ 0.1\\ 0.1\\ 0.2\end{bmatrix}$$

y_1

Class 1 $0.4\times0.6+0.2\times0.7+\ 0.1\times0.5+\ 0.1\times0.5+\ 0.2\times0.5=0.12$

Class 2 $0.4\times0.4+0.2\times0.2+\ 0.1\times0.2+\ 0.1\times0.7+\ 0.2\times0.8=0.09$

Class 3 $0.4\times0.1+0.2\times0.7+\ 0.1\times0.1+\ 0.1\times0.6+\ 0.2\times0.6=0.07$

Three Key Factors: Fusion Method

Continuous-valued Output

- Example:
  - 3 classes
  - 5 base classifiers

$$D(x) = \begin{bmatrix} 0.6 & 0.4 & 0.1 \\ 0.7 & 0.2 & 0.7 \\ 0.5 & 0.2 & 0.1 \\ 0.5 & 0.7 & 0.6 \\ 0.5 & 0.8 & 0.6 \end{bmatrix}$$

Weight Average

L x c Weight

$$w = \begin{bmatrix} 0.1 & 0.2 & 0.2 \\ 0.1 & 0.1 & 0.4 \\ 0.2 & 0.1 & 0.1 \\ 0.4 & 0.2 & 0.1 \\ 0.2 & 0.4 & 0.2 \end{bmatrix}$$

y_2

Class 1 $0.1 \times 0.6 + 0.1 \times 0.7 + 0.2 \times 0.5 + 0.4 \times 0.5 + 0.2 \times 0.5 = 0.11$

Class 2 $0.2 \times 0.4 + 0.1 \times 0.2 + 0.1 \times 0.2 + 0.2 \times 0.7 + 0.4 \times 0.8 = 0.12$

Class 3 $0.2 \times 0.1 + 0.4 \times 0.7 + 0.1 \times 0.1 + 0.1 \times 0.6 + 0.2 \times 0.6 = 0.10$

Three Key Factors: Fusion Method

Diversity

- If all base classifiers always have the same decision, no need to consider all of them
- **Diversity** is a measure of difference between base classifiers
  - An intuitive, key concept for ensemble
  - Many definitions
- Can be categorized according to output type: Label and Continuous-valued Output

Label Output

- Pairwise Method
  Consider two base classifiers D_i and D_k
- There are four different possibilities:

	D_k correct	D_k wrong
D_i correct	N^{11}	N^{10}
D_i wrong	N^{01}	N^{00}

$$N = N^{00} + N^{01} + N^{10} + N^{11}$$

N^{11} : Number of times when two base classifiers are correct
N^{10} : Number of times when a classifier is correct and another is wrong
N^{01} : Number of times when a classifier is wrong and another is correct
N^{00} : Number of times when two base classifiers are wrong
N : Total Number of times

Label Output

- Disagreement Measure
  - Probability two classifiers disagree each other
  - Range: 0 – 1 (most diverse, totally disagree)

$$\frac{N^{01} + N^{10}}{N}$$

- Double Fault Measure
  - Probability two classifiers being wrong together
  - Range: 0 – 1 (most diverse, both wrong all the time)

$$\frac{N^{00}}{N}$$

Three Key Factors: Fusion Method: Diversity

Continuous-valued Output

- Correlation Coefficient (CC)
  - CC between two classifiers' outputs (pairwise)
  - Diversity is the average of CCs of L(L-1)/2 pairs
    - 1: not diverse (identical)
    - 0: independent
    - -1: the most diverse
  - Definition: $CC(f_i, f_j) = \frac{E\left[\left(f_i - \mu_{f_i}\right)\left(f_j - \mu_{f_j}\right)\right]}{\sigma_{f_i}\sigma_{f_j}}$
    - f_i : the ith classifiers' outputs
    - μ_{f_i} and σ_{f_i} : mean and standard deviation of the ith classifiers' output on all samples

Three Key Factors: Fusion Method

Diversity

- How to make base classifiers **diversify**?
  - Implicit Method
    - Using different Training Sets
      - Samples
      - Features
    - Using different Base Classifiers
      - Learning Models
      - Training Parameters
  - Explicit Method
    - Maximize diversity during training

Ensemble Construction Method

- The most well known MCS construction methods:
  - Bagging
  - Boosting
  - Negative Correlation

Ensemble Construction Method

Bagging

- Aim to aggregated different versions of a model generated by bootstrap training samples
  - Bootstrapping: use samples of the data with repetition

- **Algorithm**
  - Random a replicate of training set with replacement
  - Train a base classifier using the replicate
  - Repeat until *L* number of base classifiers are trained
  - Finally, voting or average fusion (no weighting) method can be used

Example

- **Bagged Decision Trees**
  - Draw bootstrap samples to form sample sets
  - Train trees on each sample set
  - Average prediction of trees on unseen samples

- **Random Forests (Bagged Trees++)**
  - Draw bootstrap samples to form sample sets
  - Each set uses different feature subsets
  - Train trees on each samples
  - Average prediction of trees on unseen samples

Bagging

- Advantage:
  - Simple, easy to understand
  - Good for unstable classifier
    - If small changes in the training set causes large difference in the generated classifier
    - The algorithm has high variance
    - E.g. Decision Tree
- Disadvantage:
  - May not generating complementary base models

Boosting

- Actively generate complementary base models
  - Train the next base model based on mistakes made by previous models
- Generate a sequence of base models each focusing on previous one’s errors

Example

- **Adaptive Boosting (AdaBoost)**
  - Base models are trained by minimizing the weighted error
    - A larger weight is assigned to samples classified wrongly
  - Weighted average is used as the fusion method
    - A model with a smaller error is assigned a larger weight; vice versa

Negative Correlation

- For continuous-valued output base classifiers, e.g. MLPNN
- Explicitly consider diversity measure
- Objective Function per each base classifier:

$$\text{Objective Function} = \text{Training Error} + \boxed{\lambda}\,\boxed{\text{Diversity}}$$

λ is the tradeoff parameter

$$\frac{1}{N}\sum_{i=1}^{N}\left(f_k(x_i) - f(x_i)\left[\sum_{\substack{j=1\\ j\neq k}}^{L}\left(f_j(x_i) - f(x_i)\right)\right]\right)$$

where $f(x_i) = \frac{1}{L}\sum_{j=1}^{L} f_j(x_i)$