Data Mining

Lecture Notes for Chapter 4

Artificial Neural Networks

Introduction to Data Mining , 2nd Edition

by

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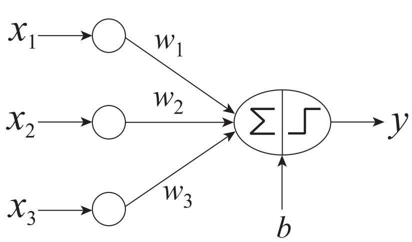
Artificial Neural Networks (ANN)

- **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



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

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

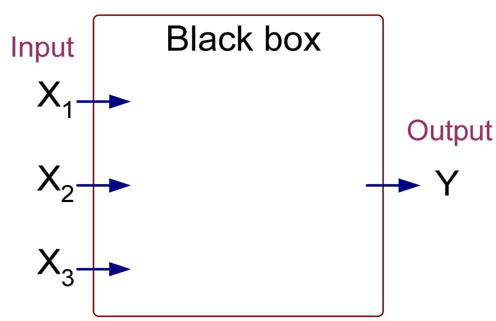
$$\hat{y} = sign(\tilde{\mathbf{w}}^T\tilde{\mathbf{x}})$$

Activation Function

- Learns linear decision boundaries
- Related to logistic regression (activation function is sign instead of sigmoid)

Perceptron Example

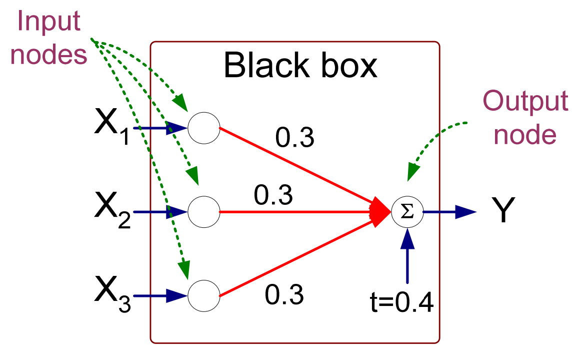
X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1



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:

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

- Until stopping condition is met
- k: iteration number; λ: learning rate

Perceptron Learning Rule

- Weight update formula:

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

- 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 x_{ij} is positive) so that $\hat{y}$ will increase
    - If y < $\hat{y}$, e=-2: weight must be decreased (assuming x_{ij} 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

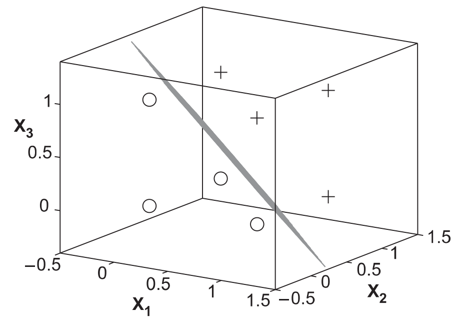
Weight updates over first epoch

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

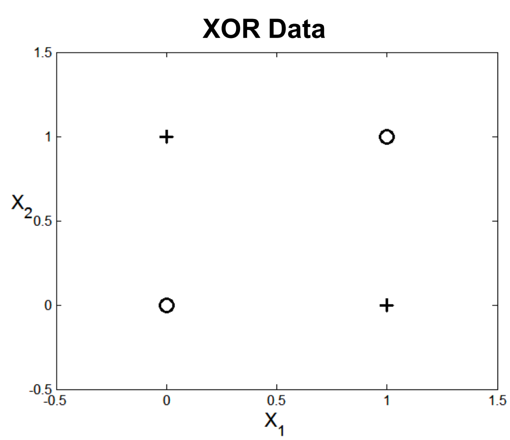


Nonlinearly Separable Data

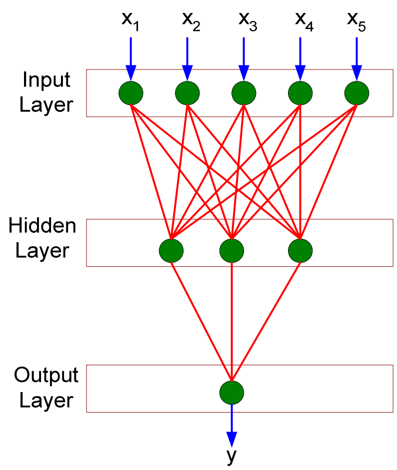
For nonlinearly separable problems, perceptron learning algorithm will fail because no linear hyperplane can separate the data perfectly

$$y = x_1 \oplus x_2$$

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"

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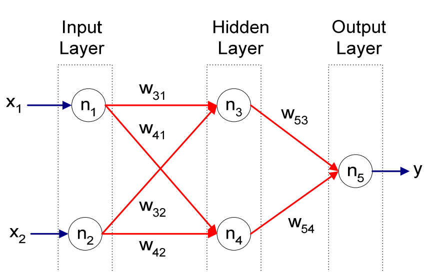
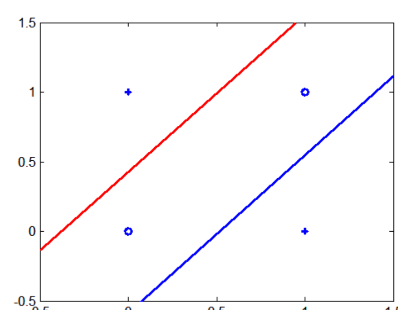
Multi-layer Neural Network

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



XOR Data



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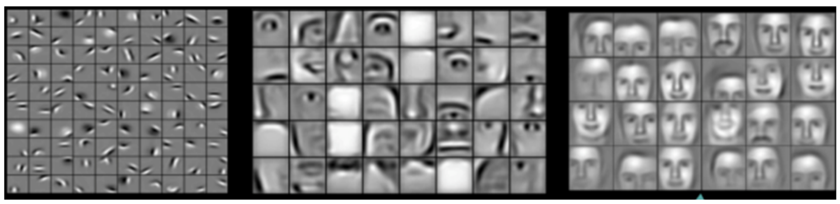
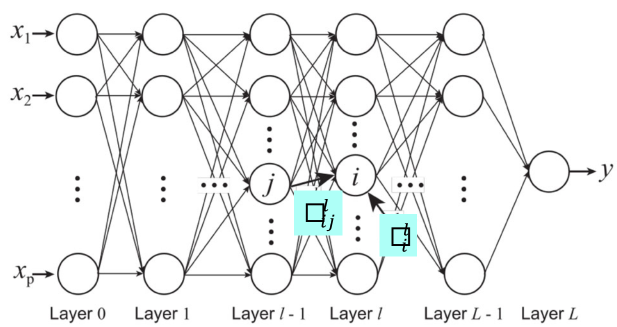
Why Multiple Hidden Layers?

- 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



$$a_i^l = f(z_i^l) = f\big(\underbrace{\sum_j w_{ij}^l a_j^{l-1} + b_i^l}_{\text{Linear Predictor}}\big)$$

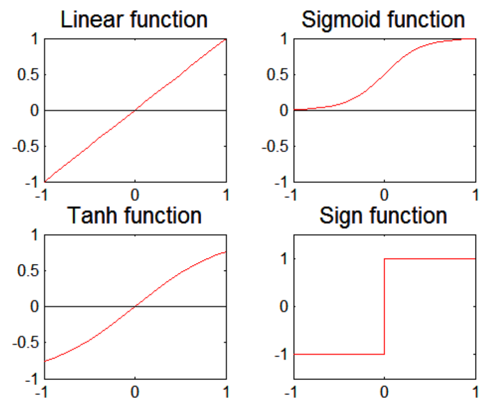
Activation value at node i at layer l

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

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

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

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

- 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