

Tutorial 4

Supervised Learning using Neural Network

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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.

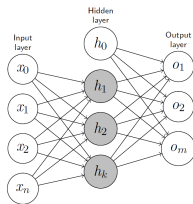
- **Feed-forward neural network (FFNN):** A directed acyclic graph, where nodes are arranged in layers from inputs to outputs.
- **Recurrent neural network (RNN):** A directed graph with cycles; nodes have additionally feedback into themselves or previous nodes.

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 $x \in \mathbb{R}^n$, hidden layer h is a vector where $h \in \mathbb{R}^k$ and output o is a vector where $o \in \mathbb{R}^m$.
- Nodes are connected by weights. These weights are learnt during the training. The weight matrices for the hidden layer is $W_0 \in \mathbb{R}^{k \times n}$, and for the output layer is $W_1 \in \mathbb{R}^{m \times k}$.
- Biases are $b_0 \in \mathbb{R}^k$ and $b_1 \in \mathbb{R}^m$, 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 be 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 $x = (x_0, x_1, \dots, x_n)^T$, where $x_0 = 1$.
- Let w be the weights on the incident edges, that $w = (w_0, w_1, \dots, w_n)^T$, where $w_0 = b$ is the bias.

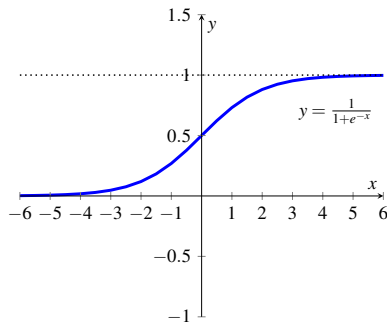
The output from this node is given by:

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

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



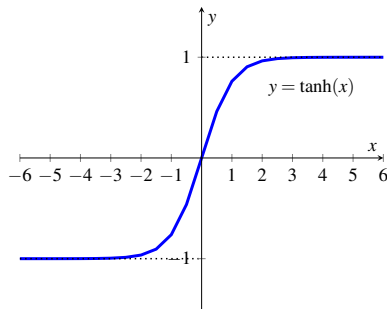
$$f(x) = \text{Sigmoid}(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$

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

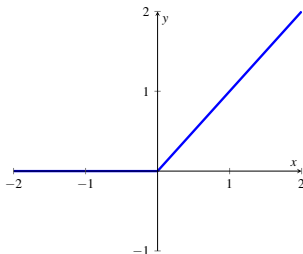


$$f(x) = \tanh(x) = \frac{\sinh(x)}{\cosh(x)} = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

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



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

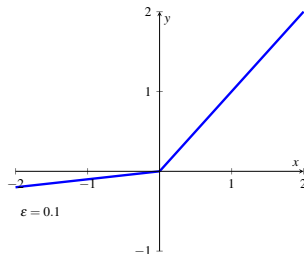
Where $f(x) \in [0, +\infty)$. The derivative is equal to:

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

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:

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

Where $f(x) \in \mathbb{R}$, and $\epsilon \in [0, 1)$ The derivative is equal to ($x = 0$ is not differentiable):

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

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)

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

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

Mean Absolute Error (MAE)

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

- 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:

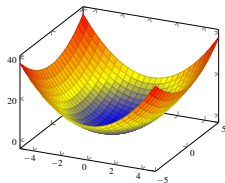
$$\frac{\partial L_i}{\partial f_k} = p_k - 1(y_i = k)$$

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).

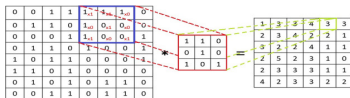


$$\text{step_size} = \text{gradient} \times \lambda$$

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

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.

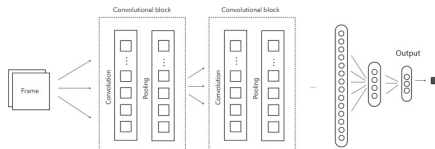
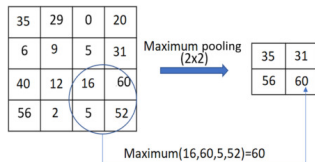
The same formula is also applied to the output width.

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 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? $2 \times 3 + 3 \times 4 = 18$
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- How many weights will you learn? $2 \times 3 + 3 \times 4 = 18$
- What will be the hypothesis returned by this neural network? $3 + 4 = 7$ biases; $7 + 18 = 25$; A matrix of 25 numbers
- What will be the hypothesis space?
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- What will be the hypothesis space? 25-dimensional space of real numbers
- If you add a second hidden layer to the neural network above, also with 3 nodes, how many weights will we learn?
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- If you add a second hidden layer to the neural network above, also with 3 nodes, how many weights will we learn? $2 \times 3 + 3 \times 3 + 3 \times 4 = 27$
- Which NN will be more apt to over fit?

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- What will be the hypothesis space? 25-dimensional space of real numbers
- If you add a second hidden layer to the neural network above, also with 3 nodes, how many weights will we learn? $2 \times 3 + 3 \times 3 + 3 \times 4 = 27$
- Which NN will be more apt to over fit? The 2nd one, because it has more degrees of freedom.

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?

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

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- single-point mutation would it take to get to 101111? 1
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- 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?
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- single-point mutation would it take to get to 111011? 1
- single-point crossover would it take to get to 111011? 2
- 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?

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- two-point crossover would it take to get to 111011? 1
- single-point mutation would it take to get to 010101? 3
- single-point crossover would it take to get to 010101? Infinite
- two-point crossover would it take to get to 010101?

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- two-point crossover would it take to get to 111011? 1
- single-point mutation would it take to get to 010101? 3
- single-point crossover would it take to get to 010101? Infinite
- two-point crossover would it take to get to 010101? Infinite

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.

- What is the probability of getting 101111 by an application of mutation?
- What is the probability of getting 101111 by an application of single-point crossover?
- What is the probability of getting 101111 by an application of two-point crossover?
- What is the combined probability?

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- What is the probability of getting 101111 by an application of mutation?
 $\frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} = 0.0277 = 2.77\%$
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 $\frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} = 0.0277 = 1.38\%$
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 $\frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{2}{6} = 0.46296\%$
- What is the combined probability?

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 $\frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{2}{6} = 0.46296\%$
- What is the combined probability? $2.77 + 1.38 + 0.46296 = 4.61\%$

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Question 3

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.

- What is the probability of getting 111011 by an application of mutation?
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 $2 \times (\frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6}) = 0.01929\%$
- What is the probability of getting 111011 by an application of two-point crossover?

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 $2 \times (\frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6}) = 0.01929\%$
- What is the probability of getting 111011 by an application of two-point crossover?
 $\frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} = 0.23148\%$

Tutorial Questions for Genetic Algorithms

Question 4

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.

- What is the probability of getting 010101 by an application of mutation?
- What is the probability of getting 010101 by an application of single-point crossover?
- What is the probability of getting 010101 by an application of two-point crossover?

Tutorial Questions for Genetic Algorithms

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- What is the probability of getting 010101 by an application of mutation?
 $\frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} = 0.0000006201814\%$
- What is the probability of getting 010101 by an application of single-point crossover?
- What is the probability of getting 010101 by an application of two-point crossover?

Tutorial Questions for Genetic Algorithms

Question 4

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- What is the probability of getting 010101 by an application of mutation?
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- What is the probability of getting 010101 by an application of single-point crossover? **Infinite**
- What is the probability of getting 010101 by an application of two-point crossover?

Tutorial Questions for Genetic Algorithms

Question 4

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.

- What is the probability of getting 010101 by an application of mutation?
 $\frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} = 0.0000006201814\%$
- What is the probability of getting 010101 by an application of single-point crossover? **Infinite**
- What is the probability of getting 010101 by an application of two-point crossover? **Infinite**