



Ensembles of Diverse Neural Networks

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Outline of the Presentation

1. Introduction
2. Background of Ensemble Construction
3. Data Sampling for Ensemble Construction
4. Candidate Ensemble Methods
5. Experimental Studies
6. Motivation to better NNE Construction

Artificial Neural Network

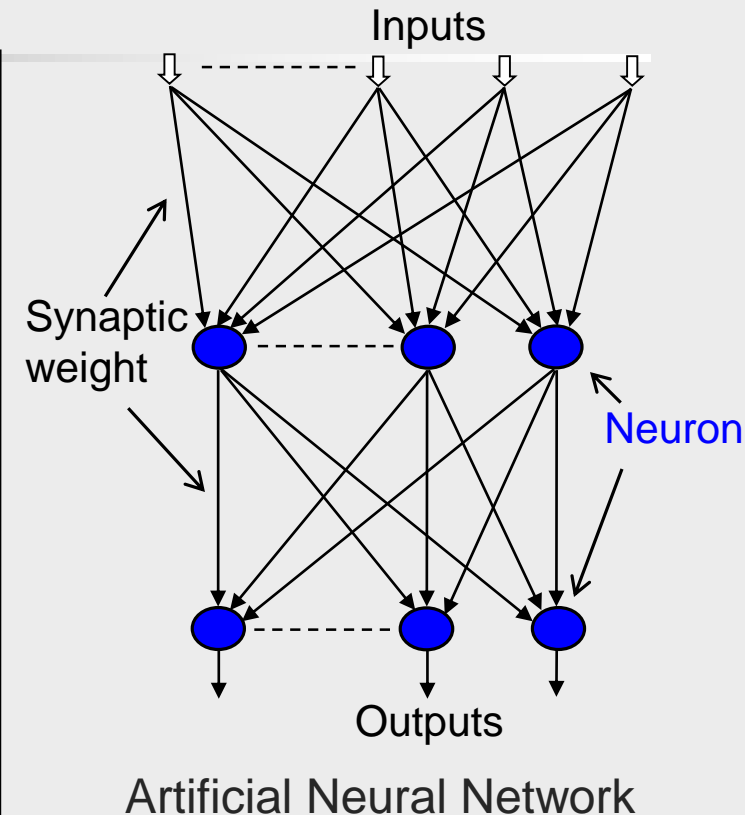
According to Haykin, an artificial neural network (NN) is a collection of simple processing units and it has ability to store experimental knowledge.

NN resembles the human brain in two respects:

- 1. Knowledge is acquired by a NN from its environment through a learning process.*
- 2. Interneuron connection strengths, known as synaptic weights, are used to store the knowledge.*

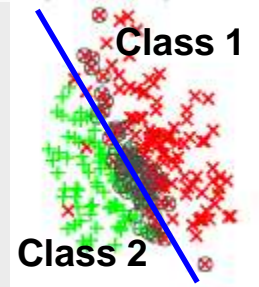
❖ **Functionality** of a NN depends on the **synaptic weight** values and the **aim of learning** is to get **proper weight set**.

NNs have been successfully applied for various task; for classification it performs well.

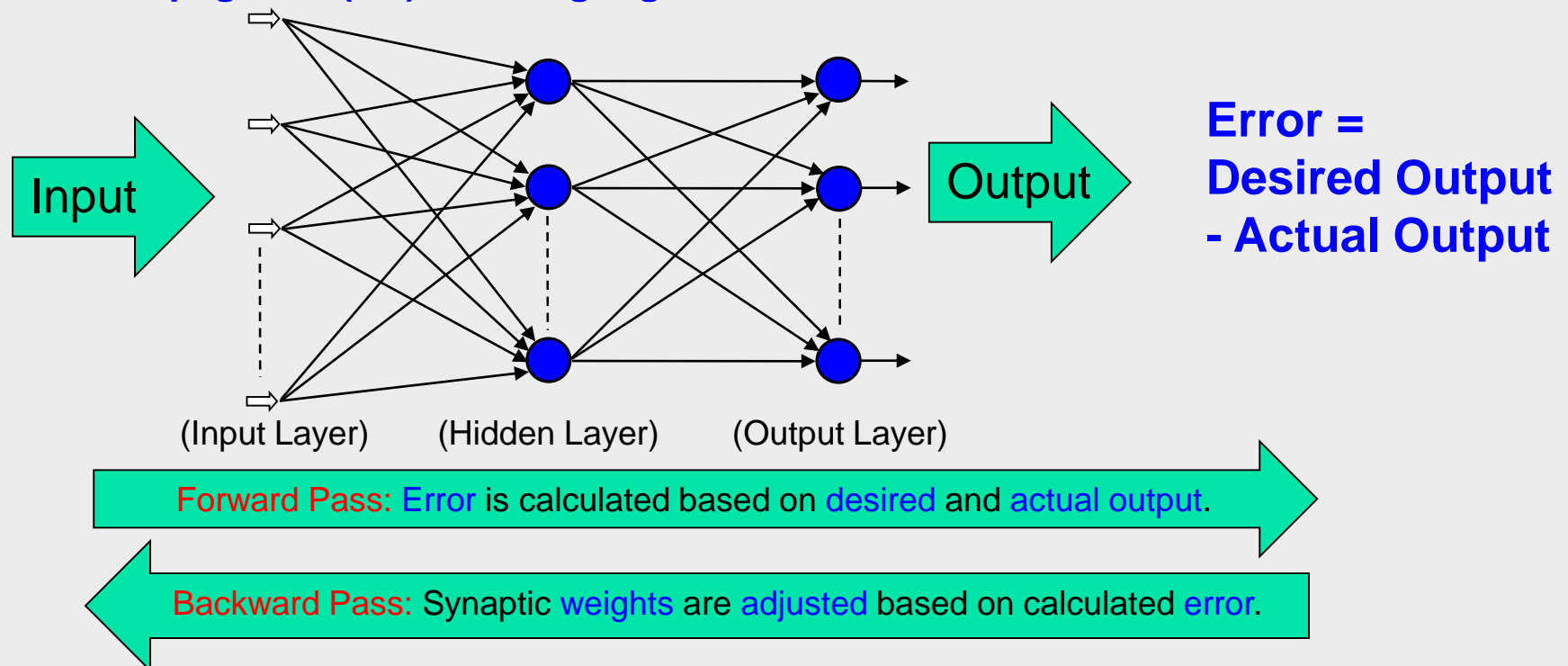


NNs for Classification Tasks

- ❖ **Classification** is one of the most frequently encountered decision making tasks of human activity.
- ❖ It occurs when an object needs to be assigned into a predefined group or class based on a number of observed attributes related to that object.



Back-Propagation (BP) Learning Algorithm for Classification



- ❖ At a time small fraction of a weight is corrected w. r. t demand correction for smooth learning; a parameter learning rate(η) defines the relative size to change.

Performance Measures

Learning and generalization are the most important topics in NN research. Learning is the ability to approximate the training data while generalization is the ability to predict well beyond the training data.

- Generalization is more desirable because the common use of a NN is to make good prediction on new or unknown objects.
- It measures on the testing set that is reserved from available data and not use in the training.
- Testing error rate (TER), i.e., rate of wrong classification on testing set, is widely acceptable quantifying measure, which value minimum is good.

$$\text{TER} = \frac{\text{Total testing set misclassified patterns}}{\text{Total testing set patterns}}$$

Available Data

Training Set
(Use for learning)

Testing Set
(Reserve to measure generalization)

Benchmark problems are used to measure TER.

Benchmark Problems for Evaluation

A **benchmark** is a **point of reference** by which **something can be measured**.

- For NN or machine learning, the **most popular benchmark dataset** collection is the University of California, Irvine (**UCI**) **Machine Learning Repository** (<http://archive.ics.uci.edu/ml/>).
- UCI **contains raw data** that **require preprocessing** to use in NN. Some preprocessed data is also available at **Proben1** (<ftp://ftp.ira.uka.de/pub/neuron/>).
- **Various persons or groups** also maintain **different benchmark datasets** for specific purpose: **Delve** (www.cs.toronto.edu/~delve/data/datasets.html), **Orange** (www.ailab.si/orange/datasets.asp), etc.
- In this study **32 benchmark problems** are considered from UCI. Well defined **benchmark methodology** is followed for preprocessing.

UCI



Machine Learning Repository

Center for Machine Learning and Intelligent Systems

Welcome to the UC Irvine Machine Learning Repository!

We currently maintain 174 data sets as a service to the machine learning community. You may [view all data sets](#) through our searchable interface. Our [old web site](#) is still available in its original format. For a general overview of the Repository, please visit our [About page](#). For information about citing data sets in publications, please read our [citation policy](#). If you would like to donate to the Repository, please read our [donation policy](#). For any other questions, feel free to [contact the Repository librarians](#). We have also set up a [mirror site](#) for the Repository.

Supported By:






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Latest News:

- 07-23-2008: [Repository mirror](#) has been set up.
- 03-24-2008: New data sets have been added!
- 06-25-2007: Two new data sets have been added: UJI Pen Characters, MAGIC Gamma Telescope
- 04-13-2007: Research papers that cite the repository have been associated to specific data sets.
- 04-09-2007: Three new data sets have been added: Poker Hand, Calit2 Building People Counts, Dodgers Loop Sensor.
- 09-08-2006: The Beta site has been launched.
- 09-01-2006: SPECTF.test has been modified by the donor.

Newest Data Sets:

- 06-26-2008:  [Parkinsons](#)
- 04-21-2008:  [Ozone Level Detection](#)
- 04-03-2008:  [Absciscic Acid Signaling Network](#)
- 03-20-2008:  [Hill-Valley](#)

Most Popular Data Sets:

- 39351: 
- 31585: 
- 26458: 
- 23553: 

Benchmark Problems

Problems Related to Human Life

Problem	Task
Breast Cancer Wisconsin	Predicts whether a tumor is benign (not dangerous to health) or malignant (dangerous) based on a sample tissue taken from a patient's breast.
BUPA Liver Disorder	Identify liver disorders based on blood tests along with other related information such as alcohol consumption.
Diabetes	Investigate whether the patient shows or not the signs of diabetes.
Heart Disease Cleveland	Predicting whether at least one of four major heart vessels is reduced in diameter by more than 50%.
Hepatitis	Anticipate status (i.e., live or die) of hepatitis patient.
Lymphography	Predict the situation of lymph nodes and lymphatic vessels.
Lungcancer	Identify types of pathological lung cancers.
Postoperative	Determine place to send patients for postoperative recovery.

Benchmark Problems

Problems Related to Finance

Problem	Task
Australian Credit Card	Classify people as good or bad credit risks depend on applicants' particulars.
Car	Evaluate cars based on price and facilities.
Labor Negotiations	Identify a worker as good or bad i.e., contract with him beneficial or not.
German Credit Card	Like Australian Card, this problem also concerns to predict the approval or non-approval of a credit card to a customer.

Problems Related to Plants

Problem	Task
Iris Plants	Classify iris plant types.
Mushroom	Identify whether a mushroom is edible or not based on a description of the mushroom's shape, color, odor, and habitat.
Soybean	Recognize 19 different diseases of soybeans.

Summary of Benchmark Problems

Abbr.	Problem	Total Examp	Input Features		NN Architecture		
			Cont.	Discr.	Inputs	Class	Hidd. Node
ACC	Australian Credit Card	690	6	9	51	2	10
BLN	Balance	625	-	4	20	3	10
BCW	Breast Cancer Wisconsin	699	9	-	9	2	5
CAR	Car	1728	-	6	21	4	10
DBT	Diabetes	768	8	-	8	2	5
GCC	German Credit Card	1000	7	13	63	2	10
HDC	Heart Disease Cleveland	303	6	7	35	2	5
HPT	Hepatitis (HPT)	155	6	13	19	2	5
HTR	Hypothyroid	7200	6	15	21	3	5
HSV	House Vote	435	-	16	16	2	5
INS	Ionosphere	351	34	-	34	2	10
KRP	King+Rook vs King+Pawn	3196	-	36	74	2	10
LMP	Lymphography	148	-	18	18	4	10
PST	Postoperative	90	1	7	19	3	5
SBN	Soybean	683	-	35	82	19	25
SNR	Sonar	208	60	-	60	2	10
SPL	Splice Junction	3175	-	60	60	3	10
WIN	Wine	178	13	-	13	3	5
WVF	Waveform	5000	21	-	21	3	10
ZOO	Zoo	101	15	1	16	7	10

Input Features of Diabetes

1. Number of times pregnant
2. Plasma glucose concentration
3. Diastolic blood pressure
4. Triceps skin fold thickness (mm)
5. 2-Hour serum insulin (mu U/ml)
6. Body mass index
7. Diabetes pedigree function
8. Age

❖ Problems show variations in number of examples, input features and classes.

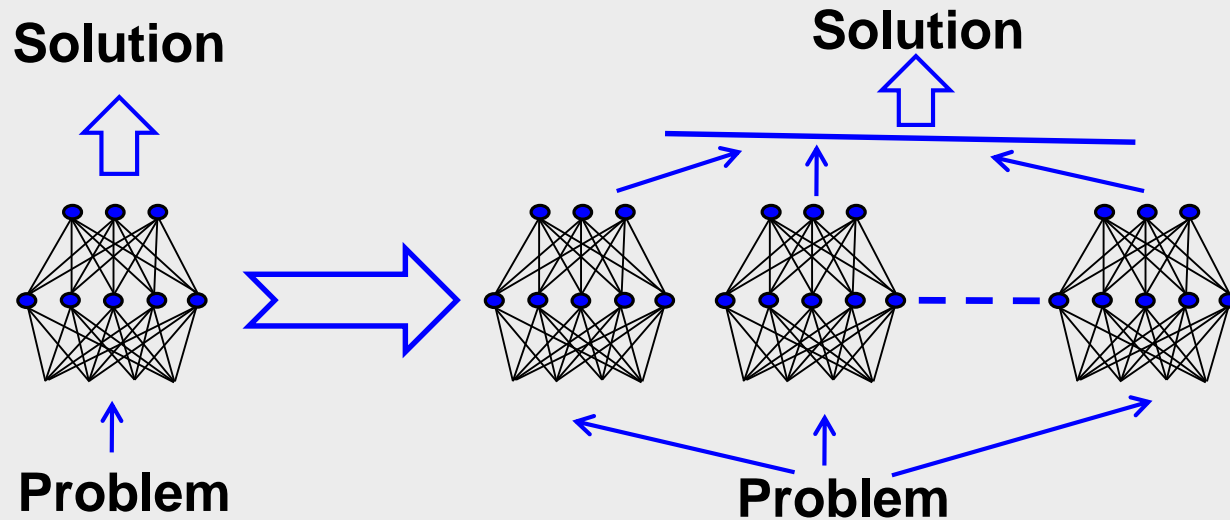
Why Ensemble of Neural Networks?

- The idea of building an **ensemble** with **several NNs** is taken from **sociology**.
- A **committee of people** for an **important task** or building **board of doctors** for a **major operation** is a common matter.
- Each **member** of the committee should be as **competent as possible**, but they should be **complementary to one another**. If **one or a few** members make an **error**, the probability is high that the **remaining members** can **correct his error**.
- **Several NNs** together might perform **better than single NN** when they **maintain proper diversity** to compensate failure of one by others.



The **goal of ensemble** is to achieve **better generalization** (i.e., lower TER) through **producing diverse NNs**.

Neural Network Ensemble (NNE)



In an NNE, **component NNs solve the problem individually** and **combine their outputs for NNE's output**. For better performance **diversity among NNs is important**.

- Diversity means **disagreement among the NNs**. Pair wise plain disagreement (**PD**) measure is the most popular among various measuring techniques.
- For a NNs pair, **diversity (div)** is equal to the **proportion of the patterns on which NNs reply different class predictions**. The total **NNE diversity (div_ens)** is the average for all the pairs.

$$div_{i,j} = \frac{1}{N} \sum_{n=1}^N Diff(C_i(x_n), C_j(x_n)),$$

$$div_ens = \frac{[div_{i,j} \text{ for all NNs pairs}]}{\text{Total NNs pair}} = \frac{\sum_{i=1}^{M-1} \sum_{j=i+1}^M div_{i,j}}{\sum_{m=1}^{M-1} m}$$

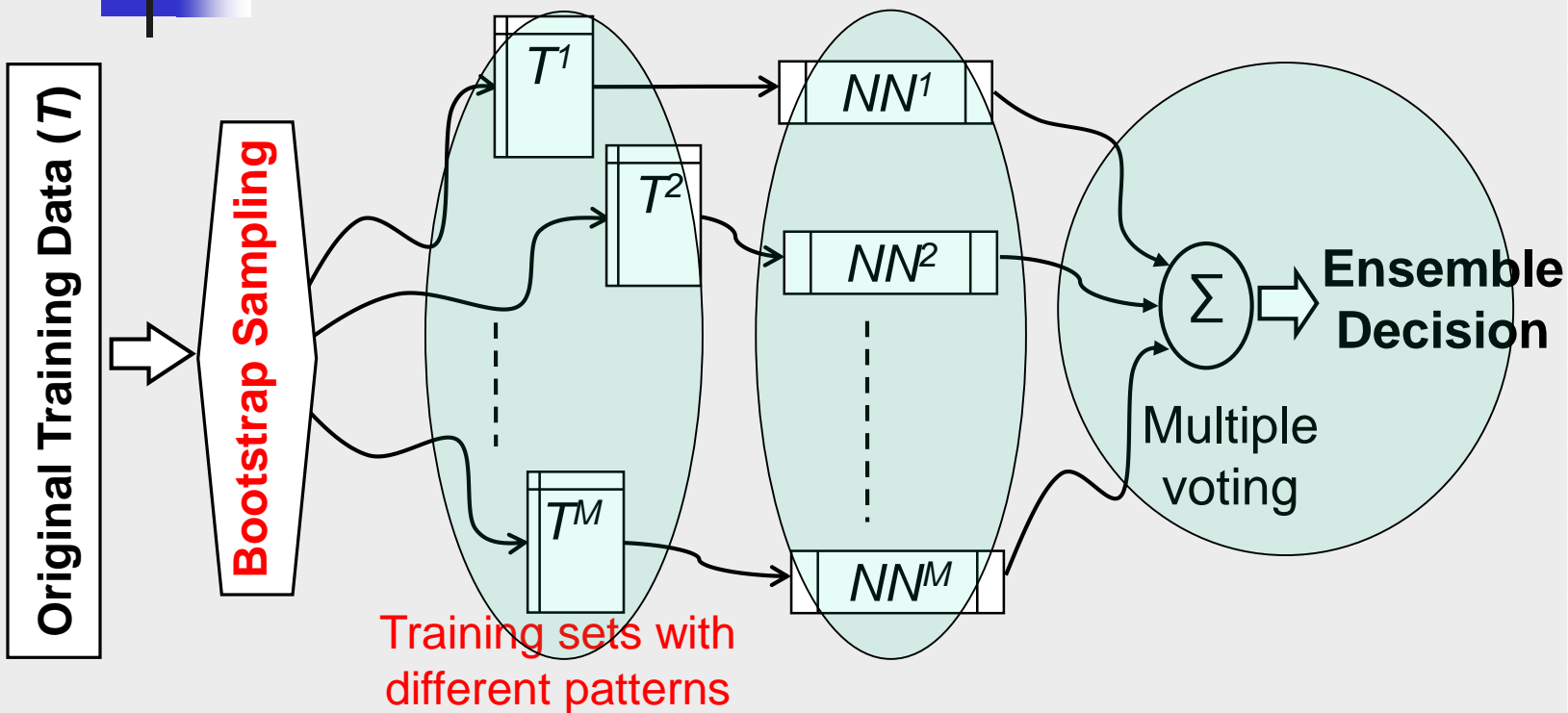
Data Sampling for NNE Construction

Proper diversity among component NNs is an important parameter for ensemble construction so that failure of one may compensate by others.

- There are various ways one can produce diverse NNs, such as varying initial random weights, algorithm employed and training data.
- Since functionality of a NN depends on its training data, data sampling is considered as the most effective for diversity than other approaches.
- Data sampling (i.e. variation in training data) involves: bootstrapping of original training data, generation artificial data, sampling of input features, etc.

1. Bagging (Breiman, 1996)

L. Breiman, "Bagging Predictors" *Machine Learning*, vol. 24, pp. 23 –140, 1996.



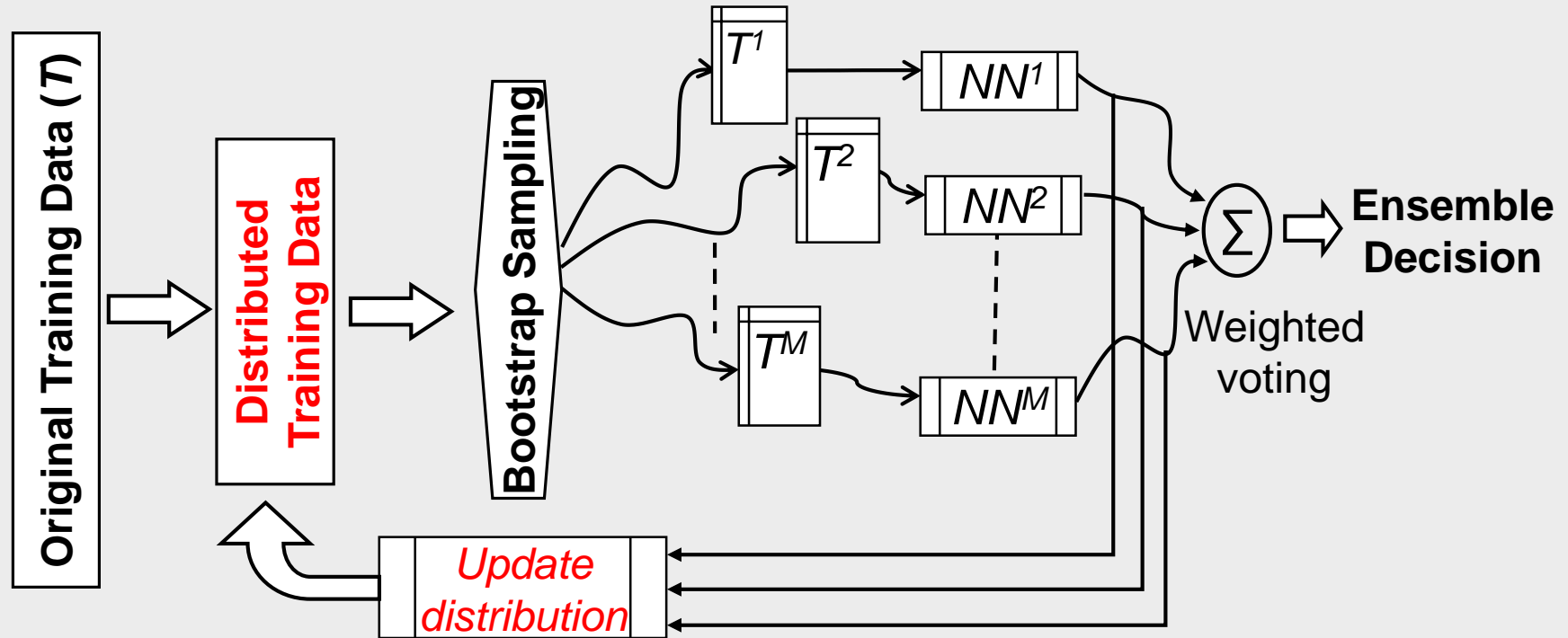
T	T^1	T^2
1	4	10
2	9	6
3	6	3
4	8	9
5	1	2
6	8	7
7	5	3
8	1	4
9	2	2
10	4	9

Bootstrap sampling: Randomly selects a pattern and replace it again in its original place for later use.

In a training set **many patterns appear multiple times** while others are left.

2. AdaBoost (Freund & Schapire, 1996)

Y. Freund and R. E. Schapire, “Experiments with a new boosting algorithm”, in *Proc. of the 13th Int. Conf. on Machine Learning* (Morgan Kaufmann, 1996), pp. 148–156



- NNs are trained **one after another sequentially** and after training a NN **distribution of training data updates**.
- Existence of previously **miss classified patterns increases** in coming training sets due to **error base distribution**.

Bagging and AdaBoost

1. Let M be the number of networks to be trained for an ensemble

Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$

2. for $i=1$ to M {

a. Make a training set, T_i by sampling N patterns uniformly at random with replacement from T

b. Train network NN_i by T_i

}

3. Ensemble decision is made in multiple voting way

Bagging

1. Let M be the number of networks to be trained for an ensemble.

Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$

Assign weight for each pattern of T , initially weights are the same, i.e., $w_1(n) = 1/N$

2. for $i=1$ to M {

a. Make a training set, T_i by sampling N patterns at random with replacement from T based on weight distribution $w_i(n)$

b. Train network NN_i with T_i

c. $\varepsilon_i = \sum_{(x(n), d(n)) \in T: NN_i(x(n)) \neq d(n)} w_i(n)$ (weighted error on training set)

d. $\beta_i = (1 - \varepsilon_i) / \varepsilon_i$

e. for each $(x(n), d(n)) \in T$,

if $NN_i(x_n) \neq d_n$ then $w_{i+1}(n) = w_i(n) \cdot \beta_i$, otherwise $w_{i+1}(n) = w_i(n)$

f. Normalize the weights of T

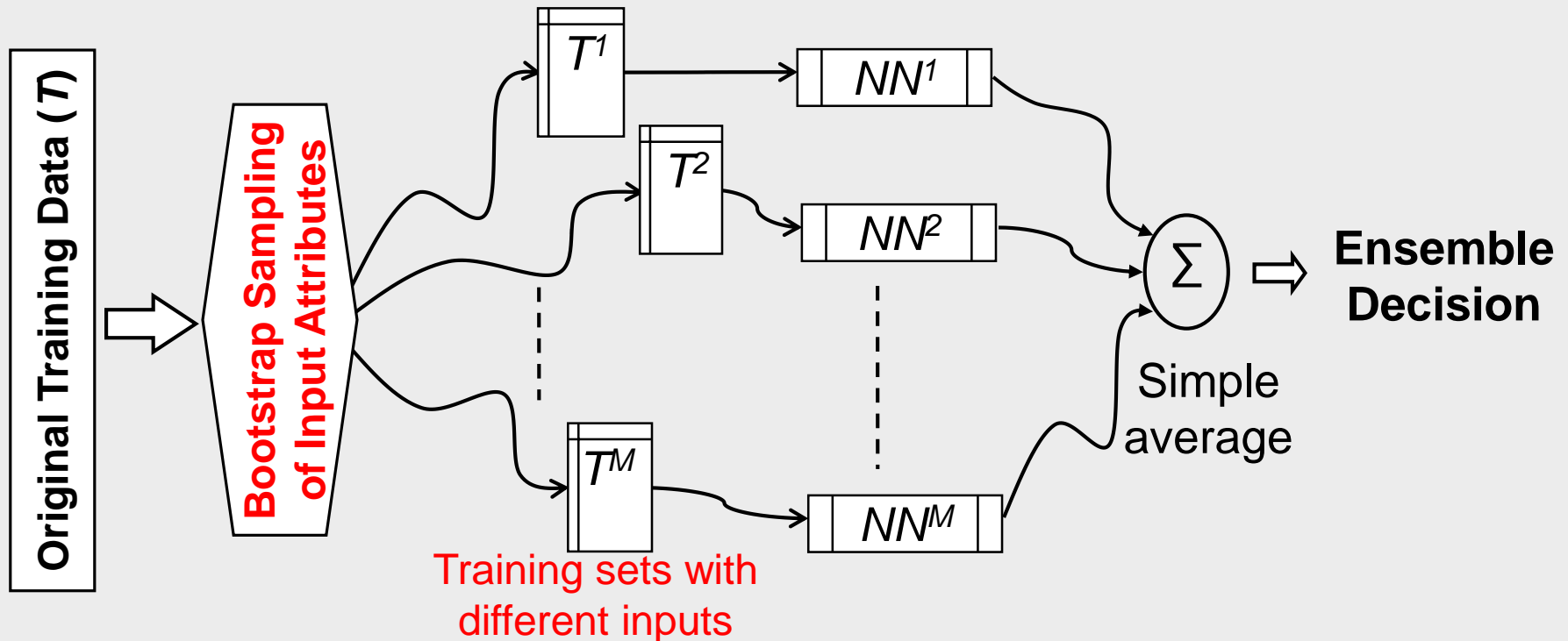
}

3. Ensemble decision is made in weighted voting way

AdaBoost

3. Random Subspace Method(RSM) (Ho, 1998)

T. K. Ho, "The random subspace method for constructing decision forests" *IEEE Trans. on Pattern Analysis and Machine Intelligence*, vol. 20, pp. 832–844, 1998



RSM require to maintain tagging with original inputs for every NN's inputs.

1. Let M be the number of networks to be trained for an ensemble

Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$ and feature set $F = \{1, 2, \dots, f\}$

2. *for* $i=1$ to M {

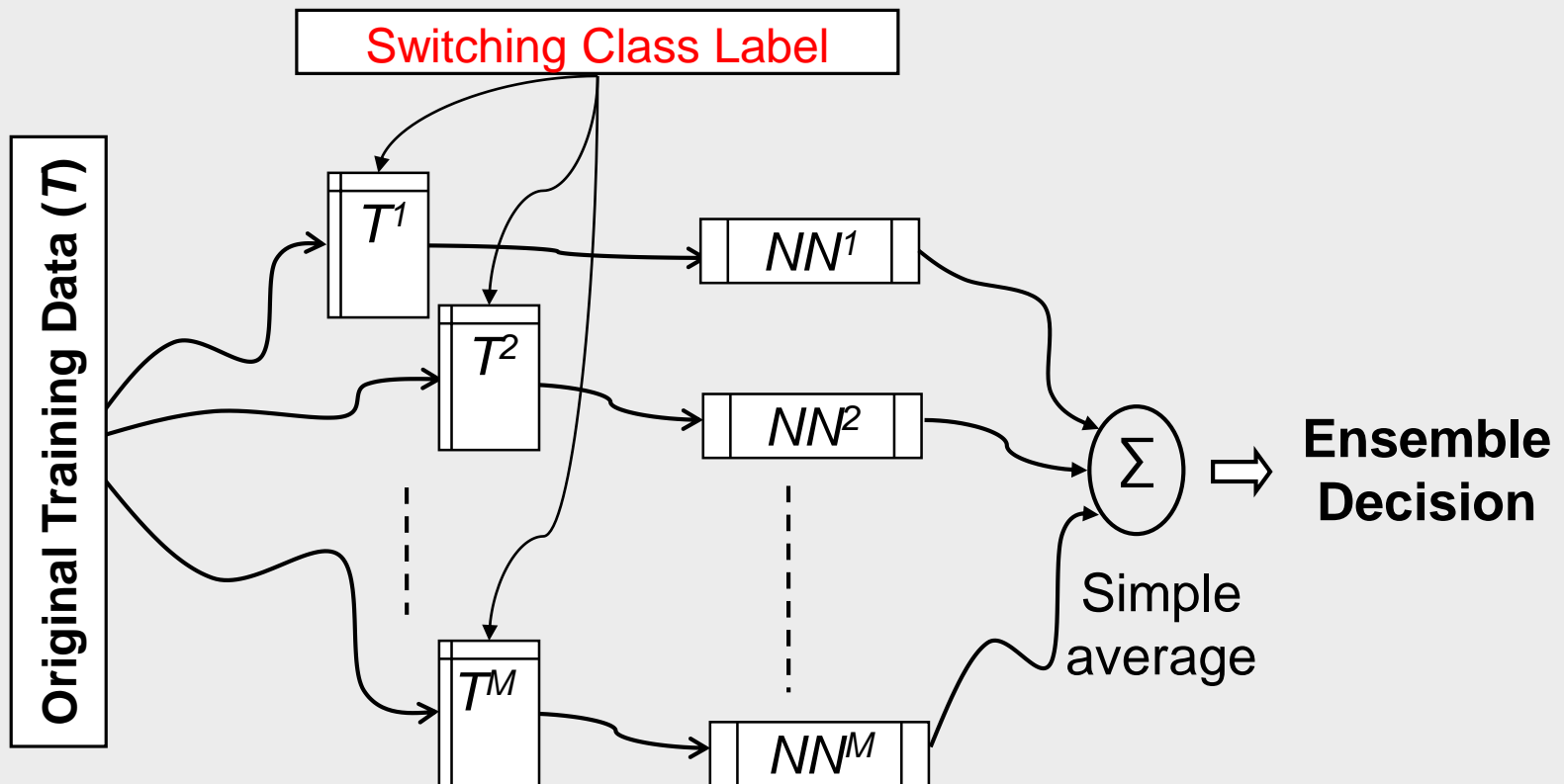
- a. Make a feature subset, F_i by sampling $|F|$ features uniformly at random with replacement from F
- b. Train network NN_i by T with feature set F_i

}

3. Ensemble decision is made in simple average way

4. Class Label Switching (Martínez-Muñoz & Suárez, 2005)

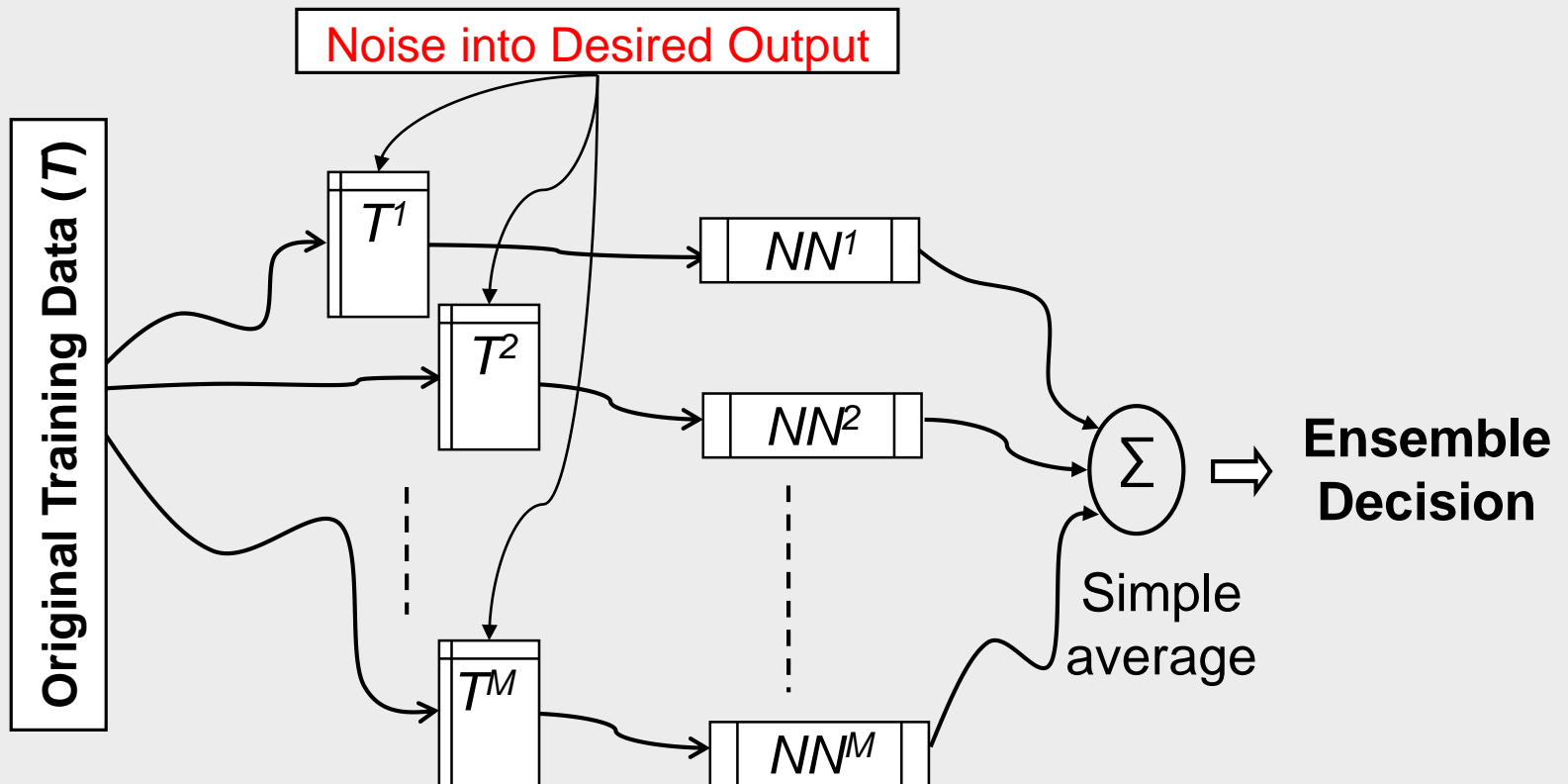
G. Martínez-Muñoz and A. Suárez, "Switching class labels to generate classification ensembles," *Pattern Recognition*, vol. 38, pp. 1483–1494, 2005.



A parameter $S_{fraction}$ maintains number of examples to change class label.

5. Smearing (Breiman, 2000)

L. Breiman, "Randomizing outputs to increase prediction accuracy," Machine Learning, vol 40, pp. 229–242, 2000.



Class Label Switching and Smearing

1. Let M be the number of networks to be trained for an ensemble
 Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$
 Take $S_{Fraction}$ -factor that determines number of pattern to alter class label
 Number of patters to switch the class label, $S = S_{Fraction} * N$
2. for $i=1$ to M {
 - a. Make a training set, $T_i = T$
 - b. Randomly select S examples in T_i and assign different class label randomly
 - c. Train network NN_i by T_i
3. Ensemble decision is made in simple average way

Class Label Switching

1. Let M be the number of networks to be trained for an ensemble
 Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$
 Compute standard deviation measure (sd_k) is each class based on Eq. (2.1)
2. for $i=1$ to M {
 - a. Make a training set, $T_i = T$
 - b. Change the desired output of T_i based on Eq. (2.2)
 - c. Train network NN_i by T_i
3. Ensemble decision is made in simple average way

If p_k is the proportion of the patterns in class k , then standard deviation measure (sd)

$$sd_k = 2 (p_k (1 - p_k))^{0.5} \quad (2.1)$$

The new desired output for the k -th class for the n -th training pattern for a network is

$$d'_k(n) = d_k(n) + z_k(n)sd_k \quad k=1, \dots, K \quad n=1, \dots, N \quad (2.2)$$

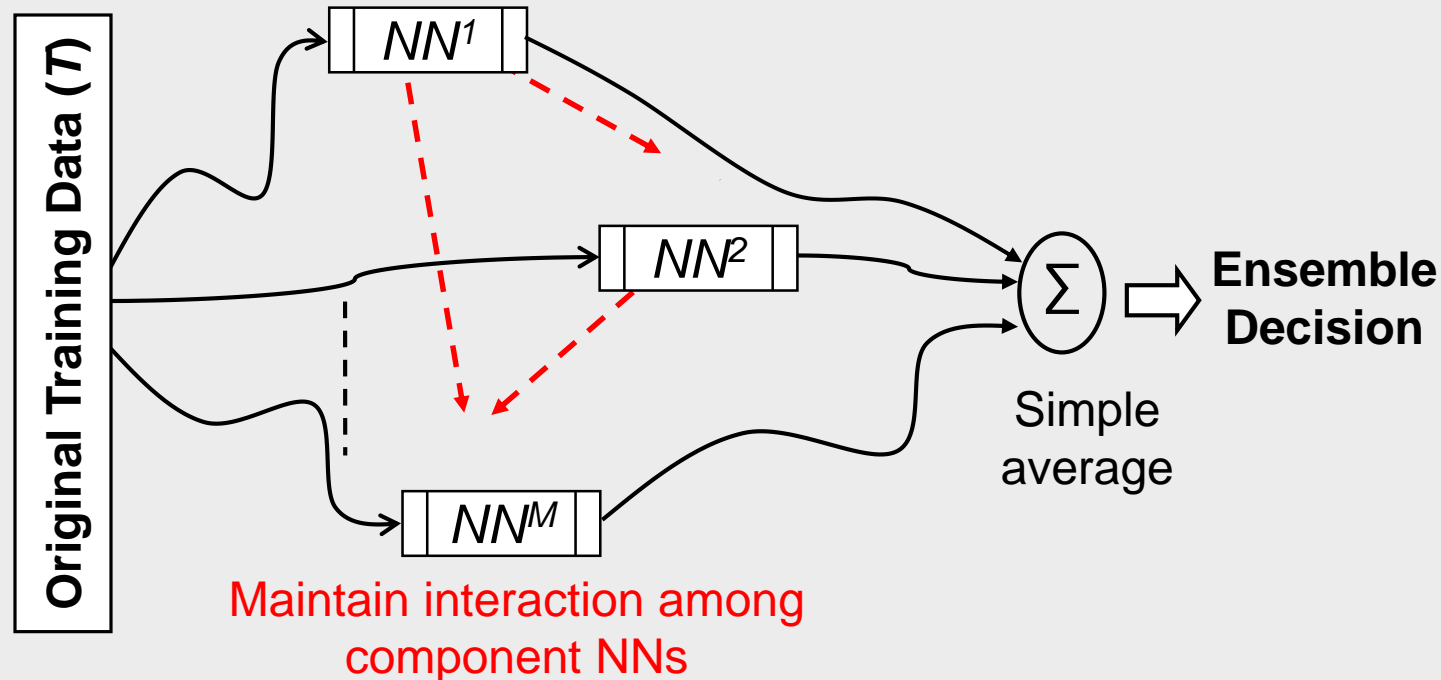
Where $z_k(n)$ is the random number from Gaussian distribution with a mean zero and a variance of one.

Smearing

6. Negative Correlation Learning(NCL) (Liu & Yao, 1999)

Y. Liu and X. Yao, "Ensemble learning via negative correlation," *Neural Networks*, vol. 12 pp. 1399–1404, 1999.

Y. Liu and X. Yao, "Simultaneous training of negatively correlated neural networks in an ensemble," *IEEE Trans. Systems, Man, and Cybernetics — Part B*, vol. 29, pp. 716–725, 1999.



$$\text{Error function, } e_i(n) = \underbrace{\frac{1}{2} (f_i(n) - d(n))^2}_{\text{Normal BP portion}} + \underbrace{\lambda \left((f_i(n) - \bar{f}(n)) \sum_{j \neq i} (f_j(n) - \bar{f}(n)) \right)}_{\text{Correlation penalty term}}$$

- ❖ Interaction produces negatively correlated NNs and therefore NNs motivate different functional spaces.
- ❖ The coefficient of the penalty term (λ) maintain strength of interaction.

Negative Correlation Learning(NCL)

1. Let M be the number of networks to be trained for an ensemble

Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$

Create M networks, NN_1 ---- NN_M

2. *for* $n=1$ *to* N {

 Prepare ensemble output for pattern n

for $i=1$ *to* M {

 Train network NN_i for pattern n using error definition of Eq. (2.3)

 }

}

3. Ensemble decision is made in simple average way

Negative Correlation Learning (NCL)

$$e_i(n) = \frac{1}{2} (d(n) - f_i(n))^2 + \lambda p_i(n) \text{ ----- Eq. 2.3}$$

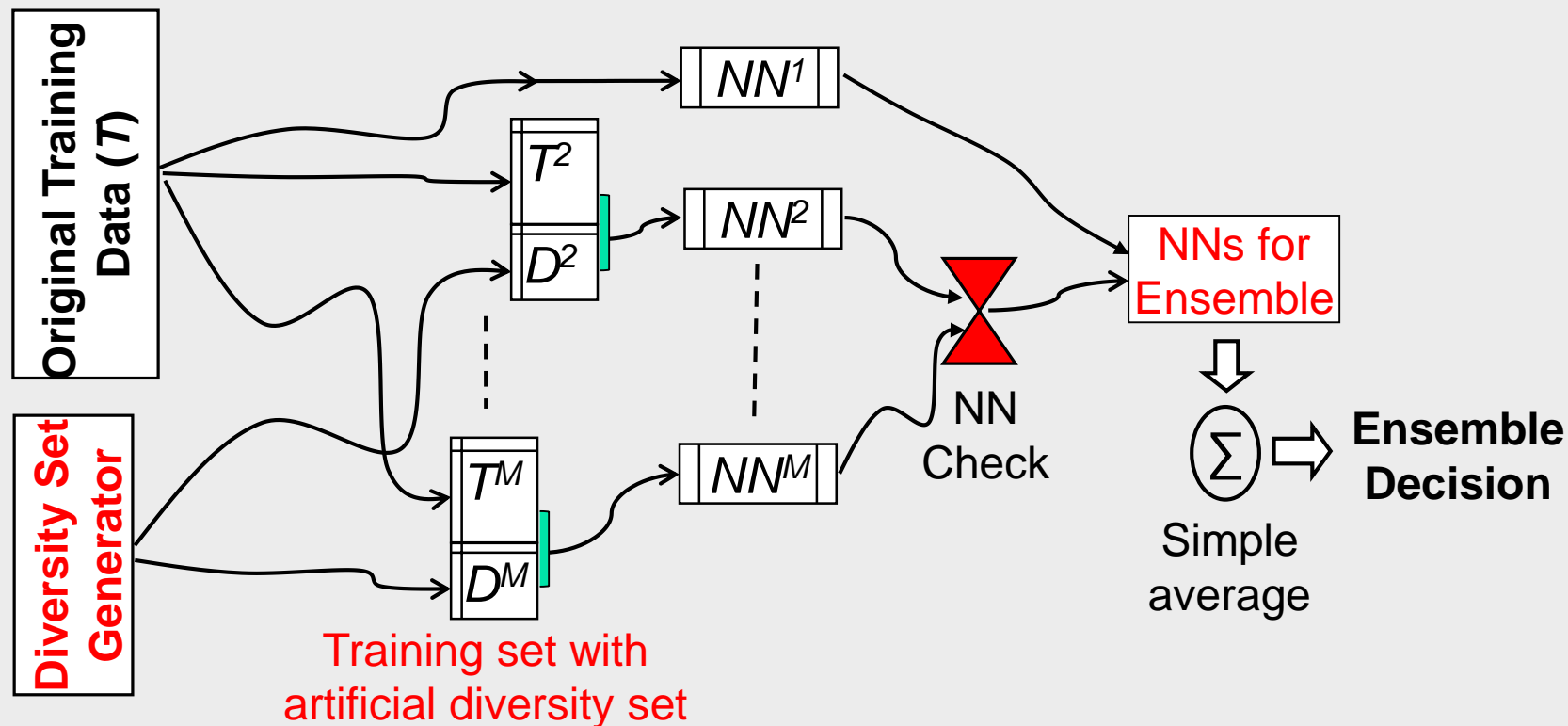
$$p_i(n) = (f_i(n) - \bar{f}(n)) \sum_{j \neq i} (f_j(n) - \bar{f}(n))$$

$$\bar{f}(n) = \frac{1}{M} \sum_{i=1}^M f_i(n)$$

7. DECORATE (Melville & Mooney, 2005)

Diverse Ensemble Creation by Oppositional Relabeling of Artificial Training Examples

P. Melville and R. J. Mooney, "Creating diversity in ensembles using artificial data," *Information Fusion*, vol. 6, pp. 99–111, 2005.



- ❖ Trains predefined large number of NNs to select NNs for final NNE
- ❖ A parameter R_{size} maintains size of diversity set.
- ❖ Training of large number of NNs and additional diversity set increase training time.

DECORATE

1. Let I_{max} be the number of networks to be trained for an ensemble and M is the desired number of networks

Take original training set $T = \{(x(1), d(1)), \dots, (x(N), d(N))\}$ with class label $d(n) \in K = \{1, 2, \dots, k\}$

Take R_{Size} -factor that determines size of diversity set

$i=1$ (for network in ensemble) and $trials = 1$ (for trial network)

Train network NN_i with T (first network is trained with original training data)

Initialize ensemble, $Ens = \{ NN_i \}$

Compute ensemble error, $\varepsilon = \left(\sum_{(x(n), d(n)) \in T: Ens(x(n)) \neq d(n)} 1 \right) / N$

2. while $trials < I_{max}$ and $i < M$ {

a. Generate $R_{Size} \times |T|$ training examples, R

b. Label examples in R with probability of class labels inversely proportional to predictions of Ens

c. Prepare training set T_i , $T_i = T \cup R$ and train network NN_i with T_i

d. $Ens = Ens \cup \{ NN_i \}$

e. Compute ε' based on Step 1

f. if $\varepsilon' \leq \varepsilon$ then $i = i + 1$ and $\varepsilon = \varepsilon'$, otherwise $Ens = Ens - \{ NN_i \}$

g. $trials = trials + 1$

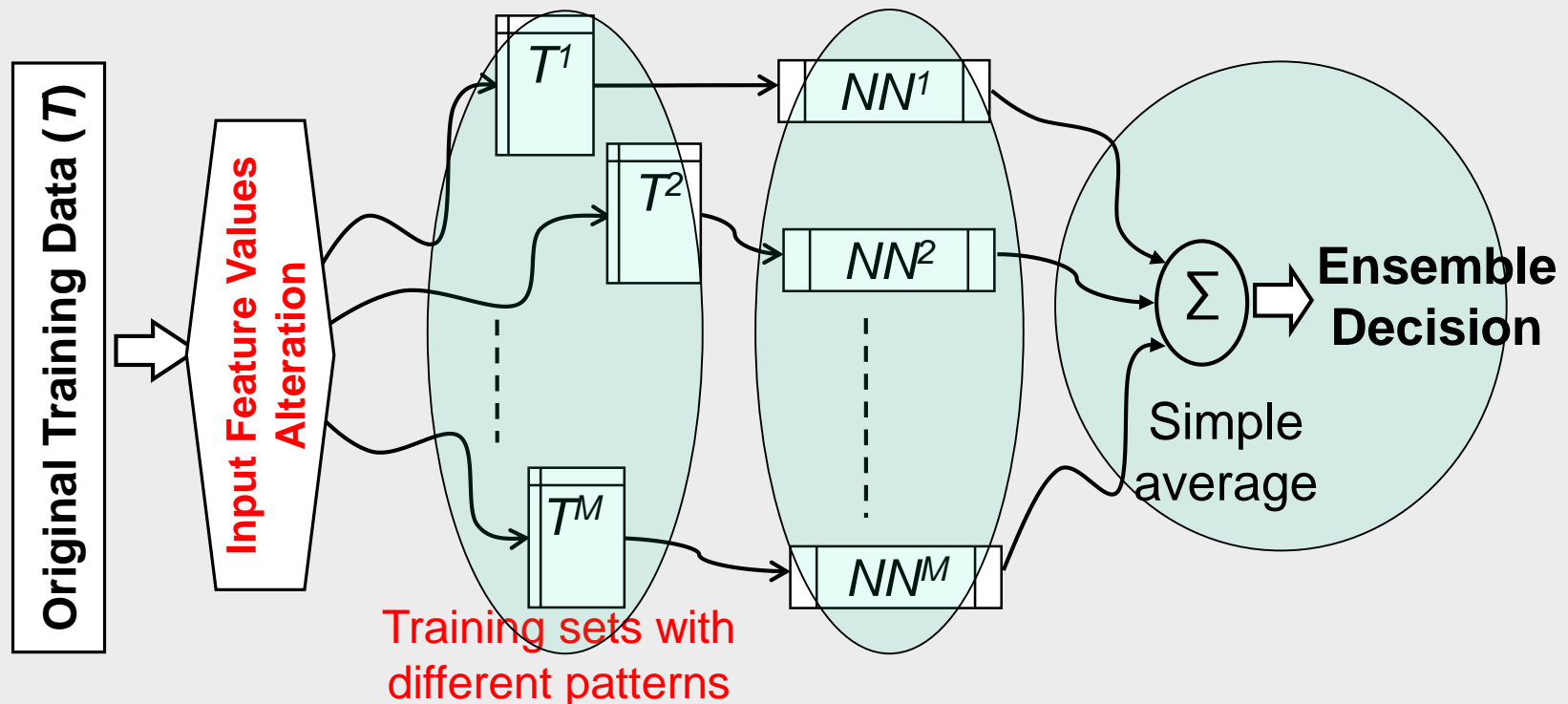
}

3. Ensemble decision is made in simple average way

8. Ensemble through Input Values Alteration (EIVA)

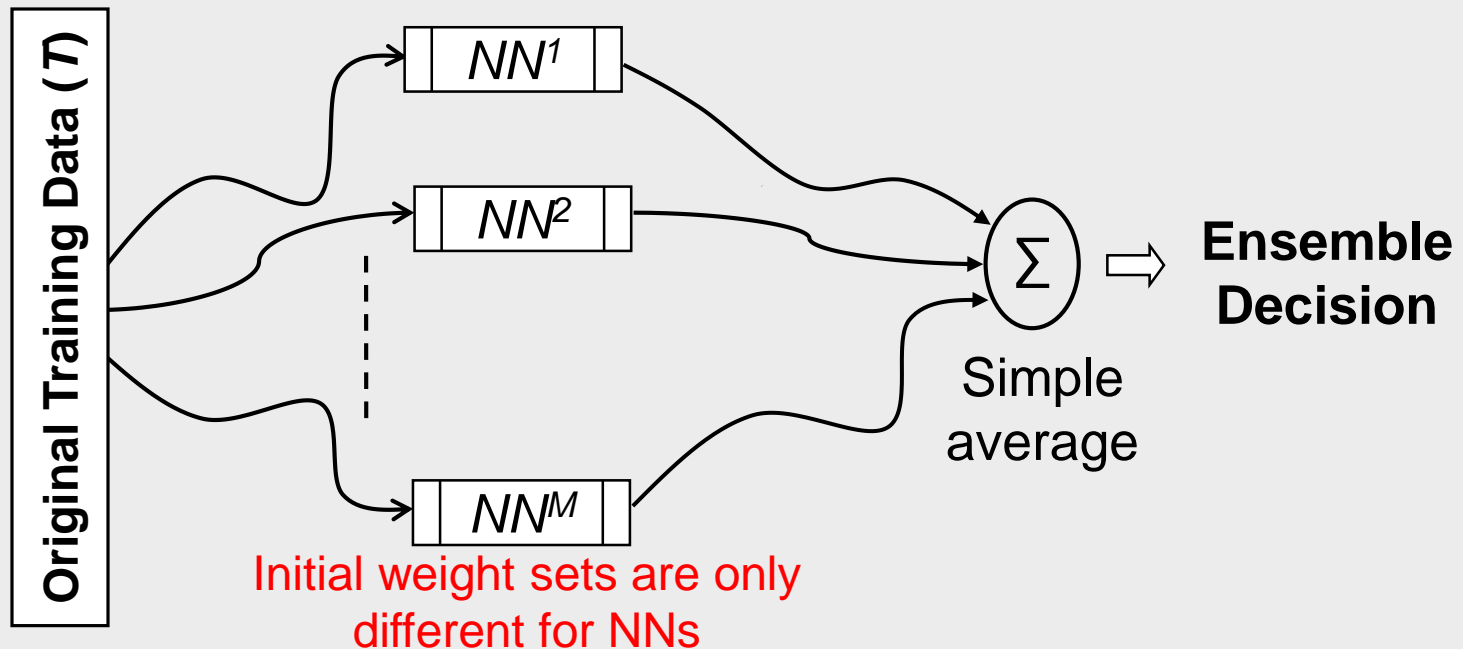
(M.A.H. Akhand & K. Murase, 2012)

M. A. H. Akhand, and K. Murase , “Ensembles of Neural Networks based on the Alteration of Input Feature Values ” *International Journal of Neural Systems*, vol. 22, no.1, pp. 77-87, 2012.



Feature Values Alteration: Randomly selects a pattern and alter some of its feature values with the value of another one.

9. Simple NNE(sNNE)



- ❖ To evaluate performance of data sampling based NNE methods, **sNNE** is considered as **base line**.
- ❖ **Less diversity** due to same data for all NNs; therefore, performance is **worse**.

Motivation to Comparative Study

- A number of ensemble methods already proposed using various data sampling techniques.
- Proposed methods are investigated on heterogeneous test bed.
- Some methods are proposed for decision trees and empirical result for NN is not available.

Comparative study of the proposed methods on a common ground is necessary to evaluate their effectiveness.

(Eight prominent NNE methods are considered for investigation.)

Experimental Studies

Common Settings:

- For an NNE 20 NNs are considered.
- Each NN is trained for equal 50 / 75 / 100 iteration.
- Learning rate of back propagation was set 0.15.
- 10-fold cross validations was followed for result presentation.

Built in Parameter Settings:

- For DECORATE R_{Size} value was 0.5, 0.75 or 1. Maximum trial NNs was 30.
- In class label switching $S_{fraction}$ was 0.1, 0.2 or 0.3.
- NCL was tested with λ value 0.25, 0.5 or 0.75.

TER Comparison over 50 Indp. Runs

Problem	sNNE 20NNs/NNE	Bagging 20NNs/NNE	AdaBoost 20NNs/NNE	DECORATE (NNs/NNE)	RSM 20NNs/NNE	Switching 20NNs/NNE	Smearing 20NNs/NNE	NCL 20NNs/NNE
ACC	0.1522	0.1417	0.1568	0.14 (8.34)	0.1461	0.1423	0.1414	0.1443
BCW	0.0348	0.0322	0.0322	0.0299(6.40)	0.0296	0.029	0.0319	0.0313
CAR	0.1128	0.0995	0.0799	0.1203(2.00)	0.1647	0.118	0.1193	0.1036
DBT	0.2379	0.2321	0.2305	0.2342(1.14)	0.2318	0.2382	0.2366	0.2308
GCC	0.2462	0.2424	0.2476	0.2652(1.88)	0.2414	0.2416	0.2482	0.2402
HDC	0.1633	0.1573	0.1653	0.152 (6.78)	0.152	0.1567	0.1567	0.1627
HPT	0.1547	0.1627	0.172	0.16(1.16)	0.1573	0.1587	0.1547	0.152
HTR	0.0531	0.0518	0.0263	0.0528(1.02)	0.0559	0.056	0.0558	0.0522
INS	0.1343	0.1297	0.1034	0.0606 (12.9)	0.1429	0.132	0.1806	0.1366
IRP	0.0267	0.0293	0.028	0.0267 (1.00)	0.0293	0.0267	0.0267	0.0267
LMP	0.1486	0.1529	0.1729	0.1371 (4.74)	0.1486	0.14	0.1586	0.15
PRM	0.068	0.068	0.072	0.066 (20.00)	0.068	0.07	0.078	0.068
SGM	0.07	0.0648	0.0432	0.0761(3.14)	0.0681	0.0724	0.0765	0.0677
SNR	0.195	0.194	0.181	0.166 (7.58)	0.20	0.201	0.209	0.195
SPL	0.1419	0.1556	0.1529	0.1823(2.36)	0.0873	0.1527	0.1725	0.1409
STL	0.144	0.1379	0.1358	0.1525(2.98)	0.1435	0.1419	0.1556	0.145
WVF	0.1327	0.1297	0.132	0.1308(4.18)	0.1352	0.1339	0.1345	0.1312

Result Summary over 30 Problems

	sNNE	Bagging	AdaBoost	DECORATE	RSM	Switching	Smearing	NCL
Average TER	0.1505	0.1393	0.1380	0.1441	0.1562	0.1512	0.1581	0.1462
Best/Worst	2/3	5/1	11/6	7/2	2/7	2/3	1/9	6/0
NNE Method	Pair Wise Win/Draw/Loss Summary							
sNNE	-	23/1/6	19/0/11	17/1/12	12/2/16	11/1/18	8/2/20	20/4/6
Bagging		-	16/1/13	11/0/19	10/2/18	7/1/22	5/0/25	10/1/19
AdaBoost			-	13/0/17	11/0/19	12/0/18	10/0/20	15/0/15
DECORATE				-	11/1/18	10/1/19	5/1/24	16/1/13
RSM					-	17/0/13	12/0/18	22/1/7
Switching						-	6/2/22	19/1/10
Smearing							-	24/1/5

Conclusions from the Comparative Study:

- ❖ No one is superior to others for all the problems.
- ❖ DECORATE performs better for problems with limited examples, e.g., INS, LPM, PRM. NCL also good for small problems.
- ❖ For large sized problems bagging and AdaBoost are the best, e.g., CAR, HRT, WVF. AdaBoost might show very good result for very large problems.
- ❖ RSM performs well for sufficient input set, e.g., SPL.

Conclusions

- Basic introduction about NNs and NNE is presented.
- Comparative study of prominent existing methods is given and identified effectiveness of the methods.
- Given an Outline for better NNE construction.