Data Mining

Lecture Notes for Chapter 4

Artificial Neural Networks

Introduction to Data Mining , 2nd Edition

by

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Artificial Neural Networks (ANN)

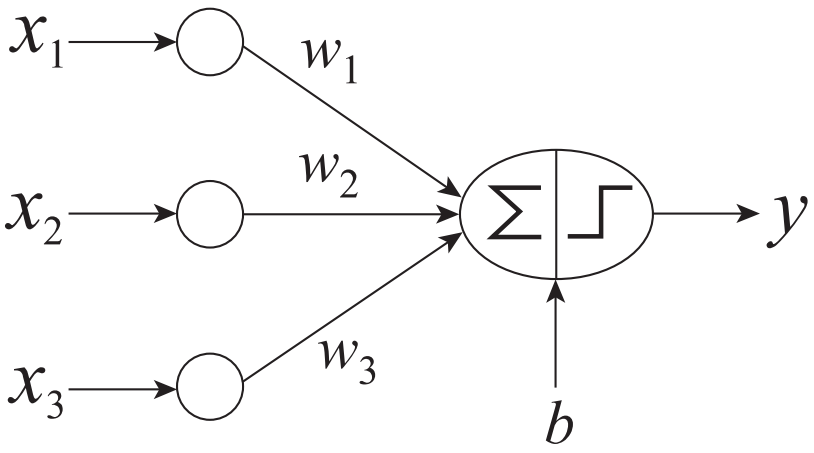
Basic Idea: A complex non-linear function can be learned as a composition of simple processing units

ANN is a collection of simple processing units (nodes) that are connected by directed links (edges)

- Every node receives signals from incoming edges, performs computations, and transmits signals to outgoing edges
- Analogous to *human brain* where nodes are neurons and signals are electrical impulses
- Weight of an edge determines the strength of connection between the nodes

Simplest ANN: **Perceptron** (single neuron)

Basic Architecture of Perceptron



$$y = \begin{cases} 1, & \text{if } \mathbf{w}^T\mathbf{x} + b > 0. \\ -1, & \text{otherwise.} \end{cases}$$

$$\tilde{\mathbf{w}} = (\mathbf{w}^T \ b)^T \qquad \tilde{\mathbf{x}} = (\mathbf{x}^T \ 1)^T$$

$$\hat{y} = sign(\tilde{\mathbf{w}}^T\tilde{\mathbf{x}})$$

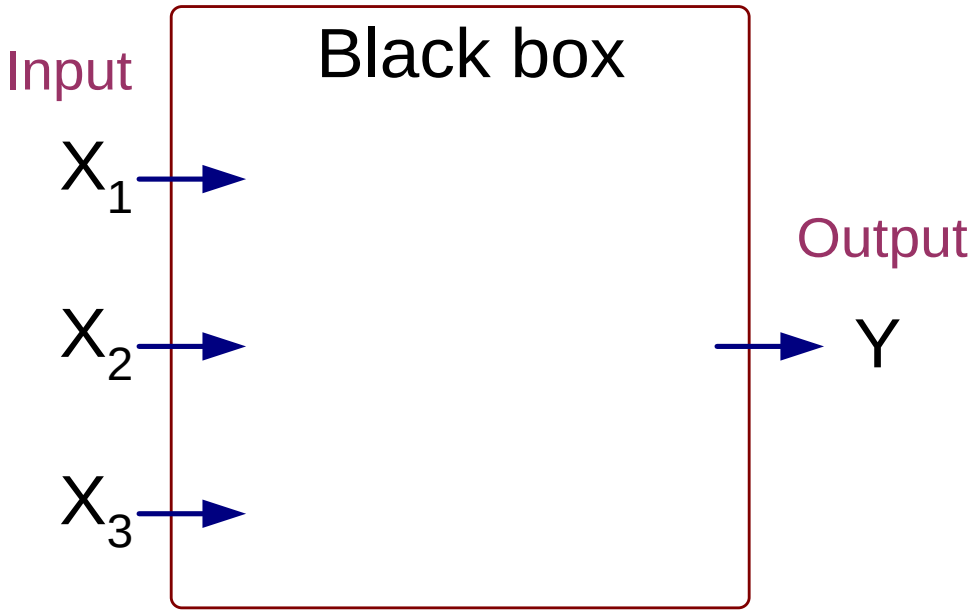
Activation Function

Learns linear decision boundaries

Related to logistic regression (activation function is sign instead of sigmoid)

Perceptron Example

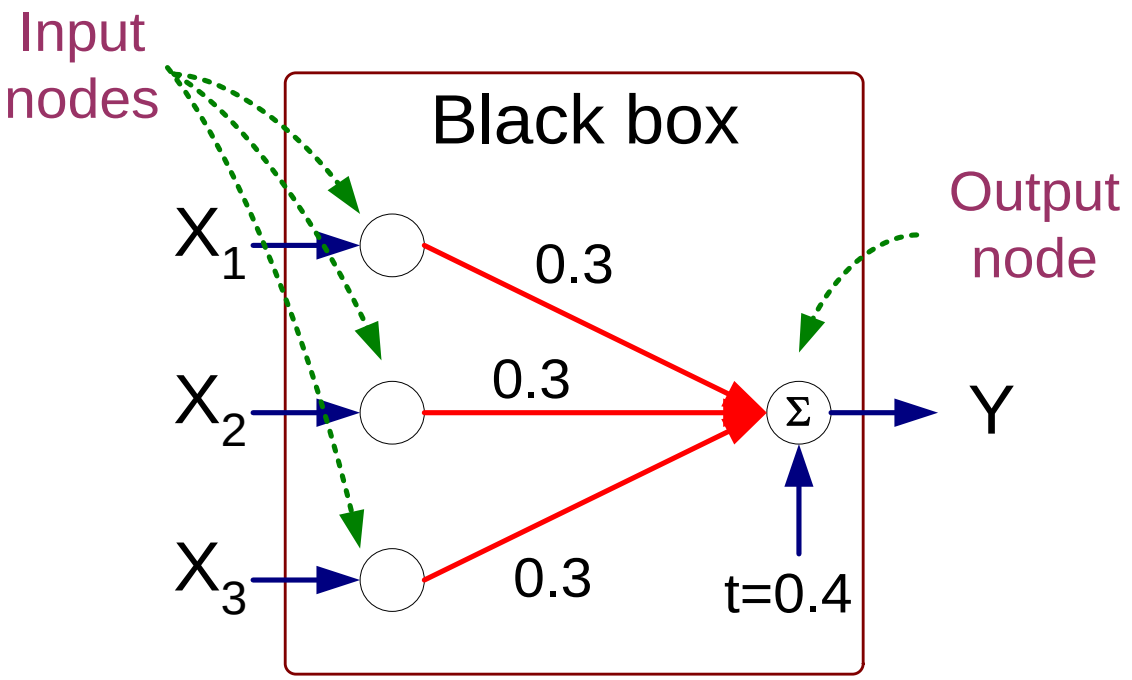
X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1



Output Y is 1 if at least two of the three inputs are equal to 1.

Perceptron Example

X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1



$$Y = sign(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4)$$

$$\text{where } sign(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0 \end{cases}$$

Perceptron Learning Rule

Initialize the weights (w_0, w_1, …, w_d)

Repeat

- For each training example (x_i, y_i)
  - Compute $\hat{y}_i$
  - Update the weights:

$$w_j^{(k+1)} = w_j^{(k)} + \lambda\left(y_i - \hat{y}_i^{(k)}\right)x_{ij}$$

Until stopping condition is met

k: iteration number; λ: learning rate

Perceptron Learning Rule

Weight update formula:

$$w_j^{(k+1)} = w_j^{(k)} + \lambda\left(y_i - \hat{y}_i^{(k)}\right)x_{ij}$$

Intuition:

- Update weight based on error: e = $(y_i - \hat{y}_i)$
  - If y = $\hat{y}$, e=0: no update needed
  - If y > $\hat{y}$, e=2: weight must be increased (assuming Xij is positive) so that $\hat{y}$ will increase
  - If y < $\hat{y}$, e=-2: weight must be decreased (assuming Xij is positive) so that $\hat{y}$ will decrease

Example of Perceptron Learning

$$\lambda = 0.1$$

X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1

	w_0	w_1	w_2	w_3
0	0	0	0	0
1	-0.2	-0.2	0	0
2	0	0	0	0.2
3	0	0	0	0.2
4	0	0	0	0.2
5	-0.2	0	0	0
6	-0.2	0	0	0
7	0	0	0.2	0.2
8	-0.2	0	0.2	0.2

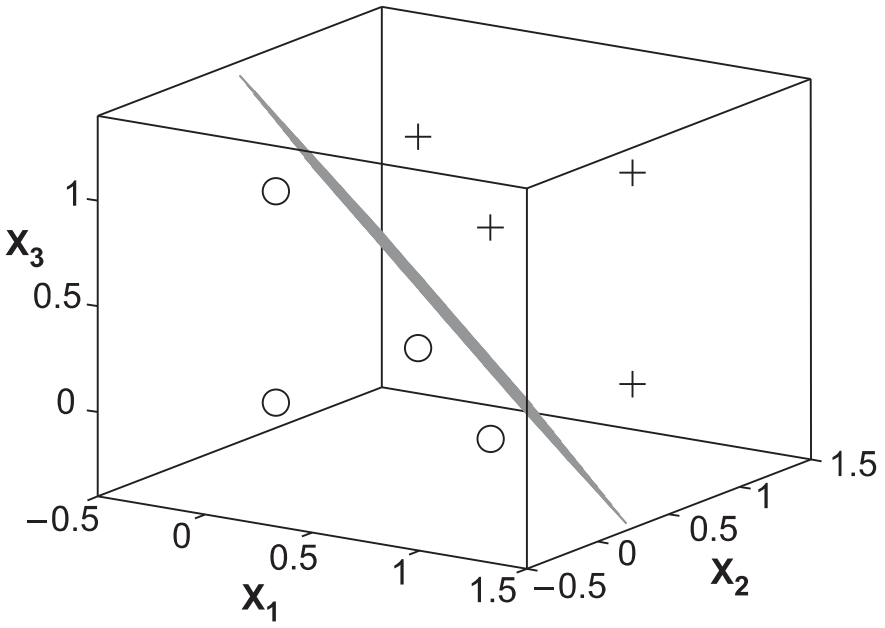
Weight updates over first epoch

Epoch	w_0	w_1	w_2	w_3
0	0	0	0	0
1	-0.2	0	0.2	0.2
2	-0.2	0	0.4	0.2
3	-0.4	0	0.4	0.2
4	-0.4	0.2	0.4	0.4
5	-0.6	0.2	0.4	0.2
6	-0.6	0.4	0.4	0.2

Weight updates over all epochs

Perceptron Learning

Since y is a linear combination of input variables, decision boundary is linear

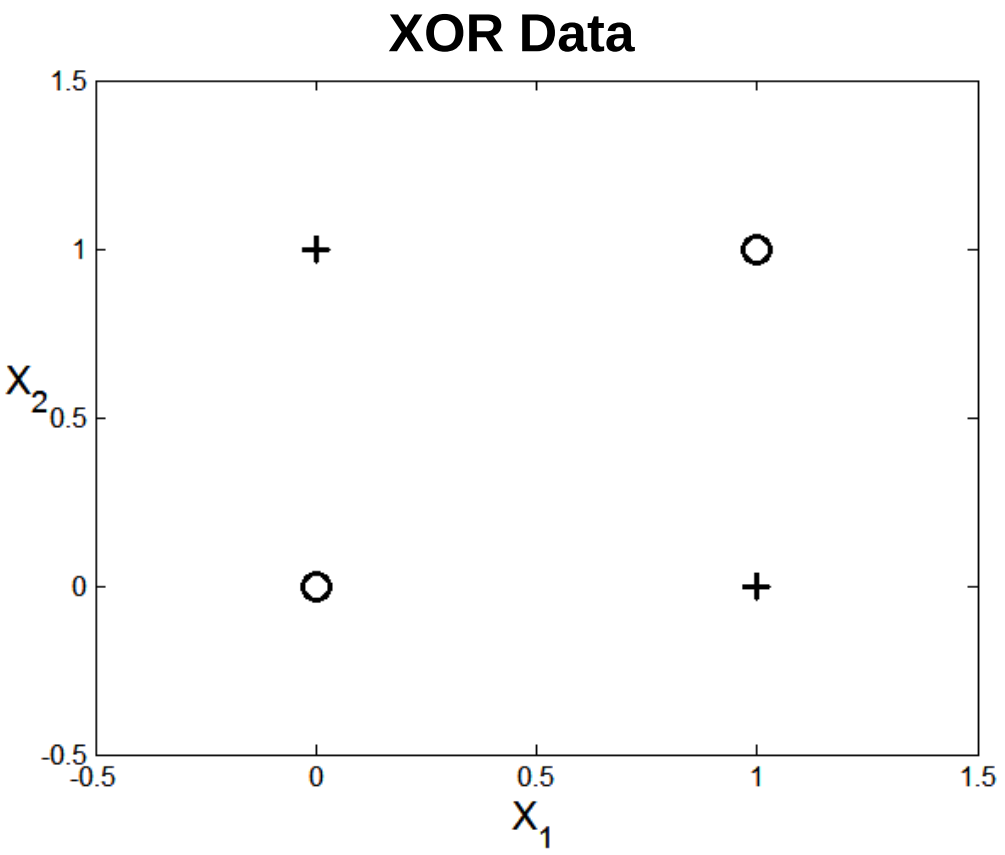


Nonlinearly Separable Data

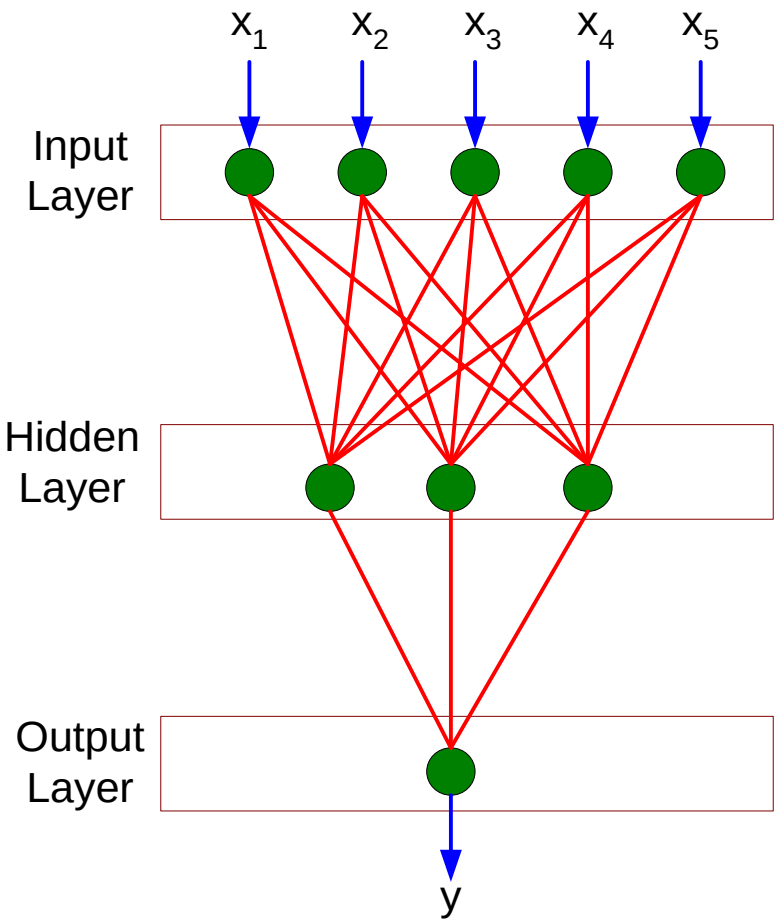
For nonlinearly separable problems, perceptron learning algorithm will fail because no linear hyperplane can separate the data perfectly

$$y = x_1 \oplus x_2$$

x_1	x_2	y
0	0	-1
1	0	1
0	1	1
1	1	-1



Multi-layer Neural Network



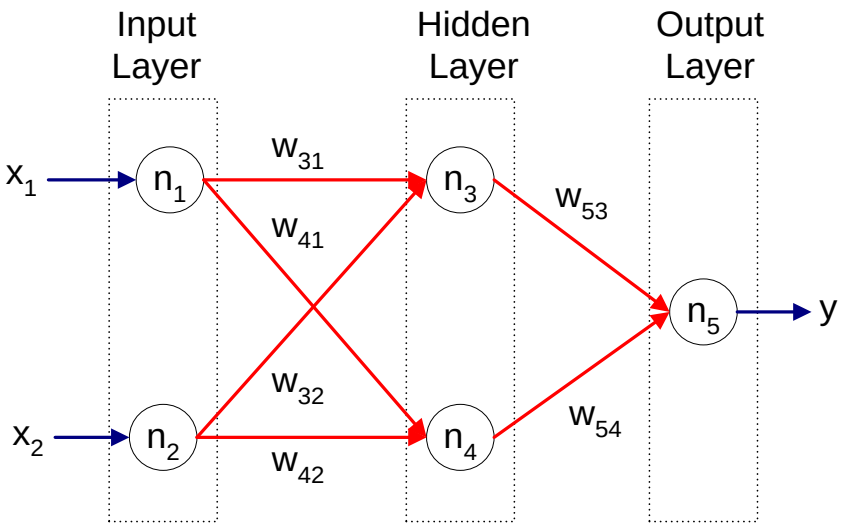
More than one *hidden layer* of computing nodes

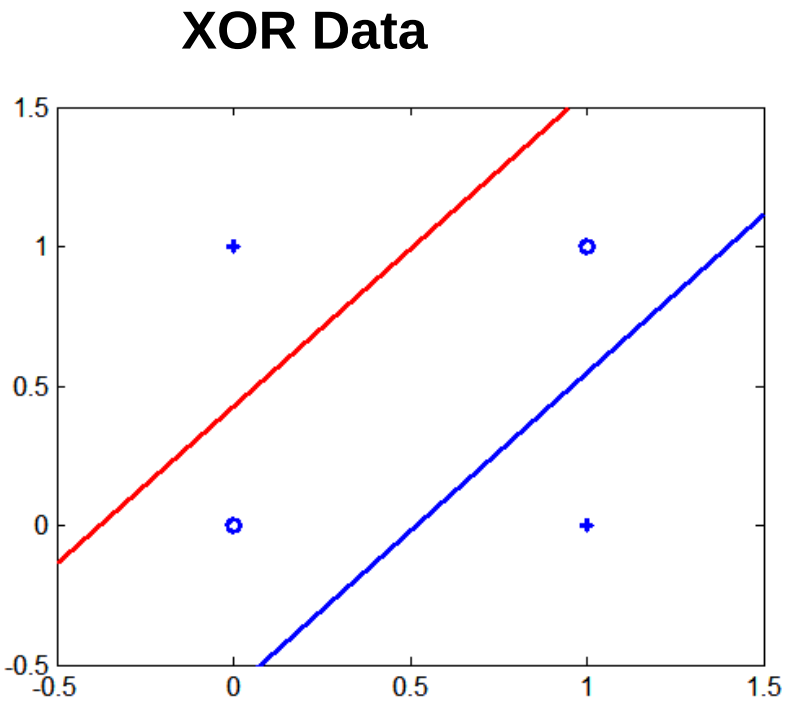
Every node in a hidden layer operates on activations from preceding layer and transmits activations forward to nodes of next layer

Also referred to as "feedforward neural networks"

Multi-layer Neural Network

Multi-layer neural networks with at least one hidden layer can solve any type of classification task involving nonlinear decision surfaces



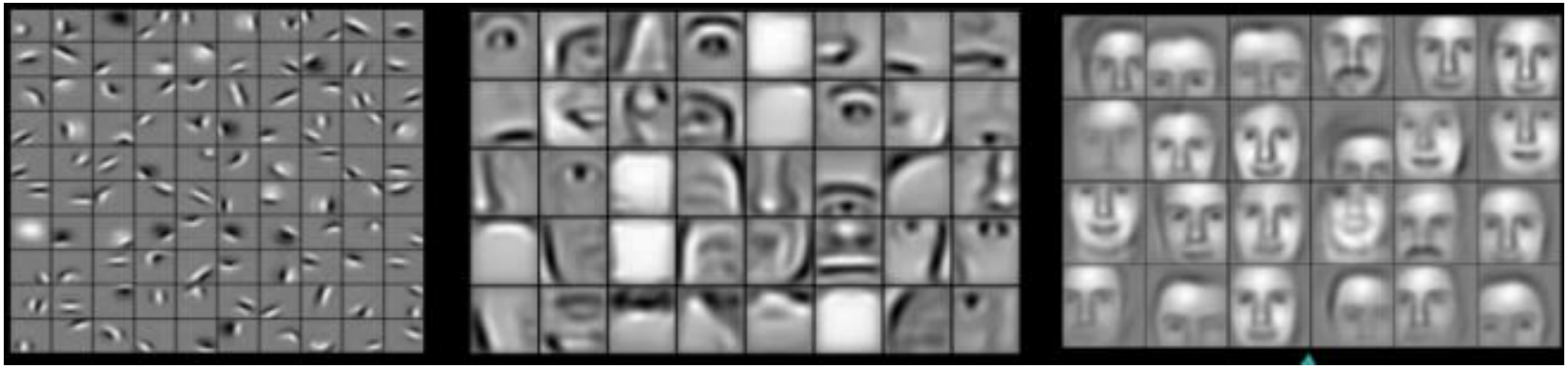


Why Multiple Hidden Layers?

Activations at hidden layers can be viewed as features extracted as functions of inputs

Every hidden layer represents a level of abstraction

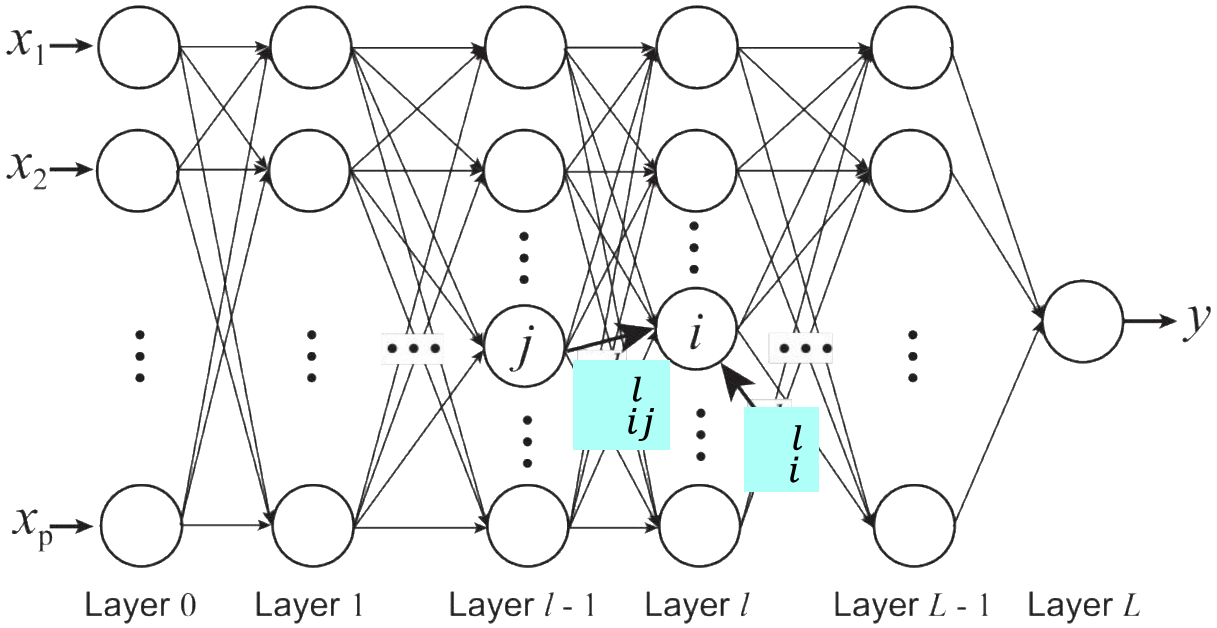
- *Complex features are compositions of simpler features*



Number of layers is known as **depth** of ANN

- *Deeper networks express complex hierarchy of features*

Multi-Layer Network Architecture



$$a_i^l = f(z_i^l) = f\left(\sum_j w_{ij}^l a_j^{l-1} + b_i^l\right)$$

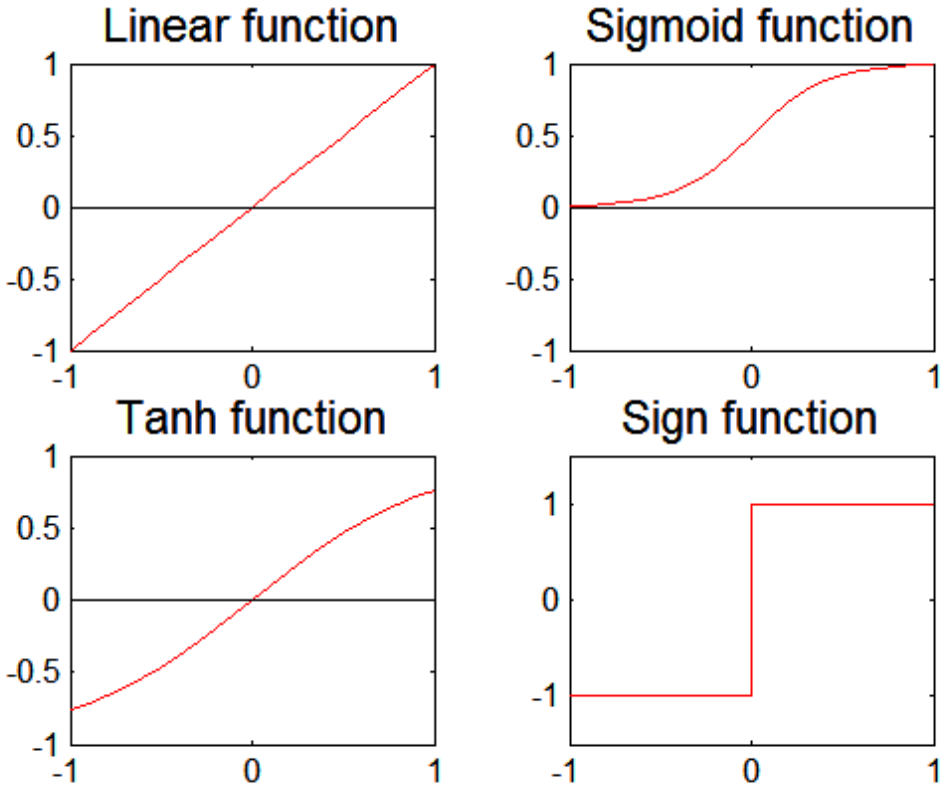
Activation value
at node i at layer l

Activation Function

Linear Predictor

Activation Functions

$$a_i^l = f(z_i^l) = f\Big(\sum_j w_{ij}^l a_j^{l-1} + b_i^l\Big)$$



$$a_i^l = \sigma(z_i^l) = \frac{1}{1+e^{-z_i^l}}.$$

$$\frac{\partial a_i^l}{\partial z_i^l} = \frac{\partial\ \sigma(z_i^l)}{\partial z_i^l} = a_i^l(1-a_i^l)$$

Learning Multi-layer Neural Network

Can we apply perceptron learning rule to each node, including hidden nodes?

- Perceptron learning rule computes error term e = y - $\hat{y}$ and updates weights accordingly
  - Problem: how to determine the true value of y for hidden nodes?
- Approximate error in hidden nodes by error in the output nodes
  - Problem:
    - Not clear how adjustment in the hidden nodes affect overall error
    - No guarantee of convergence to optimal solution

Gradient Descent

Loss Function to measure errors across all training points

$$E(\mathbf{w}, \mathbf{b}) = \sum_{k=1}^{n} \text{Loss } (y_k, \ \hat{y}_k)$$

Squared Loss:

$$\text{Loss } (y_k, \ \hat{y}_k) = (y_k - \hat{y}_k)^2.$$

Gradient descent: Update parameters in the direction of "maximum descent" in the loss function across all points

$$w_{ij}^l \longleftarrow w_{ij}^l - \lambda \frac{\partial E}{\partial w_{ij}^l},$$

$$b_i^l \longleftarrow b_i^l - \lambda \frac{\partial E}{\partial b_i^l},$$

λ: learning rate

Stochastic gradient descent (SGD): update the weight for every instance (minibatch SGD: update over min-batches of instances)

Computing Gradients

$$\frac{\partial E}{\partial w_{ij}^l} = \sum_{k=1}^{n} \frac{\partial \text{ Loss } (y_k,\ \hat{y_k})}{\partial w_{ij}^l}.$$

$$\hat{y} = a^L$$

$$a_i^l = f(z_i^l) = f\left(\sum_j w_{ij}^l a_j^{l-1} + b_i^l\right)$$

Using chain rule of differentiation (on a single instance):

$$\frac{\partial \text{ Loss}}{\partial w_{ij}^l} = \frac{\partial \text{ Loss}}{\partial a_i^l} \times \frac{\partial a_i^l}{\partial z_i^l} \times \frac{\partial z_i^l}{\partial w_{ij}^l}.$$

For sigmoid activation function:

$$\frac{\partial \text{ Loss}}{\partial w_{ij}^l} = \delta_i^l \times a_i^l(1 - a_i^l) \times a_j^{l-1},$$

$$\text{where } \delta_i^l = \frac{\partial \text{ Loss}}{\partial a_i^l}.$$

How can we compute δ_i^l for every layer?

Backpropagation Algorithm

At output layer L:

$$\delta^L = \frac{\partial \text{ Loss}}{\partial a^L} = \frac{\partial \ (y - a^L)^2}{\partial a^L} = 2(a^L - y).$$

At a hidden layer l (using chain rule):

$$\delta_j^l = \sum_i (\delta_i^{l+1} \times a_i^{l+1}(1 - a_i^{l+1}) \times w_{ij}^{l+1}).$$

- Gradients at layer l can be computed using gradients at layer l + 1
- Start from layer L and "backpropagate" gradients to all previous layers

Use gradient descent to update weights at every epoch

For next epoch, use updated weights to compute loss fn. and its gradient

Iterate until convergence (loss does not change)

Design Issues in ANN

Number of nodes in input layer

- One input node per **binary/continuous** attribute
- k or $\log_2$ k nodes for each **categorical** attribute with k values

Number of nodes in output layer

- One output for binary class problem
- k or $\log_2$ k nodes for k-class problem

Number of hidden layers and nodes per layer

Initial weights and biases

Learning rate, max. number of epochs, mini-batch size for mini-batch SGD, …

Characteristics of ANN

Multilayer ANN are universal approximators but could suffer from overfitting if the network is too large

- Naturally represents a hierarchy of features at multiple levels of abstractions

Gradient descent may converge to local minimum

Model building is compute intensive, but testing is fast

Can handle redundant and irrelevant attributes because weights are automatically learnt for all attributes

Sensitive to noise in training data

- This issue can be addressed by incorporating model complexity in the loss function

Difficult to handle missing attributes

Deep Learning Trends

Training **deep** neural networks (more than 5-10 layers) could only be possible in recent times with:

- Faster computing resources (GPU)
- Larger labeled training sets

Algorithmic Improvements in Deep Learning

- Responsive activation functions (e.g., RELU)
- Regularization (e.g., Dropout)
- Supervised pre-training
- Unsupervised pre-training (auto-encoders)

Specialized ANN Architectures:

- Convolutional Neural Networks (for image data)
- Recurrent Neural Networks (for sequence data)
- Residual Networks (with skip connections)

Generative Models: Generative Adversarial Networks