Tutorial 4

Supervised Learning using Neural Network

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Objectives

Overview on Neural Network

Where does neural network (NN) shine?

- Commonly used in supervised learning where data has a lot of instances and feature space is large.
- It scales well when data size increases.

An (artificial) neural network is a direct graph.

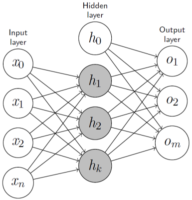
- **Feed-forward neural network (FFNN):** A directed acyclic graph, where nodes are arranged in layers from inputs to outputs.
- **Recurrent neural network (RNN):** A directed graph with cycles; nodes have additionally feedback into themselves or previous nodes.

Motivation

To combat **gradient vanishing** problem, *feedback nodes* in the hidden layers are commonly used in large-scale deep neural networks.

A basic NN with 1 hidden layer

- The data has n features, and the outputs have m classes.
- k hidden neurons in the hidden layer.
- Let x be the input vector where $x \in^{\mathrm{n}}$, hidden layer h is a vector where $h \in^{\mathrm{k}}$ and output o is a vector where $o \in^{\mathrm{m}}$.
- Nodes are connected by weights. These weights are learnt during the training. The weight matrices for the hidden layer is $W_0 \in^{\mathrm{k} \times \mathrm{n}}$, and for the output layer is $W_1 \in^{\mathrm{m} \times \mathrm{k}}$.
- Biases are $b_0 \in^{\mathrm{k}}$ and $b_1 \in^{\mathrm{m}}$, where $x_0 = h_0 = 1$.



$o = f(W_1 \cdot f(W_0 \cdot x + b_0) + b_1)$, where f is the activation function, applied element-wise.
Note: The last activation function should based on the desired outputs. (Eg: One-hot encoding, regression)

Activation Functions

The activation function must be **non-linear**.

For a given non-input node h:

- Suppose there are n nodes connect to h.
- Let x be the column vector input to the node, that $x = (x_0, x_1, \ldots, x_n)^T$, where $x_0 = 1$.
- Let w be the weights on the incident edges, that $w = (w_0, w_1, \ldots, w_n)^T$, where $w_0 = b$ is the bias.

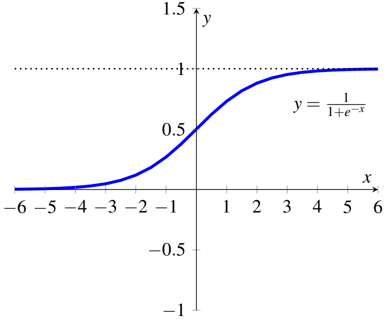
The output from this node is given by:

$$f(w^T x) = f(\sum_{i=0}^{n} w_i x_i) = f(\sum_{i=1}^{n} w_i x_i + b)$$

Where f is the activation function for this node.

If the activation function is linear, we can merge multiple hidden layers into one layer. The structure is equivalent to linear regression.

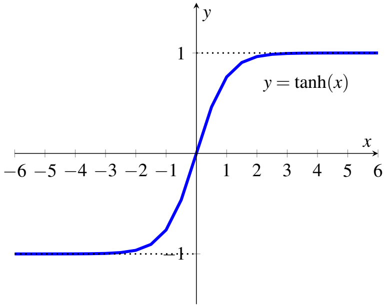
Sigmoid Function



$$f(x) = \text{Sigmoid}(x) = \sigma(x) = \frac{1}{1+e^{-x}}$$

Where $f(x) \in (0,1)$, and the derivative is $f'(x) = f(x)(1-f(x))$.
Rarely used in hidden layers for state-of-the-art models.
Often used in the last hidden layer to produce logistic outputs.

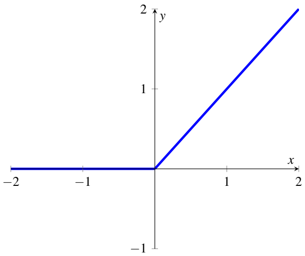
Hyperbolic Tangent (tanh) Function



$$f(x) = \tanh(x) = \frac{\sinh(x)}{\cosh(x)} = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

Where $f(x) \in (-1, 1)$, and the derivative is $f'(x) = 1 - f(x)^2$
Similar to Sigmoid function, but faster to converge.

Rectified Linear Unit (ReLU) Function



$$f(x) = \mathrm{ReLU}(x) = (x)^+ = \max(0, x)$$

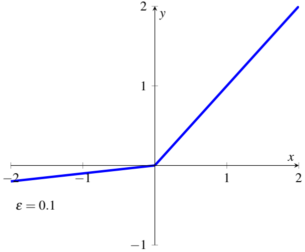
Where $f(x) \in [0, +\infty)$. The derivative is equal to:

$$f'(x) = \begin{cases} 0, & \text{if } x < 0 \\ 1, & \text{if } x > 0 \end{cases}$$

Where $x = 0$ is not differentiable.

ReLU is the most common activation function for hidden layers in recent deep learning.

Leaky ReLU



Let ε be the negative slope:

$$f(x) = \text{LeakyReLU}(x) = \max(0,x) + \varepsilon \times \min(0,x) = \begin{cases} x, & \text{if } x \geq 0 \\ \varepsilon \times x, & \text{otherwise} \end{cases}$$

Where $f(x) \in$, and $\varepsilon \in [0,1)$ The derivative is equal to ($x = 0$ is not differentiable):

$$f'(x) = \begin{cases} \varepsilon, & \text{if } x < 0 \\ 1, & \text{if } x > 0 \end{cases}$$

Similar to ReLU, but overcomes the "dead neuron" problem.

Loss/Cost Functions - MSE

The goal of training is to minimize a loss function. An objective function is a loss function.

Mean Squared Error (MSE)

$$\ell(X, y|W) = \text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

- Squared L2-norm error;
- Loss is computed forward,
- W are the weights.
- X are the data.
- y are the target labels.
- Minimizing ℓ using backpropagation with stochastic gradient descent (SGD) algorithm.

Mean Absolute Error (MAE)

$$\ell(X,y|W) = \text{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

- Minimizing L1-norm error
- Compare with MSE, L1-norm is more robust to outliers.
- Compare with MSE, the solution from L1-norm is unstable, so it is harder to optimize.

When use as regularization:

- L1-regularization prefers sparse outputs.
- L2-regularization prefers smaller weights and distributes the weights more evenly.

Softmax Function

Softmax function is defined as:

$$\text{Softmax}(x_i) = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$

- The outputs from a NN can be negative or above 1.
- Softmax function rescales them so that the elements of a n-dimensional output lie in the range $[0, 1]$ and sum to 1.

Negative Log Likelihood (NLL) Loss

NLL Loss is useful to train a classification problem with multiple output classes.

Let p be a vector of probabilities (after Softmax function).

$$p_k = \frac{\exp(f_k)}{\sum_j \exp(f_j)}$$

The Loss for one example is:

$$L_i = -\log(p_{y_i})$$

The partial derivative is extremely simple:

$$\frac{\partial L_i}{\partial f_k} = p_k - 1(y_i = k)$$

Example:

	Class	**Prediction**	**df**
Alpaca	0	0.2	**0.2**
Cat	1	0.3	**-0.7**
Dog	0	0.5	**0.5**

Optimization

Convolution Layers

Pooling Layers

Recurrent Layers

Tutorial Questions