Artificial Neural Networks

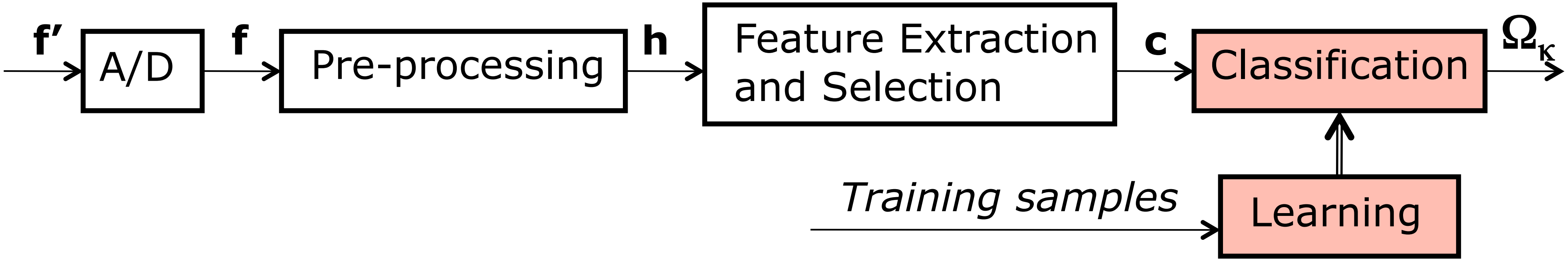
Radial Basis Function Networks

Dr. Elli Angelopoulou

Lehrstuhl für Mustererkennung (Informatik 5)

Friedrich-Alexander-Universität Erlangen-Nürnberg

Pattern Recognition Pipeline



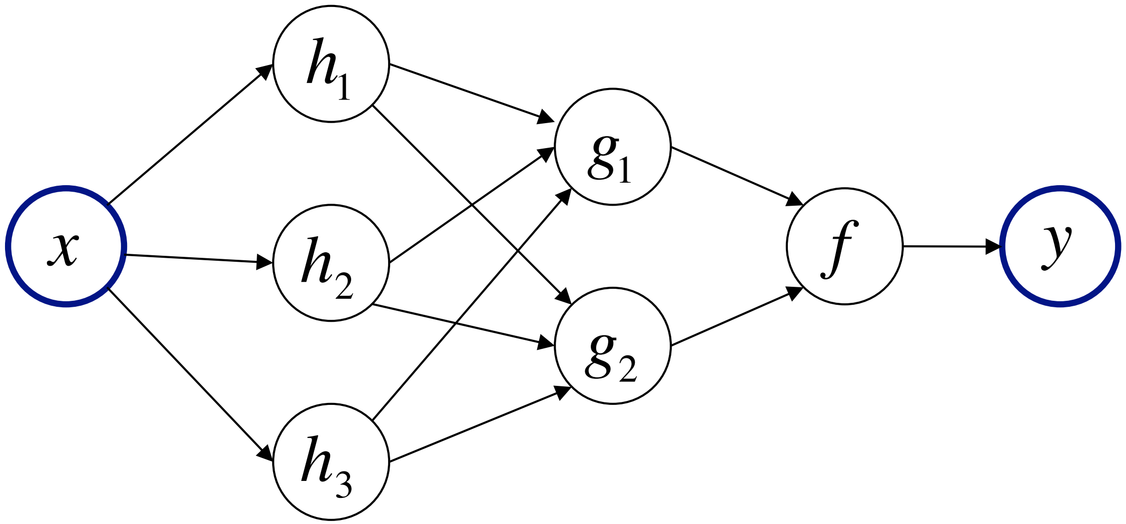
- Classification
  - Statistical classifiers
    - Bayesian classifier
    - Gaussian classifier
  - Polynomial classifiers
  - Non-Parametric classifiers
    - k-Nearest-Neighbor density estimation
    - Parzen windows
    - Artificial neural networks

Artificial Neural Network (ANN)

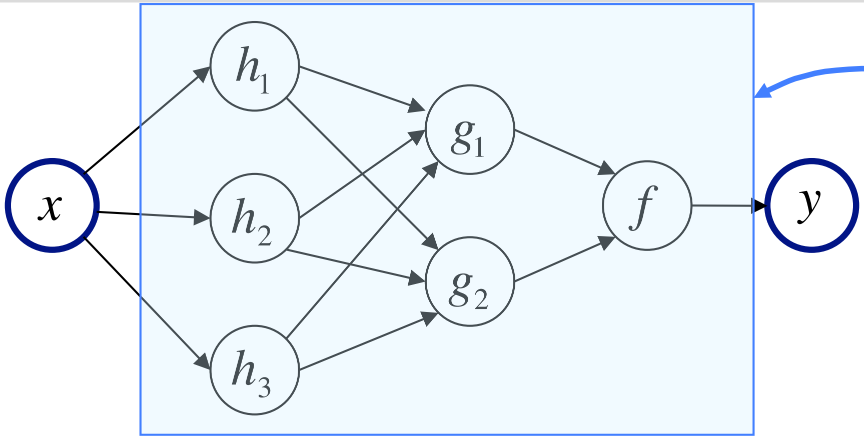
- There is no precise agreed definition among researchers as to what is an artificial neural network.
- Most would agree that it involves a network of simple processing elements (neurons), which can exhibit complex global behavior, determined by
  - the connections between the processing elements and
  - the element parameters.
- In a neural network model, simple nodes (*neurons*, or *processing elements* or *units*) are connected together to form a network of nodes.

ANN Operation

- In general an ANN operates as a function $f : x \rightarrow y$.
- The "network" arises because the function $f(x)$ is defined as a composition of other functions $g_i(x)$, which can further be defined as a composition of other functions, e.g. $h_j(x)$.



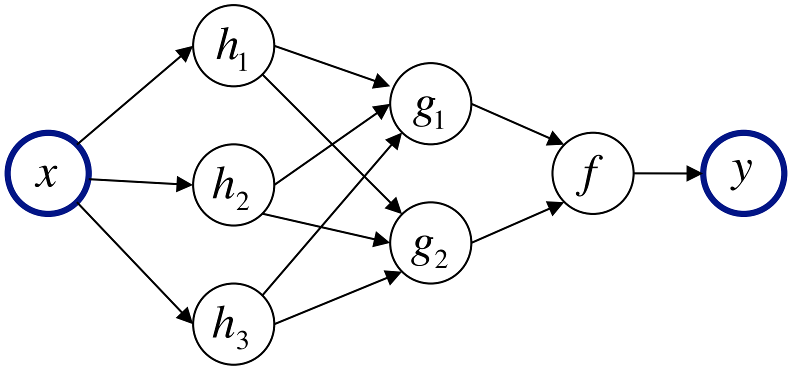
General Form of ANN



Sometimes the network is abstracted as an ANN black box.

- There is great variation in ANNs, depending on:
  - The number of layers
  - Whether there are hidden layers or not
  - The connectivity (We could have feedback loops.)
  - The adaptability
- An ANN does not have to be adaptive. In practice, part of their strength comes from adapting, changing the weights of the connections in order to produce a desired signal flow.

Mathematical Description of an ANN



- A widely used type of composition is the nonlinear weighted sum:

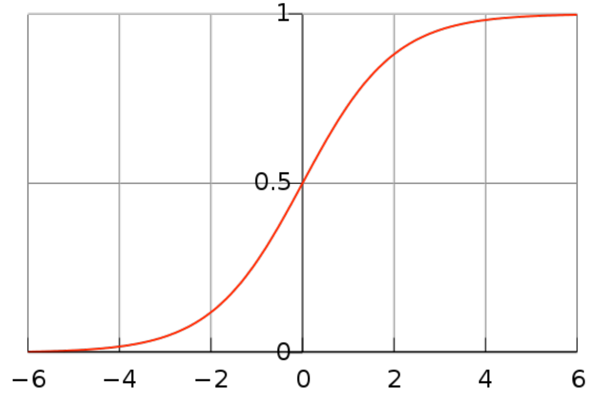
$$f(x) = \phi\left(\sum_i w_i g_i(x)\right)$$

  where ϕ is a predefined function that forces the output of a neuron to be in a certain range, typically [0,1] or [-1,1].
- ϕ is often referred to as an activation function.

Activation Function

- An activation function tries to mimic the firing of the neuron if the incoming signal is sufficiently strong.
- Mathematically, this is usually achieved with a sigmoid function, e.g.:

$$\phi(t) = \frac{1}{1+e^{-t}}$$



- Sigmoid functions have the following characteristic properties:
  - They are differentiable
  - They have 1 inflection point
  - They have a pair of horizontal asymptotes
- Another typical sigmoid function employed in ANNs is the hyperbolic tangent, $\phi(t) = \tanh(t)$.

ANN and Classification

- The ANNs that we will examine are used in computing discriminant functions.
- Recall that, a discriminant function for class Ω_κ is a polynomial that evaluates to 1 if the feature vector belongs to that class. Otherwise it evaluates to zero.

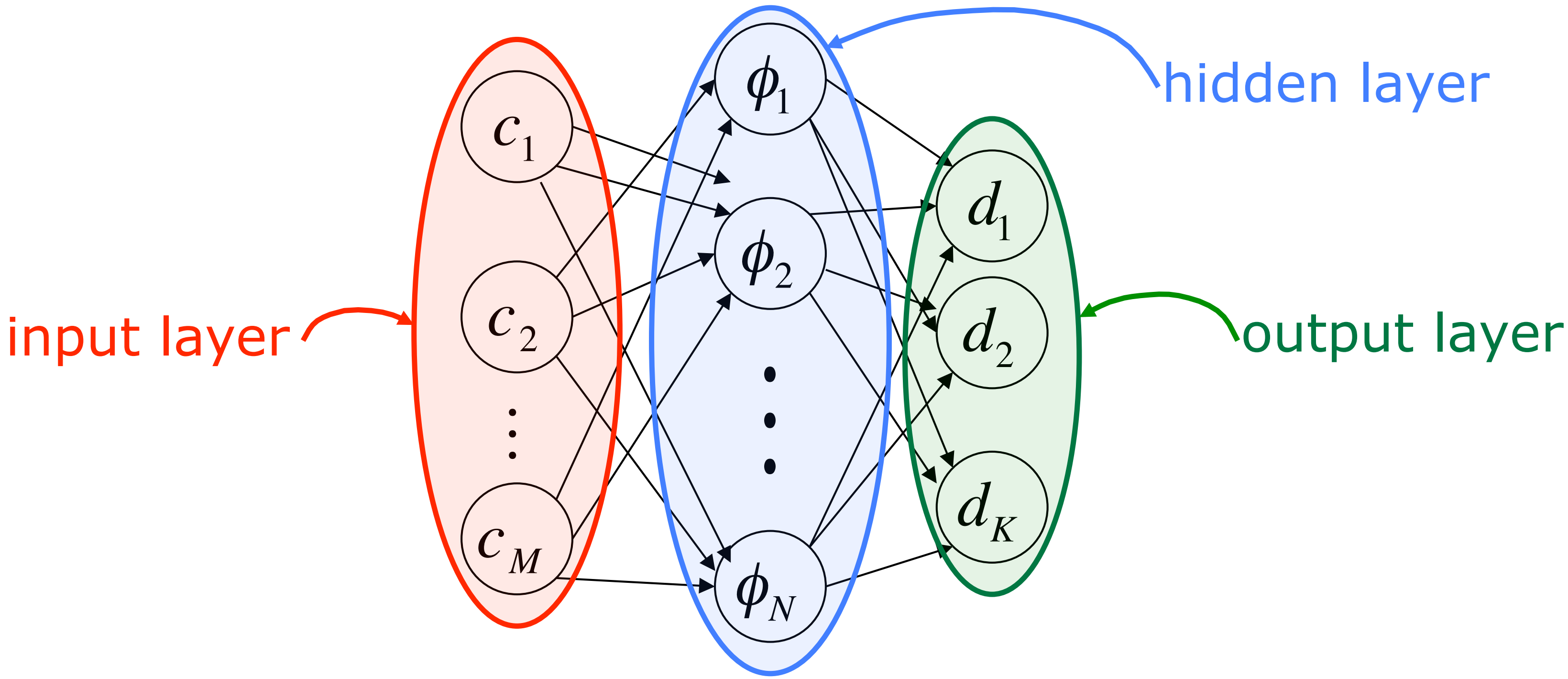
$$d_\kappa(\vec{c}) = \begin{cases} 1 & \text{if } \vec{c} \in \Omega_\kappa \\ 0 & \text{otherwise} \end{cases}$$

- The input of such an ANN is a feature vector $\vec{c}$ and the output is a discriminant vector, $\vec{d} = (d_1, d_2, \ldots, d_K)$.

$$\vec{c} \longrightarrow \boxed{\text{ANN}} \longrightarrow \vec{d}$$

Radial Basis Function ANNs

- Radial Basis Function (RBF) networks use Radial Basis Functions as their activation function.
- An RBF network is a feed-forward 3 layer network:
  - input layer, $\vec{c}$ in our case
  - a hidden layer, where each node ϕ_i is a separate RBF
  - an output layer, which is a weighted sum of the hidden layers.



Radial Basis Functions

- Radial basis functions were first used in 1987 by Powell.
- He introduced RBFs as a means of mapping an input vector to an output vector.
- A radial basis function (RBF) is a real-valued function whose value depends only on the distance from the origin, so that

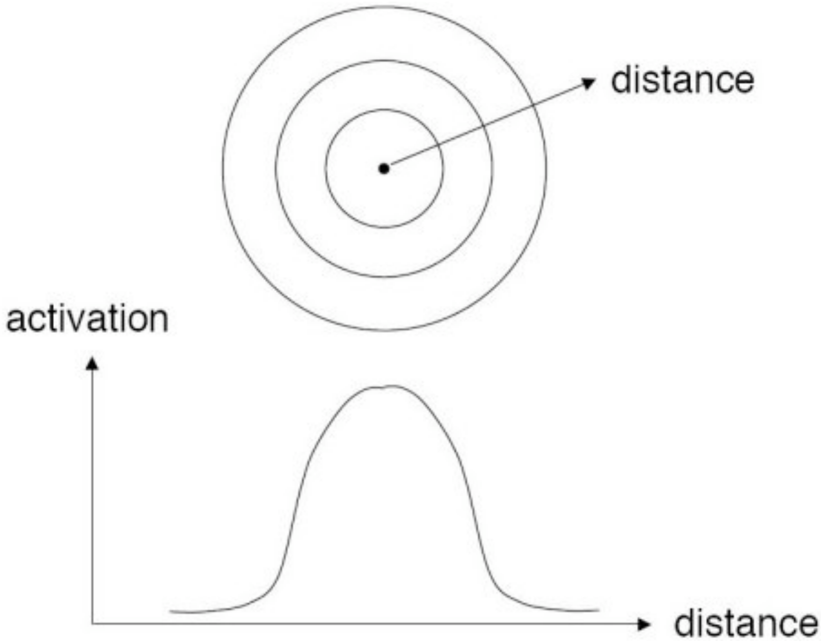
$$\phi(\vec{x}) = \phi(\|\vec{x}\|)$$

- Alternatively, the RBF can be based on the distance from some other point $\vec{q}$, called a center:

$$\phi(\vec{x},\vec{q}) = \phi(\|\vec{x} - \vec{q}\|)$$

Radial Basis Functions - continued

- So RBFs are a type of distance function.
- As a distance function, RBFs have the key characteristic that response decreases monotonically with distance from a central point.
- Its response radially decreases.



Different RBFs

- Any distance function that decreases radially can be considered a radial basis function. Some commonly used RBFs are:
- Two different forms of Gaussians:

$$\phi(\|\vec{x}-\vec{q}\|) = e^{-\frac{(\|\vec{x}-\vec{q}\|)^2}{\sigma^2}} \qquad \phi(\|\vec{x}-\vec{q}\|) = \frac{1}{\sqrt{2\pi\Sigma}} e^{-\frac{1}{2}(\|\vec{x}-\vec{q}\|)^T \Sigma^{-1}(\|\vec{x}-\vec{q}\|)}$$

- Multiquadric:

$$\phi(\|\vec{x}-\vec{q}\|) = \sqrt{r^2 + \|\vec{x}-\vec{q}\|^2} \Big/ r^2$$

- Spline (a.k.a Logarithmic):

$$\phi(\|\vec{x}-\vec{q}\|) = \|\vec{x}-\vec{q}\|^2 \log\left(\|\vec{x}-\vec{q}\|\right)$$

RBF and Classification

- Within the context of classification, RBFs work as follows.
- We are given a set of *N* training samples $\vec{c}_1, \vec{c}_2, \ldots, \vec{c}_N$ and we want to find the best discriminant functions.
- One radial basis function (RBF) approach is to use a set of *N* basis functions, each centered around one of the training samples, i.e. $\vec{q}_i = \vec{c}_i$.
- Given a new feature vector $\vec{c}$ we use RBFs to compute how far away it is from each of the training samples.

$$\phi(\vec{c} - \vec{c}_i) = \phi_i(\vec{c})$$

RBF and Classification – continued

- The discriminant function is then treated as a linear combination of these radial basis functions.

$$d_\kappa(\vec{c}) = \sum_{i=1}^{N} w_i \phi(\|\vec{c} - \vec{c}_i\|) = \sum_{i=1}^{N} w_i \phi_i(\vec{c})$$

- In this type of RBFs training corresponds to the estimation of the weights w_i from the training data.
- In more detail, recall that each $d_\kappa(\vec{c})$ is a binary function. Thus the training set has the form:

$$T = \left\{ \left(\vec{c}_l, d_{\kappa(l)}(\vec{c}_l) \right), l = 1, 2, \ldots, N \right\}$$

where $d_{\kappa(l)}(\vec{c})$ is the discriminant function of the class $\Omega_{\kappa(l)}$ to which the sample $\vec{c}_l$ belongs.

RBFN Training

- So for each training pair $\left(\vec{c}_l, d_{\kappa(l)}(\vec{c}_l)\right)$ we have:

$$d_{\kappa(l)}(\vec{c}_l) = \sum_{i=1}^{N} w_i \phi(\|\vec{c}_l - \vec{c}_i\|)$$

- This can be written as a vector product:

$$d_{\kappa(l)}(\vec{c}_l) = \left(w_1, w_2, \ldots, w_N\right) \begin{bmatrix} \phi(\|\vec{c}_l - \vec{c}_1\|) \\ \phi(\|\vec{c}_l - \vec{c}_2\|) \\ \vdots \\ \phi(\|\vec{c}_l - \vec{c}_N\|) \end{bmatrix}$$

$$d_{\kappa(l)}(\vec{c}_l) = \left(\phi(\|\vec{c}_l - \vec{c}_1\|), \phi(\|\vec{c}_l - \vec{c}_2\|), \ldots, \phi(\|\vec{c}_l - \vec{c}_N\|)\right) \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix}$$

RBFN Training - continued

- Since there are *N* samples in my training set, I have *N* such equations.

$$d_{\kappa(1)}(\vec{c}_1) = \left(\phi(\|\vec{c}_1 - \vec{c}_1\|), \phi(\|\vec{c}_1 - \vec{c}_2\|), \ldots, \phi(\|\vec{c}_1 - \vec{c}_N\|)\right) \vec{w}$$

$$d_{\kappa(2)}(\vec{c}_2) = \left(\phi(\|\vec{c}_2 - \vec{c}_1\|), \phi(\|\vec{c}_2 - \vec{c}_2\|), \ldots, \phi(\|\vec{c}_2 - \vec{c}_N\|)\right) \vec{w}$$

$$\vdots$$

$$d_{\kappa(N)}(\vec{c}_N) = \left(\phi(\|\vec{c}_N - \vec{c}_1\|), \phi(\|\vec{c}_N - \vec{c}_2\|), \ldots, \phi(\|\vec{c}_N - \vec{c}_N\|)\right) \vec{w}$$

which can be written more compactly as:

$$\vec{d}' = \Phi \, \vec{w}$$

$$\Rightarrow \vec{w} = \Phi^{+} \vec{d}'$$

Important Comment on RBFN Training

- If we have many feature vectors in our training data and we have an RBF estimate for each individual training sample we end up with too many RBFs, too many nodes => Slow training and **Overfitting!!**

- Solution: Use centers of clusters of feature vectors for the RBFs, instead of the individual feature vectors.

- Each RBF is now centered around $\vec{\mu}_j,\ j = 1,2,\ldots,s$ instead of $\vec{c}_i,\ i = 1,2,\ldots,N$:

$$\phi(\vec{c} - \vec{\mu}_j) = \phi_j(\vec{c})$$

Updated Training of RBFNs

- 2-stage process:

1. Unsupervised selection of RBF centers $\vec{\mu}_j$

   K-means:

   pick *s* $\vec{\mu}_j$ values at random.

   Assign each training sample to its nearest $\vec{\mu}_j$.
   Recompute $\vec{\mu}_j$ as the mean value of the samples of cluster *j*.

   Repeat this process until the $\vec{\mu}_j$s are stabilized.

   If using a Gaussian RBF, use MLE to compute Σ_j

2. The estimation of $\vec{w}$ can be done as before via linear algebra methods (e.g. SVD)

Weaknesses of the 2-stage Approach

- The estimation of $\vec{\mu}_j$ and Σ_j is not guided by the discriminant function that is used to compute $\vec{w}$.
- Hence we have a non-symmetric approach.
- Stage 2 relies on the results of Stage 1.
- Thus, we have a propagation of estimation errors which often means an amplification of errors.
- Better solution: use an integrated, fully supervised approach like the Orthogonal Least Squares approach.

RBFN Training via Orthogonal Least Squares

- Main idea of OLS: Do not cluster as a preprocessing step.
- Rather do a sequential selection of the centers $\vec{\mu}_j$ which leads to the largest reduction in the sum of squared errors.
- Which sum of squared error (SSD)?
- The difference between the computed and the expected result (value) of the discriminant functions:

$$SSD = \sum_{i=1}^{N} \left(\hat{\vec{d}}_i - \vec{d}_i \right)$$

Orthogonal Least Squares Algorithm

1. Start with *N* pairs $\left(\vec{c}_l, d_{\kappa(l)}(\vec{c}_l)\right)$ and *s*=0
3. For each training pair *i* of the n=N-s features vectors

   2a. Add the current feature $\vec{c}_i$ to the *s* centers

   The new vector becomes an additional $\vec{\mu}_j$

   2b. Compute the weights $\vec{w}$

   Use linear algebra as previously described.

   2c. Compute the sum of squared differences, SSD.
3. Out of the n pairs, add the feature vector with the smallest SSD to *s.*
4. s++;

Repeat until all the desired # of clusters is reached.

References

1. The sigmoid function plot is courtesy of Wikipedia http://en.wikipedia.org/wiki/File:Logistic-curve.svg
2. The RBF graph is courtesy of P. Sherrod http://www.dtreg.com/rbf.htm