### 4.4 Introduction to special neural network architectures

### 4.4.1 Determining the optimal Structure

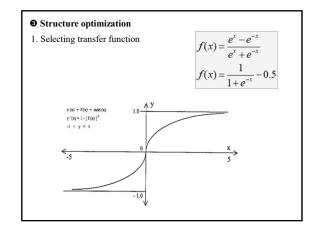
• Empirical Formula

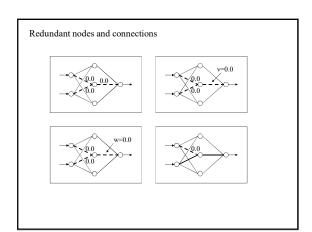
The number of nodes in the hidden layer:

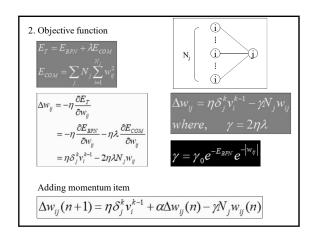
$$k = 10.43 \, sn + 0.12 \, n^2 + 2.54 \, s + 0.77 \, n + 0.35 + 0.5$$

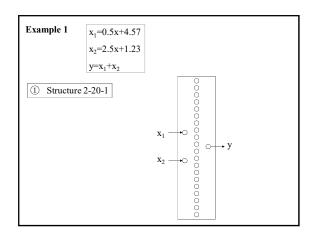
- s: No. of nodes in the input layer
- n: No. of nodes in the output layer
- 2 Identifying redundant node

 $\delta_{I}\!\!=\!\!E_{without\ node\ I}\text{--}E_{with\ node\ i}$ 

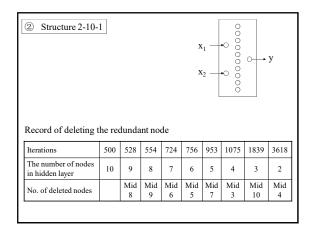


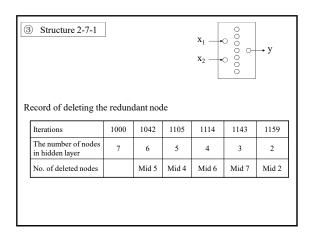


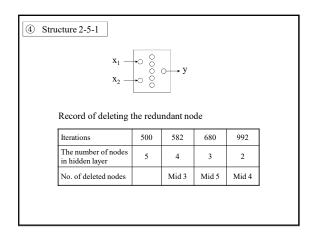


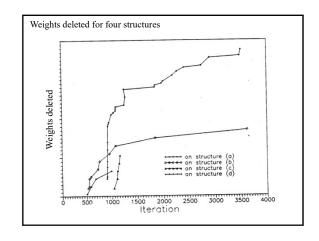


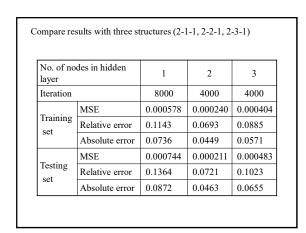
Iterations	900	901	912	913	918	920	924	996
The number of nodes in hidden layer	20	18	17	16	14	13	11	10
No. of deleted nodes		Mid 19,20	Mid 13	Mid 4	Mid 14,17	Mid 18	Mid 15,16	
Iterations	1273	1747	2183	2269	240	6 29	900	3507
The number of nodes in hidden layer	9	8	7	6	5		3	2
No. of deleted nodes	Mid 8	Mid 12	Mid 11	Mid 10	Mie 9	Mid N		Mid 2

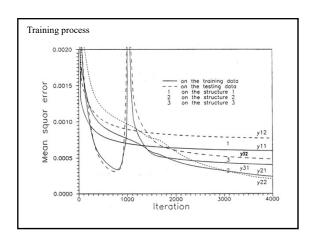


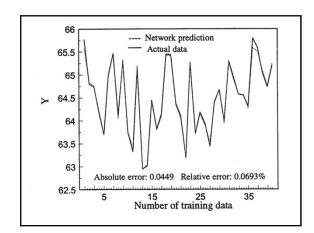


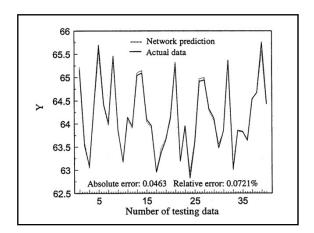


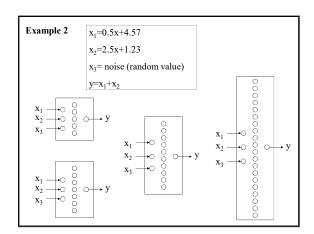


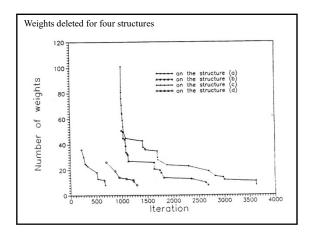


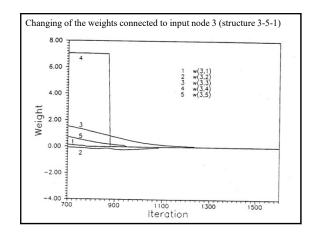


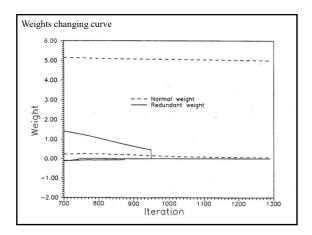






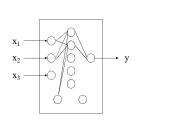






### Example

Final structure 1



Reco	rd for r	edundaı	nt weigl	nts dele	ted with	differe	ent weig	ght dead	llines
W <sub>0</sub> =±0.001 W <sub>0</sub> =±		0.005	05 W <sub>0</sub> =±0.01		W <sub>0</sub> =±0.05		W <sub>0</sub> =±0.1		
Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted
771	1	768	1	765	1	742	1	700	1
904	2	886	2	866	2	775	2	716	2
956	3	953	3	949	3	874	7	723	3
1292	4	1083	4	1027	4	948	12	780	8
1339	5	1167	5	1109	5	1088	13	855	13
1378	8	1206	6	1147	6	1223	14	1002	18
1460	9	1223	9	1150	9	1231	15		
1523	14	1410	10	1287	13	1290	18		
1532	18	1440	14	1372	14				
		1515	18	1492	18				

Record for redundant weights deleted with different  $\gamma_0$ 

γ <sub>0</sub> =0	0.005	$\gamma_0 = 0$	.0005	γ <sub>0</sub> =0	.0001	$\gamma_0 = 0.$	00005	
Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted	
700	1	704	1	742	1	766	1	
701	8	713	3	775	2	901	2	
703	14	738	8	874	7	1097	7	
1922	15	740	9	948	12	1114	12	
2880	16	901	10	1088	13	1281	13	
2883	17	1480	11	1223	14	1629	14	
3305	18	1509	12	1231	15	1654	15	
		2082	15	1290	18	5083	18	
		2517	16					
		3064	18					

Record for redundant weights deleted with different E<sub>0</sub>

E <sub>0</sub> =0	$E_0 = 0.005$		E <sub>0</sub> =0.0005		.0001	E <sub>0</sub> =0.00005	
Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted	Iteration	Weights deleted
765	1	765	1	765	1	765	1
866	2	866	2	866	2	866	2
949	3	949	3	949	3	949	3
1140	4	1027	4	1027	4	1027	4
1231	5	1109	5	1109	5	1109	5
1533	6	1147	6	1147	6	1147	6
3020	7	1887	9	1150	9	1150	9
3166	8	1903	10	1287	13	1287	13
3968	9	1904	11	1372	14	1372	14
4127	11	1981	14	1492	18	1492	18
6422	14	2025	18				
6597	18						
10000	18	4000	18	4000	18	4000	18

## 4.4.2 Autoassociative Networks

Two main applications:

- (1) Data compression and filtering
- (2) Dimensionality reduction of an input vector

Two main categories:

- (1) Signal-processing networks
- (2) Image-processing networks

The most commonly used NN for signal processing is the autoassociative backpropagation network

- $\ensuremath{\mathfrak{B}}$  reduce the amount of random noise in the input signal
- \* filter gross errors in data resulting from sensor-malfunctions, drift and bias.

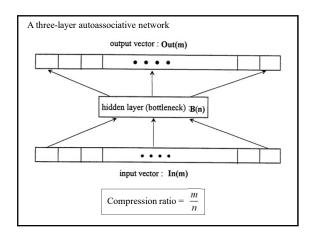
The input signal has three distinct components:

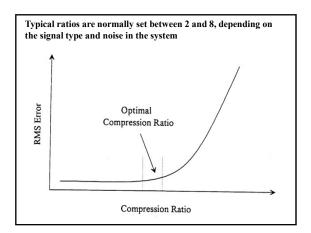
- (1) A pure signal (p)
- (2) Measurement noise (n)
- (3) Measurement error (e)

Thus, we may represent the input vector as a linear combination of the three components:

$$In(m)=In_p(m)+In_n(m)+In_e(m)$$

The objective of filtering a process signal is to map only the pure signal  $(In_p(m))$  onto the output vector, while removing all measurement noise  $(In_n(m))$  and measurement errors  $(In_e(m))$ .





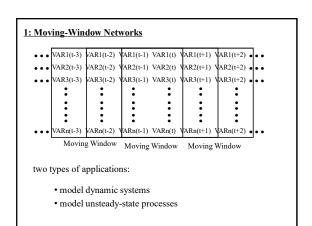
# 4.4.3 Hierarchical Neural Networks The input vector is divided into groups that have similar effects on the output responses Output Layer Hidden Layer Subnet # 1 Subnet # 2 Subnet # 3

### Advantages:

- use more nodes with fewer weight factors, improving efficiency. Therefore, network training requires fewer examples and less time.
- (2) well-defined subnetworks of related variables provides hints that help the network learn in the right direction.
- (3) isomorphic to expert systems or model-based algorithms for the same task. We can map each useful subnetwork to a rule (or small set of rules) or a model-based local analysis.

The following sections describe two significant types of hierarchical networks used in process system engineering.

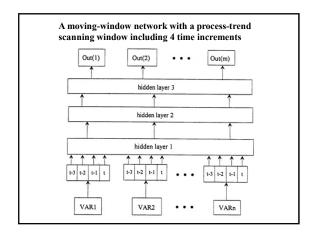
- (1) moving-window networks for time-dependent processes
- (2) input-compression networks for working with large input variable sets



## Key challenge problems:

- (1) Choose the "time-window width"
- (2) Choose the time between data sampling point
- (3) Use average moving-window values as input to the network

$$\overline{VAR_{j}}(t) = \frac{\sum_{n=0}^{3} VAR_{j}(t - n\Delta t)}{A}$$

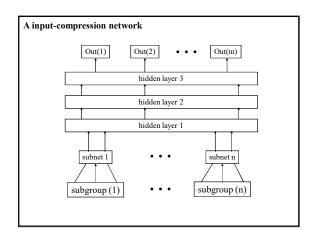


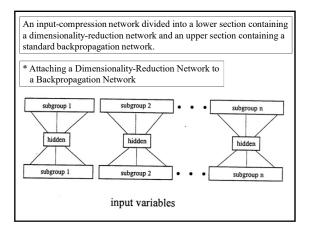
### 2: Input-Compression Networks

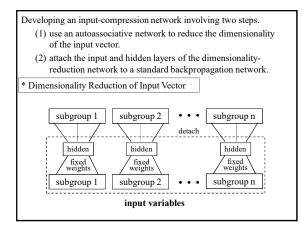
Neural networks can become very large and difficult to train if they have a large number of input variables that influence the output responses.

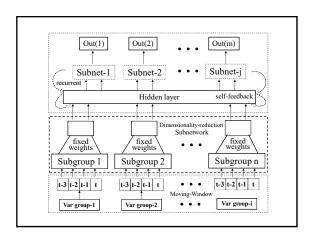
### Auto-assoicate hierarchical neural network

The input layer in the input-compression network consists of n property groups, where each group includes input variables with similar effects on the output responses. Each property group is compressed into a corresponding subnetwork to create a more compact representation of the input variables without losing any essential information.









### Example:

Feature Clustering-FC

Feature Target Correlation -FTC

# Data Attributes Decompostion method

### DATASETS FROM UCI RESPOSITORY AND PRODUCTION

Dataset	Dataset Character Quality							
Name	Instances	Attributes	Outputs	Default Task				
Ionosphere	351	34	1	Classification				
Breast Cancers	569	30	1	Regression /Classification				
PTA	260	17	1	Regression				

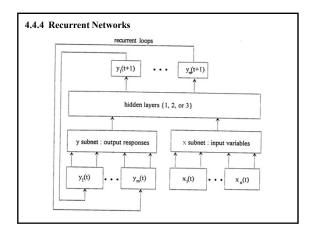
### FEATURE SETS ENSEMBLES FROM TEST DATA SETS

ъ м	Feature Sets Ensemble Steps					
Dataset Name	Feature Target Correlation	Feature Clustering				
Ionosphere	{22,27,30,32,34} {1,220,21,23,24,25,26,28, 29,31,33}	{2,18,20,24,26,28} {1,3,5,7,9,29,31} {22,27,30,32,34} {4,6,8,10,12,14,16,33} {11,13,15,17,19,21,23,25}				
Breast Cancers	{10,12,15,19} {1,2,3,4,5,6,7,8,9,11,13,14,1 6,17,18,2030}	{3,23} {4,24} {10,12,15,19} {1,2,5,7,822,2530}				
PTA	{3,4,8,10,13} {1,2,5,6,7,9,11,12,14,15,16,1 7}	{7,9,11,12,14} {15,16,17} {1,2,5,6} {3,4,8,10,13}				

### Comparison results

D-44 N	Methods Comparison(Err/Sta)						
Dataset Name	BP	DAD-AHNN	DAD-THNN				
T l	8.1468	3.9423	4.4179				
Ionosphere	0.2669	0.1239	0.1168				
Breast Cancers	5.1059	2.4075	4.0621				
Breast Cancers	0.1665	0.1348	0.1568				
PTA	0.4426	0.4247	0.3609				
PIA	0.0037	0.0033	0.0030				

AHNN--Auto-assoicate Hierarchical Neural Network THNN--Treetyped Hierarchical Neural Network

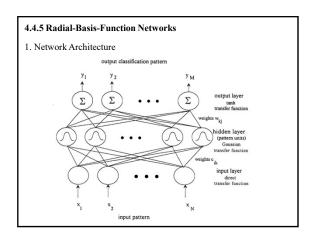


# Definition:

A recurrent network combines the feedback and feedforward connections of neural networks. It is simply a neural network with loops connecting the output responses to the input layer.

# Applications:

The recurrent network provides a modeling technique that can be used for process optimization and adaptive process control of time-dependent processes.



(1) Input Layer

The output of the node equals the input.

(2) Hidden Layer

Its nodes satisfy the unique property of being radially symmetric.

- (a) A center vector c<sub>k</sub> in the input space, made up of cluster center, with elements c<sub>ik</sub>(i=1 to N). The vector is typically stored as the weight factors from the input layer to the hidden layer.
- (b) A distance measure to determine how far an input vector  $\mathbf{x}$ , with elements  $\mathbf{x}_i$  (i=1 to N), is from the center vector  $\mathbf{c}_k$ . We use the standard Euclidean distance measure between  $\mathbf{x}$  and  $\mathbf{c}_k$  to define a Euclidean summation,  $I_k$ (k=1 to L), where L is the number of nodes in hidden layer.

$$I_k = ||x - c_k|| = \sqrt{\sum_{i=1}^{N} (x_i - c_{ik})^2}$$

(c) A transfer function which transforms the Euclidean summation  $I_k$  (k=1 to L) to give an output for each node.

$$v_k = e^{\frac{\left\|x - c_k\right\|^2}{2\sigma_k^2}}$$

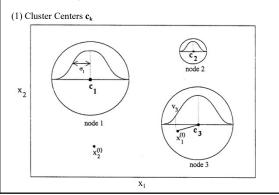
Where Sigma  $\boldsymbol{\sigma}_k$  is a width of the Gaussian function

(3) Output Layer

There are weight factors  $w_{kj}$  (k=1 to L; j=1 to M) between the  $k^{th}$  node in the hidden layer and the  $j^{th}$  node in the output layer.

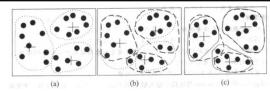
$$y_j = \sum_{k=1}^{L} w_{kj} v_k \qquad j = 1 \quad to \quad M$$

2. Network Development



Using K-means clustering algorithm

- We start by assuming an initial set of L cluster centers, i.e.,center vector c<sub>k</sub>, which corresponds to the L nodes in the hidden layer.
- The elements,  $c_{ik}$  (i=1 to N; k=1 to L) of  $c_k$  are stored as the weight factors between the input and hidden layers.
- Assume that there are T training examples available to the input layer with N nodes, and represent them by training vectors x<sup>(t)</sup> with x<sub>i</sub><sup>(t)</sup> (i=1 to N; t=1 to T).
- The adaptive K-means clustering algorithm then iteratively finds a desirable set of L center vectors c<sub>k</sub> that will minimize the sum of the squares of the distance between T training vectors x<sup>(t)</sup> and their nearest L centers c<sub>k</sub>(k=1 to L).



Example of K-means clustering algorithm

- a. We arbitrily choose three objects as the three initial cluster centers, where clusters are marked by a "+". Each object is distributed to a cluster based on the cluster center to which it is the nearest.
- b. The mean value of each cluster is recalculated based on the objects in the cluster. Relative to these new centers, objects are redistributed to the cluster domains based on which cluster center is the nearest.
- c. This process iterate, leading to Figure @. Eventually, no redistribution of the objects in any cluster occurs and so the process terminates.

(a) Initialization step

 Assume a set of cluster centers, c<sub>k</sub>, for the L nodes in the hidden layer, with the elements c<sub>k</sub> (i=1 to N; k=1 to L) stored as the weight factors between the input and hidden layers.

(b) Iterative Steps:

- Read the next training vector x<sup>(t)</sup> with elements x<sub>i</sub><sup>(t)</sup> (i=1 to N) into the input layer as t increases from 1 to T.
- Modify only the cluster center  $c_k$  (k=1 to L) closest to the training vector  $\mathbf{x}^{(t)}$  in the Euclidean distance:

$$c_k^{(new)} = c_k^{(old)} + \alpha(x^{(t)} - c_k^{(old)})$$

where  $\alpha$  is a learning rate which decreases as t increases from 1 to T.

• Continue this process for a fixed number of iterations.

(2) Gaussian Function, Sigma  $\sigma_k$ 

Using P-nearest neighboring heuristic.

- consider a given center vector  $\mathbf{c}_{\mathbf{k}}$  (k=1 to L)
- assume that  $c_{k1},\,c_{k2},\,\ldots,\,c_{kp}(1{\le}k_1,\,k_2\,,\ldots\,k_p\,{\le}L)$  are the P nearest neighboring centers.

$$\sigma_{\boldsymbol{k}} = \sqrt{\frac{1}{P} \sum_{p=1}^{P} \left\| \boldsymbol{c}_{\boldsymbol{k}} - \boldsymbol{c}_{\boldsymbol{k} p} \right\|^2}$$

(3) The resulting output from the  $k^{\text{th}}$  node in the hidden layer,  $\boldsymbol{v}_k,$  is:

$$v_k = e^{-\frac{\left\|x - c_k\right\|^2}{2\sigma_k^2}}$$

$$y_{j} = \sum_{k} w_{kj} v_{k} - T_{j}$$

$$y_{j} = f(\sum_{k} w_{kj} v_{k} - T_{j})$$

Using BP algorithm: 
$$w_{kj}(t+1) = w_{kj}(t) + \beta(y_j^d - y_j)v_k$$

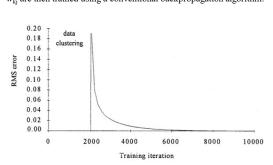
(5) Network training

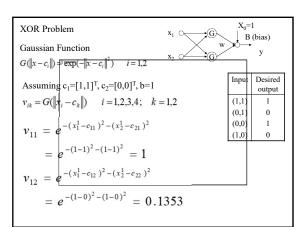
First, do not use any desired output to train the input connects to the hidden layer.

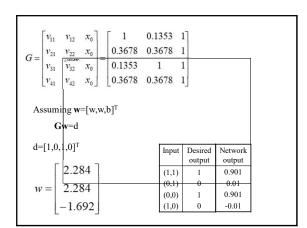
 $\boldsymbol{Second},$  for any given training example expressed by the  $t^{th}$ training vector  $\mathbf{x}^{(t)}$  with elements  $\mathbf{x}_{i}^{(t)}$  (i=1 to N), we iteratively modify only one cluster center  $c_k$  (k=1,2,..., or L) closest to the  $t^{th}$  training vector  $\mathbf{x}^{(t)}$  in the Euclidean distance.

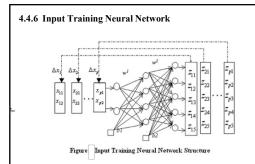
Over this same time period, no training of the weight factors,  $\boldsymbol{w}_{kj}$  , from hidden layer to output layer, occurs. We call this initial period the data-clustering phase.

For example, after the  $2000^{th}$  iteration, the weight factors,  $c_{ik}$ , are fixed for the remainder of the training procedure. The weight factors wki are then trained using a conventional backpropagation algorithm.









Let:  $t_{pk}$  is the value of the kth observed variable in the pth sample,  $z_{pk}$  is the corresponding output of IT-NN.

The aim of training IT-NN is

to minimize the following objective function:

$$\min E(X, W) = \min \sum_{p} \sum_{k} (Z_{pk} - t_{pk})^2$$

The steepest descent direction for optimizing network inputs  $\Delta X_{pi}$   $\Delta X_{pi} = -\frac{\partial E}{\partial X_{pi}} = \sum_k (t_{pk} - Z_{pk}) \frac{\partial Z_{pk}}{\partial X_{pi}}$ 

$$\Delta X_{pi} = -\frac{\partial E}{\partial X_{pi}} = \sum_{k} (t_{pk} - Z_{pk}) \frac{\partial Z_{pk}}{\partial X_{pi}}$$

The steepest descent direction for optimizing network weights  $\Delta W_{ji}$  is  $\Delta W_{ji} = -\frac{\partial E}{\partial W} = \sum_k (t_{pk} - Z_{pk}) \frac{\partial Z_{pk}}{\partial W_{ji}}$ 

$$\Delta W_{ji} = -\frac{\partial E}{\partial W} = \sum_{i} (t_{pk} - Z_{pk}) \frac{\partial Z_{pk}}{\partial W}$$

The network output is given by
$$Z_{pk} = \sigma(f_k + \sum_j w_{kj}^2 \sigma(b_j + \sum_j w_{ji}^1 X_{pi}))$$

where  $\sigma(.)$  is sigmoidal function,

 $b_j$ ,  $f_k$  are the bias of the *j*th hidden node and kth output node,  $w_{kj}$ ,  $w_{ji}$  are the weights of IT-NN.

The steepest descent direction for training network is

$$\Delta X_{pi} = \sum_{j} w_{ji}^{1} \delta_{pj}$$

where  $\,\delta_{pj} is$  the propagated error at the hidden layer.

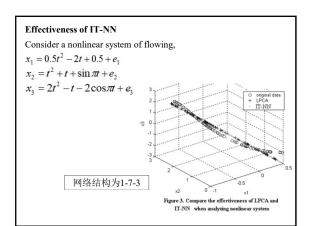
$$\delta_{pj} = \sigma'(b_j + \sum_i w_{ji}^1 X_{pi})$$

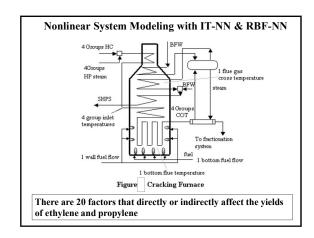
$$\delta_{pj} = \sigma'(b_{j} + \sum_{i} w_{ji}^{1} X_{pi}) \bullet$$

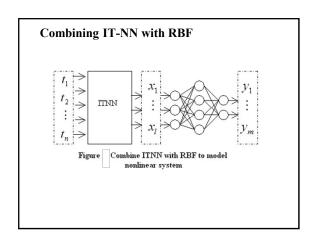
$$\sum_{k} w_{kj}^{2} (t_{pk} - Z_{pk}) \sigma'[f_{k} + \sum_{j} w_{kj}^{2} \sigma(\sum_{i} w_{ji}^{1} X_{pi})]$$

Weight adjusting is given by

$$\Delta w_{ji} = \sum_{p} X_{pi} \delta_{pj}$$

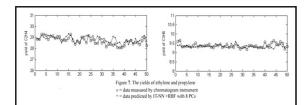




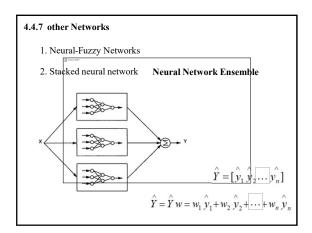


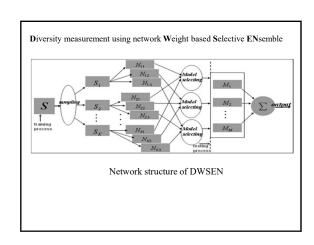
Num. Of Input nodes	10	9	8	7	6	5
e <sub>max</sub> (%)	2.1432	3.4599	2.7845	3.6290	4.3221	5.8745
e <sub>min</sub> (%)	0.0007	0.0030	0.0051	0.0033	0.0065	0.0103
e <sub>mse</sub> (%)	0.0923	0.1065	0.1565	0.1903	0.5329	1.3785

Num. of	Num. of nonlinear PCs		10	9	8	7	6	5
Training period C <sub>3</sub> H <sub>6</sub>		$e_{max}$	0.1055	0.1771	0.1730	0.2036	0.7814	0.9631
	$\mathrm{C_2H_4}$	$e_{min}$	0.0000	0.0001	0.0007	0.0010	0.0105	0.0489
		$e_{mse}$	0.0106	0.0130	0.0144	0.0555	0.1001	0.3901
		$e_{max}$	0.2373	0.3672	0.3829	0.6300	0.8100	1.485
	$C_3H_6$	$e_{min}$	0.0002	0.0001	0.0005	0.0023	0.0090	0.1068
		$e_{mse}$	0.0835	0.0902	0.0995	0.1300	0.1689	0.2155
		$e_{max}$	2.7501	2.2456	2.3780	2.4998	2.7599	5.1613
	$\mathrm{C_2H_4}$	$e_{min}$	0.0095	0.0092	0.0089	0.0104	0.0196	0.1079
Predicting period		$e_{mse}$	0.5933	0.6318	0.6770	0.8317	0.8965	1.4086
periou		$e_{max}$	3.0477	3.7034	3.9861	4.1960	4.3435	6.7936
	$C_3H_6$	$e_{min}$	0.0104	0.0108	0.0153	0.0230	0.0267	0.023
		$e_{mse}$	0.6053	0.6539	0.6900	0.90	1.09	1.7540



We can see that the IT-NN with 8 nonlinear PCs will be the best choice. Fewer PCs (7, 6 and 5) cause information lost, and more PCs (10 and 9) increase the input nodes of RBF.





# Weight Vector

$$\vec{D}_i = (w_{i1}, w_{i2}, ..., w_{iH})$$
 All weights in the ith network

Distance between Ni and Nj:

$$d\left(N_{i},N_{j}\right)=d(\overrightarrow{D}_{i},\overrightarrow{D}_{j})=\left\|\overrightarrow{D}_{i}-\overrightarrow{D}_{j}\right\|_{2}=\overline{\sum_{h=1}^{H}\left(w_{ih}-w_{jh}\right)^{2}}$$

### Weight Matrix

$$\begin{bmatrix} \overrightarrow{D}_1 \\ \overrightarrow{D}_2 \\ \vdots \\ \overrightarrow{D}_{m-1} \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \dots & w_{1H} \\ w_{21} & w_{22} & \dots & w_{2H} \\ \vdots & \vdots & \ddots & \vdots \\ w_{N1} & w_{N2} & \dots & w_{NH} \end{bmatrix}_{N*H}$$

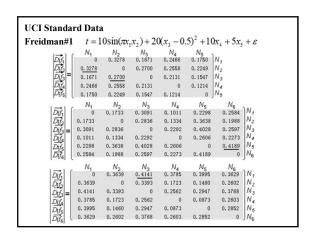
## Definition of the diversity

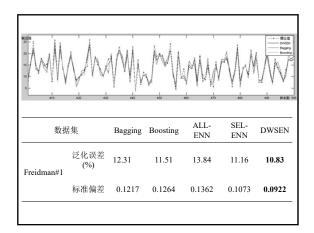
$$c = dif\left(N_{i}, N_{j}\right) = dif\left(\overrightarrow{D}_{i}, \overrightarrow{D}_{j}\right) = \frac{\left\|\overrightarrow{D}_{i} - \overrightarrow{D}_{j}\right\|_{2}}{\left\|\overrightarrow{D}_{i}\right\|_{2} + \left\|\overrightarrow{D}_{j}\right\|_{2}}$$

$$(0 \le c \le 1)$$

# **Diversity Matrix**

$$\begin{bmatrix} \overrightarrow{dif_1} \\ \overrightarrow{dif_2} \\ \vdots \\ \overrightarrow{dif_N} \end{bmatrix} = \begin{bmatrix} 0 & dif(N_1, N_2) & \dots & dif(N_1, N_N) \\ dif(N_2, N_1) & 0 & \dots & \dots \\ \vdots \\ \vdots \\ dif(N_N, N_1) & \dots & \dots & 0 \\ \end{bmatrix}_{N^2N}$$





### 4.5 Applications

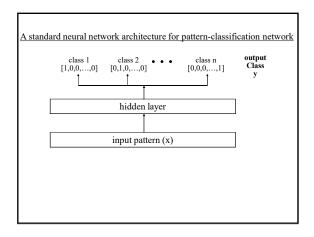
### 4.5.1 Classification

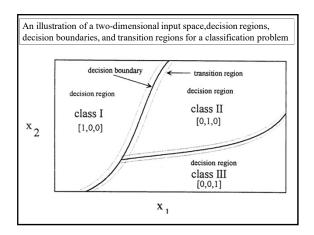
Two major areas:

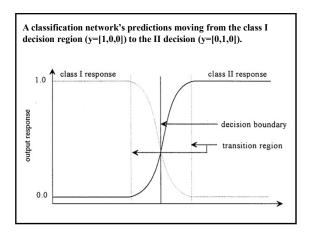
- (1) Identification of process faults based on the operating conditions of given process
- (2) Prediction of the most likely categorical group for a given input pattern

Two basic types of pattern classifiers:

Parametric and nonparametric

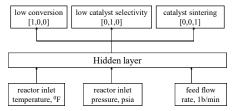




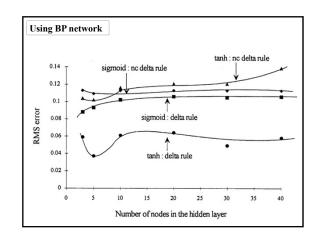


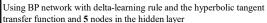
The two most commonly used network architectures for classification problems are the BP network and the RBF network.

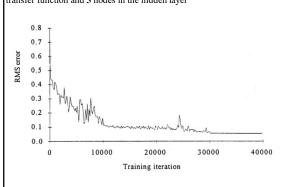
Illustrative example of fault diagnosis of a chemical reactor

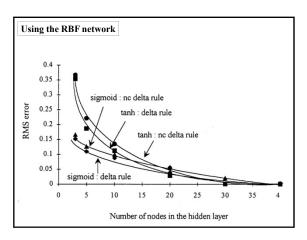


Next, we use a example to compare the BP network with the RBF network. In addition, we compare different transfer functions(e.g. sigmoid and hyperbolic tangent) and network training rules(e.g., delta rule and normalized cumulative delta rule, nc-delta).









### Comparison of the BP network and RBF network

- (1) RBF networks perform better than BP networks for classification problems
- (2) The RBF network's RMS error approaches 0 as the number of nodes increases, while the BP network has a much larger RMS error of 0.037.
- (3) BP network has a much more compact system representation than the RBF network, and has significantly lower RMS error for smaller networks(e.g. less than 5 nodes).
- (4) The RBF network also trains faster requiring only 7000 iterations, versus 30000 for the BP network.

# 4.5.2 Data compression

Using four simulated cell-growth curves spanning the entire range of possible cell-growth profiles, having maximum normalized cell concentrations of 0.2, 0.4, 0.6, and 0.8, respectively.

