Classification

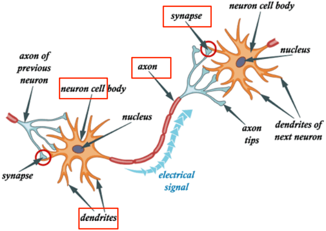
Artificial Neural Network (ANN)

Huiping Cao

Outline

Motivation

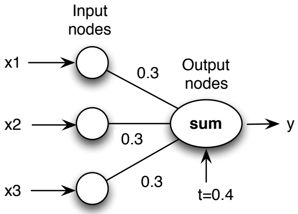
- Inspired by biological neural systems
  - We are interested in replicating the **biological function**
  - The first step is to replicate the **biological structure**



  - From the bird to plane
  - **Neurons**: nerve cells
  - **Axons**: strands of fibers, for linking neurons
  - **Dendrites**: extensions from the cell body of the neuron, connects neurons and axons
  - **Synapse**: the contact point between a dendrite and an axon

Perceptron Model – 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



Perceptron Model – Concepts

- A **perceptron** is a single processing unit of a neural net.
- **Nodes** in a neural network architecture are commonly known as **neurons** or units.
  - Input nodes: represent the input attributes
  - Output node: represent the model output
- **Weighted links**: emulate the strength of synaptic connection between neurons.

$$\hat{y} = \begin{cases} 1, & \text{if } 0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 > 0 \\ -1, & \text{if } 0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 < 0 \end{cases}$$

- **Activation functions**

$$\hat{y} = sign[w_d x_d + w_{d-1} x_{d-1} + \cdots + w_1 x_1 + w_0 x_0] = sign[\mathbf{w} \cdot \mathbf{x}]$$

where $w_0 = -t$ and $x_0 = 1$.

Perceptron Model – General Formalization

```
x1---------w1-------\
                     \
     ...wj...         > in ----> g ---> output
                     /
xn---------wn----- -/
```

- A perceptron takes *n* inputs x_1 to x_n. Each input x_j has an associated weight w_j.
- The output of the perceptron is produced by a **two-stage process**.
  - The first stage computes a quantity which is the weighted sum of the inputs $in = \sum_{j=1}^{n} w_j x_j$.
  - The second stage applies an **activation function g** to *in*. For perceptrons, the activation function used is the *threshold activation function*

$$\hat{y} = g(in) = \begin{cases} 1 & \text{if } in > \text{threshold } \sigma \\ -1 & \text{otherwise} \end{cases}$$

Perceptron Model – Activation Function

- The threshold σ is a parameter of the activation function.

$$\hat{y} = g(in) = \begin{cases} 1 & \text{if } in > \text{threshold } \sigma \\ -1 & \text{otherwise} \end{cases}$$

- An alternative way of encoding a threshold activation function is to create a special input x_0.
  - This input will always be fixed at -1 for every instance.
  - The weight w_0 associated with this input can then be used in space of the threshold σ (i.e., $w_0 = \sigma$).

  Thus,

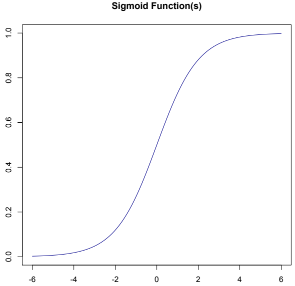
$$in = \sum_{j=0}^{n} w_j x_j$$

  where $x_0 = -1$ and $w_0 = \sigma$

$$\hat{y} = g(in) = \begin{cases} 1 & \text{if in} > 0 \\ -1 & \text{otherwise} \end{cases}$$

Activation functions

- Sigmoid function $sigmoid(s) = \theta(s) = \frac{e^s}{1+e^s}$. Its output is between 0 and 1. Its shape looks like a flattened out 's'. It is



also called a *logistic function*.

- Hyperbolic tangent function: $tanh(s) = \frac{e^s - e^{-s}}{e^s + e^{-s}}$

Learning Perceptron Model

Perceptron Learning Algorithm (PLA)

- **Training a perceptron model**: adapting the weights of the links until they fit the input-output relationships of the underlying data.

- Input: $D = \{(\mathbf{x}_i, y_i) | i = 1, 2, \cdots, N\}$ be the set of training examples
- Initialize the weight vector with random values $\mathbf{w}^{(\mathbf{0})}$.
- **repeat** (iteration no is k)
  - **for** each training point $(\mathbf{x}_i, y_i) \in D$ **do**
    - Compute the predicted output $\hat{y}_i^{(k)}$
    - **for** each weight w_j
    - Update $w_j^{(k+1)} = w_j^{(k)} + \lambda(y_i - \hat{y}_i^{(k)})x_{ij}$
- **until** stopping condition is met

Perceptron Learning Algorithm (PLA)

- **Weight update formula**: new weight is a combination of the old weight $w_j^{(k)}$ and a term proportional to the prediction error $(y_i - \hat{y}_i^{(k)})$.

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

- λ**: learning rate**, $\in [0, 1]$; It can be fixed or adaptive.
- The model is **linear** in its parameters $\mathbf{w}$ and attributes $\mathbf{x}$.

Perceptron Model – Linearly Separable

- A perceptron is a classifier, which takes *n* continuous inputs, and returns a Boolean classification (+1 or -1).
- All the points s.t. $in(\mathbf{x}) = 0$ defines a hyperplane in the space of inputs.
  - On one side of this hyperplane, all points are classified as +1.
  - On the other side, they are classified as -1.
- **Decision boundary**: A surface that divides the input space into regions of different classes.
- Perceptrons always have a linear decision boundary.
- **Linearly separable**: a classification function with a linear decision boundary.

Perceptron examples – Linearly Separable

- Perceptrons can represent many (but not ALL) Boolean functions on two inputs.
- A perceptron can represent the AND function by setting the weights to be $+1$ and the threefold to 1.5.

Perceptron examples – Non-linearly Separable

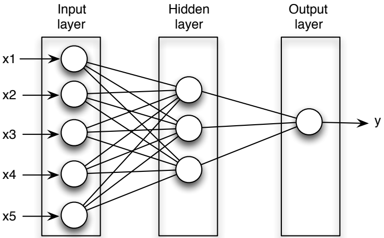
- XOR function on two inputs?
- Intuitively: we cannot find a line that can separate the four points with the points on one side having the same class labels.
- Formally:
  - Suppose that we can represent XOR using weights $\mathbf{w} = (w_0, w_1, w_2)$.
  - (1) $(x_1 = -1) \wedge (x_2 = -1)$, output is -1: $-w_0 - w_1 - w_2 \leq 0$
  - (2) $(x_1 = -1) \wedge (x_2 = 1)$, output is 1: $-w_0 - w_1 + w_2 > 0$
  - So, w_2 is positive.

  - (3) $(x_1 = 1) \wedge (x_2 = 1)$, output is -1: $-w_0 + w_1 + w_2 \leq 0$
  - (4) $(x_1 = 1) \wedge (x_2 = -1)$, output is 1: $-w_0 + w_1 - w_2 > 0$
  - So, w_2 is negative.
  - Contradiction!

Perceptron Properties

- If the problem is **linearly separable**, PLA is guaranteed to **converge** to an optimal solution.
- If the problem is **not linearly separable**, the algorithm **fails to converge**.

The neural network



- **Hidden layer, hidden nodes**
- **Feed-forward NN**: the nodes in one layer are connected only to the nodes in the next layer.
- **Recurrent NN**: the links may connect nodes within the same layer or nodes from one layer to the previous layers.
- **Activation functions**: sign, linear, sigmoid (logistic), hyperbolic tangent

Learning the ANN model

- **Target function**: the goal of the ANN learning algorithm is to determine a set of weights $\mathbf{w}$ that minimize the total sum of squared errors.

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

- When $\hat{y}$ is a linear function of its parameters, we can replace $\hat{y} = \mathbf{w} \cdot \mathbf{x}$ into the above equation, then the error function becomes quadratic in its parameters.

Gradient descent

- In most cases, the output of an ANN is a **nonlinear function** of its parameters because of the choice of its activation functions (e.g., *sigmoid* or *tanh* function)
- It is no longer straightforward to derive a solution for $\mathbf{w}$ that is guaranteed to be globally optimal.
- **Greedy algorithm** (e.g., based on **gradient descent methods**) are typically developed.
- Update formula

$$w_j = w_j - \lambda \frac{\partial E(\mathbf{w})}{\partial w_j}$$

Gradient descent

- For hidden nodes, the computation is not trivial because it is difficult to assess their error term $\frac{\partial E(\mathbf{w})}{\partial w_j}$ without knowing what their output values should be.
- **Back-propagation** technique: two phases in each iteration
  - **forward** phase: at the ith iteration, $\mathbf{w}^{(i-1)}$ are used to calculate the output value of each neuron in the network.
    Outputs of neurons at level k are computed before computing the outputs at level $k+1$. I.e., $k \rightarrow k+1$
  - **backward** phase: update of $\mathbf{w}^{(i)}$ is applied in the reverse direction.
    Weights at level $k+1$ are updated before the weights at level k are updated. I.e., $k+1 \rightarrow k$

Design issues in ANN learning

- Assign an input node to each numerical or binary input variable.
- **Output nodes**: for two-class problem, one output node; k-class problem, k output nodes.
- **Target function representation** factors: (1) weights of the links, (2) the number of hidden nodes and hidden layers, (3) biases in the nodes, and (4) type of activation function
- Finding the right **topology** is not easy.
- The **initial weights and biases** can come from random assignments.
- Fix the **missing values** first.

Characteristics of ANN

- Universal **approximators**: they can be used to approximate any target functions.
- Can handle **redundant features**.
- Sensitive to the presence of **noise**.
- The gradient descent method often converges to **local minimum**. One way: add a momentum term to the weight update formula.
- **Training** is time consuming.
- **Testing** is rapidly.

References

- Chapter 4: Introduction to Data Mining (2nd Edition) by Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar
- Python Perceptron model: https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Perceptron.html