Tutorial 4

Supervised Learning using Neural Network

Luke Chang

The University of Auckland

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Objectives

1. Overview on Neural Network
2. Activation Functions
3. Loss Functions
4. Optimization
5. Different Types of Layers
6. Tutorial Questions

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.

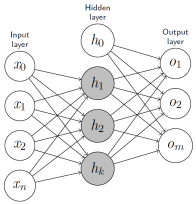
- **Feed-forward neural network (FFNN):** A directed acyclic graph, where nodes are arranged in layers from inputs to outputs.
- **Recurrent neural network (RNN):** A directed graph with cycles; nodes have additionally feedback into themselves or previous nodes.

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.

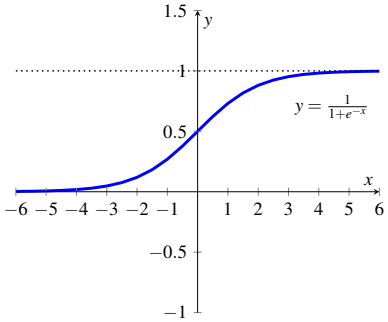
The output from this node is given by:

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

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.

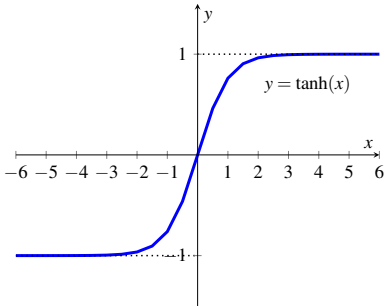
Sigmoid Function



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

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.

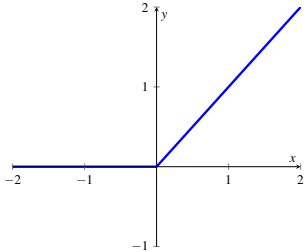
Hyperbolic Tangent (tanh) Function



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

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



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

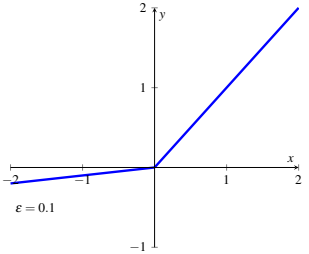
Where $f(x) \in [0, +\infty)$. The derivative is equal to:

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

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:

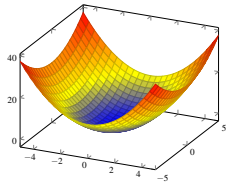
$$\frac{\partial L_i}{\partial f_k} = p_k - 1(y_i = k)$$

Example:

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

Optimization - Stochastic Gradient Descent (SGD)

- Gradient Descent: Minimizing the loss function by computing the gradient of the error and adjust the weights to descend the landscape into an error minima.
- Iterative algorithm
- Starts from a random point and travels down its slope with **learning rate** λ until it reaches the lowest point.
- Stochastic Gradient Descent (SGD) - Stochastic means **random**; Randomly select one instance at each iteration to reduce the computation cost;
- SGD works well with **mini-batch**, where the entire training data is divided into multiple random batches (without replacement, usually between 32 and 256).

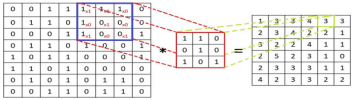


$$\text{step\_size} = \text{gradient} \times \lambda$$

$$W^{[i+1]} = W^{[i]} - \text{step\_size}$$

Convolutional Neural Network (CNN) - Convolutional Layers

- Convolutional Neural Network (CNN) is commonly applied to image datasets.
- CNN is a type of DNN.
- Convolutional layers is the fundamental building blocks for CNN.
- Convolutional layers convolve the input and pass its result to the next layer. (Convolution operation: $f * g$)
- Similar to apply an image filter, but all weights in the kernel are learnt during the training.



The height of the output is:

$$H_{\text{out}} = \lfloor \frac{H_{\text{in}} - K + 2P}{S} + 1 \rfloor$$

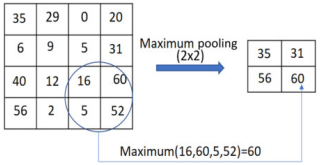
Where K is kernel size, S is stride, and P is zero padding.
The same formula is also applied to the output width.

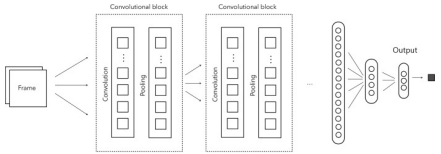
Convolutional Neural Network (CNN) - Pooling Layers

Pooling layers of a CNN implement a spatial dimensionality reduction operation designed to reduce the number of trainable parameters for the next layers.

Different types of pooling layer:

- Average pooling
- Max. pooling
- Adaptive max. pooling: Similar to Max. pooling, but define `output_size` instead of kernel size.





Tutorial Questions for Neural Networks

Question 1

Suppose you have a fully connected Neural Network with 2 variable inputs, 1 hidden layer with 3 nodes and an output layer with 4 nodes.

- How many weights will you learn?
- What will be the hypothesis returned by this neural network?
- What will be the hypothesis space?
- If you add a second hidden layer to the neural network above, also with 3 nodes, how many weights will we learn?
- Which NN will be more apt to over fit?

Tutorial Questions for Genetic Algorithms

Question 1

Suppose you have a population of two individuals 111111 and 101010.

How many applications of:

- single-point mutation would it take to get to 101111?
- single-point crossover would it take to get to 101111?
- two-point crossover would it take to get to 101111?
- single-point mutation would it take to get to 111011?
- single-point crossover would it take to get to 111011?
- two-point crossover would it take to get to 111011?
- single-point mutation would it take to get to 010101?
- single-point crossover would it take to get to 010101?
- two-point crossover would it take to get to 010101?

Tutorial Questions for Genetic Algorithms

Question 2

A population of two individuals 111111 and 101010. And the probability of choosing each parent is $1/2$ and the probability of choosing mutation, single-point crossover or two-point crossover is $1/3$. The mutation flips the bit and has a uniform chance of being applied to each bit. Single-point and two-point crossover have a uniform chance of choosing each location. Once crossover or mutation is done there is a 50% of replacing each parent randomly.

Given $x \in \{101111, 111011, 010101\}$:

- What is the probability of getting x by an application of mutation?
- What is the probability of getting x by an application of single-point crossover?
- What is the probability of getting x by an application of two-point crossover?
- What is the combined probability?