Mathematical Foundations for Machine Learning and Data Science

Overview of Perceptron Classifier, Logistic Regression and Neural Networks

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https://www.zubairkhalid.org/ee212_2021.html
Outline

- Perceptron and Perceptron Classifier
Classification

Recap:
• We assume we have training data $D$ given by

$$D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\} \subseteq \mathcal{X}^d \times \mathcal{Y}$$

Binary or Binomial Classification:
• $\mathcal{Y} = \{0, 1\}$ or $\mathcal{Y} = \{-1, 1\}$
  - Disease detection, spam email detection, fraudulent transaction, win/loss prediction, etc.

Multi-class (Multinomial) Classification:
• $\mathcal{Y} = \{1, 2, \ldots, M\}$ (M-class classification)
  - Emotion Detection.
  - Vehicle Type, Make, model, of the vehicle from the images streamed by road cameras.
  - Speaker Identification from Speech Signal.
  - Sentiment Analysis (Categories: Positive, Negative, Neutral), Text Analysis.
  - Take an image of the sky and determine the pollution level (healthy, moderate, hazard).
Overview:
- Linear Separability
  - Linearly Separable
  - NOT Linearly Separable

- Linear Classifiers
  \[ h(x) = \theta^T x + \theta_0 \]
  - line in 2D, plane in 3D, hyper-plane in higher dimensions.
Perceptron Classifier

**McCulloch-Pitts (MP) Neuron:**
- McCulloch (neuroscientist) and Pitts (logician) proposed a computational model of the biological neuron in 1943.

**Biological Neuron (Simplified illustration):**

- **Dendrites:** input node, receive signal from other neurons
- **Soma:** combines and processed signal
- **Axon:** output node, transmits processed signal
- **Synapses:** connected to the dendrites of other neurons

- Neuron is fired or transmits the signal when it is activated by the combination of input signals.

**McCulloch-Pitts (MP) Neuron:**

- \(d\) number of boolean inputs \(x^{(1)}, x^{(2)}, \ldots, x^{(d)} \in \{0, 1\}\).
- Boolean output, \(y \in \{0, 1\}\).
- If sum of inputs is less than \(\theta\), the output is zero and one otherwise.
- \(\theta\) is a thresholding parameter that characterizes the neuron.
- Mathematically,

\[
  y = \begin{cases} 
    1 & \text{if } \sum_{i=1}^{d} x^{(i)} \geq \theta \\
    0 & \text{if } \sum_{i=1}^{d} x^{(i)} < \theta 
  \end{cases}
\]

- Idea: Fire the neuron if at least \(\theta\) number of inputs are active.

**Perceptron Classifier**

**McCulloch-Pitts Neuron (MP) - Examples:**

- **OR of two inputs.**

  ![OR Diagram]

  \[ y = \begin{cases} 
  1 & \text{if } x^{(1)} + x^{(2)} \geq 1 \\
  0 & \text{if } x^{(1)} + x^{(2)} < 1 
  \end{cases} \]

- **AND of two inputs.**

  ![AND Diagram]

  \[ y = \begin{cases} 
  1 & \text{if } x^{(1)} + x^{(2)} \geq 2 \\
  0 & \text{if } x^{(1)} + x^{(2)} < 2 
  \end{cases} \]

Perceptron Classifier

McCulloch-Pitts Neuron (MP) - Examples:

- OR of three inputs.
  \[
  y = \begin{cases} 
  1 & \text{if } x^{(1)} + x^{(2)} + x^{(3)} \geq 1 \\
  0 & \text{if } x^{(1)} + x^{(2)} + x^{(3)} < 1 
  \end{cases}
  \]

- AND of three inputs.
  \[
  y = \begin{cases} 
  1 & \text{if } x^{(1)} + x^{(2)} + x^{(3)} \geq 3 \\
  0 & \text{if } x^{(1)} + x^{(2)} + x^{(3)} < 3 
  \end{cases}
  \]

Source: McCulloch-Pitts Neuron — Mankind’s First Mathematical Model Of A Biological Neuron | by Akshay L Chandra | Towards Data Science
Perceptron Classifier

McCulloch-Pitts (MP) Neuron – Limitations:

- Can classify if inputs are *linearly* separable with respect to the output.
  - How to handle the functions/mappings that are not linearly separable e.g., XOR?

- Can handle only boolean inputs.
  - Gives equal or no weightage to the inputs
  - How can we assign different weights to different inputs?
  - We hand-code threshold parameter
  - Can we automate the learning process of the parameter?

- To overcome these limitations, another model, known as perception model or perceptron, was proposed by Frank Rosenblatt (1958) and analysed by Minsky and Papert (1969).
  - Inputs real valued, weights used in aggregation
  - Learning of weights and threshold is possible.
Perceptron Classifier

**Perceptron:**
- $d$ number of real-valued inputs $x^{(1)}, x^{(2)}, \ldots, x^{(d)} \in \mathbb{R}$. *(Difference from MP Neuron)*
- Boolean output, $y \in \{0, 1\}$.
- If sum of inputs is less than $\theta$, the output is zero and one otherwise.
- Threshold $\theta$ and weights $w_1, w_2, \ldots, w_d$ are model parameters. *(Difference from MP Neuron)*

\[
\sum_{i=1}^{d} w_i x^{(i)} \begin{cases} 
1 & \text{if } \sum_{i=1}^{d} w_i x^{(i)} \geq \theta \\
0 & \text{if } \sum_{i=1}^{d} w_i x^{(i)} < \theta
\end{cases}
\]

- $\theta$, threshold represents a bias here.
- $\theta$ can be considered or absorbed as a weight.
- This will make aggregation/thresholding independent of any parameters.

Source: Perceptron: The Artificial Neuron (An Essential Upgrade To The McCulloch-Pitts Neuron) | by Akshay L Chandra | Towards Data Science
Perceptron Classifier

Perceptron:

\[ x^{(0)} = 1 \]

\[ w_0 = -\theta \]

\[ x^{(1)} \to -\theta \]

\[ w_1 \]

\[ x^{(2)} \to w_2 \]

\[ \vdots \]

\[ x^{(d)} \to w_d \]

\[ \sum \]

\[ y = \begin{cases} 
1 & \text{if } \sum_{i=1}^{d} w_i x^{(i)} - \theta \geq 0 \text{ or } \sum_{i=0}^{d} w_i x^{(i)} \geq 0 \\
0 & \text{if } \sum_{i=1}^{d} w_i x^{(i)} - \theta < 0 \text{ or } \sum_{i=0}^{d} w_i x^{(i)} < 0 
\end{cases} \]

Note:
Threshold is zero here.
Threshold has been absorbed as a model weight.

Alternative (Compact) Representation:

- \( \mathbf{x} = [x^{(0)}, x^{(1)}, \ldots, x^{(d)}] \)
- \( \mathbf{w} = [w_0, w_1, \ldots, w_d] \)

\[ x^{(0)} = 1 \]

\[ w_0 = -\theta \]

\[ x^{(1)} \to w_1 \]

\[ x^{(2)} \to w_2 \]

\[ \vdots \]

\[ x^{(d)} \to w_d \]

\[ y = \begin{cases} 
1 & \text{if } \mathbf{w}^T \mathbf{x} \geq 0 \\
0 & \text{if } \mathbf{w}^T \mathbf{x} < 0 
\end{cases} \]
Perceptron Classifier

Classification using Perceptron:

- Since $\mathbf{w}^T \mathbf{x} = 0$ represents a hyper-plane in the $d$-dimensional space, we can use perceptron as a binary classifier if the classes are linearly separable.

- How is this different from MP neuron?
  - Inputs are real-valued.
  - We have real-valued weights in the process of aggregation.
  - We can learn the weights.

$$x^{(0)} = 1, \quad w_0 = -\theta$$

$$x^{(1)}, w_1$$

$$x^{(2)}, w_2$$

$$\vdots$$

$$x^{(d)}, w_d$$

$$y = \begin{cases} 
1 & \text{if } \mathbf{w}^T \mathbf{x} \geq 0 \\
0 & \text{if } \mathbf{w}^T \mathbf{x} < 0
\end{cases}$$

Remark:

*If classes are labeled as 1 and -1*

$$y = \begin{cases} 
1 & \text{if } \mathbf{w}^T \mathbf{x} \geq 0 \\
-1 & \text{if } \mathbf{w}^T \mathbf{x} < 0
\end{cases}$$

We often write output as

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

$\text{sign}()$ returns sign of the argument.
Outline

- Perceptron and Perceptron Classifier
- Logistic Regression Classifier
Overview:
- kNN: Instance based Classifier
- **Logistic Regression**: Discriminative Classifier
  - Estimate $P(y|x)$ directly from the data
- ‘Logistic regression’ is an algorithm to carry out classification.
  - Name is misleading; the word ‘regression’ is due to the fact that the method attempts to fit a linear model in the feature space.
- Instead of predicting class, we compute the probability of instance being that class.

- Mathematically, model is characterized by variables $\theta$.
  \[
  h_\theta(x) = P(y|x) \quad \text{Posterior probability}
  \]
- A simple form of a neural network.
Consider a binary classification problem.
- We have a multi-dimensional feature space (d features).
- Features can be categorical (e.g., gender, ethnicity) or continuous (e.g., height, temperature).
- Logistic regression model:

\[
\begin{align*}
\text{Logistic Regression} \\
\sum h_\theta(x) &= \theta_0 + \theta^T x \\
h_\theta(x) &> 0 \quad \text{class 1} \\
h_\theta(x) &\leq 0 \quad \text{class 0}
\end{align*}
\]

Regression
**Model:**
- Consider a binary classification problem.
- We have a multi-dimensional feature space (d features).
- Features can be categorical (e.g., gender, ethnicity) or continuous (e.g., height, temperature).
- Logistic regression model:

$$h_{\theta}(x) = \theta_0 + \theta^T x$$

$$\text{Real-valued output here!}$$

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

$$\text{Logistic/Sigmoid function}$$

$$\frac{1}{1+e^{-h_{\theta}(x)}}$$

$$\text{Activation function}$$
Logistic Regression

**Logistic (Sigmoid) Function**

\[
\sigma(z) = \frac{1}{1 + e^{-z}}
\]

- Interpretation: maps \((-\infty, \infty)\) to \((0, 1)\)
- Squishes values in \((-\infty, \infty)\) to \((0, 1)\)
- It is differentiable.
- Generalized logistic function:

\[
\sigma(z) = \frac{L}{1 + e^{-k(z-z_0)}}
\]

- Sigmoid: because of S shaped curve
Logistic Regression

Change in notation:
- Treat bias term as an input feature for notational convenience.

\[
\begin{align*}
\mathbf{h}_\theta(\mathbf{x}) &= \sigma(\mathbf{\theta}^T \mathbf{x}) \\
&= \frac{1}{1 + e^{-\mathbf{\theta}^T \mathbf{x}}} \\
\sum_{i=0}^{d} \theta_i x_i
\end{align*}
\]

Linear function. Linear Regression.
Logistic Regression

Classification:

\[ h_\theta(x) = P(y = 1|x) \] represents the probability of class membership.

Assign class by applying threshold as

\[ \hat{y} = \begin{cases} 
\text{Class 1} & \sigma(\theta^T x) > 0.5 \\
\text{Class 0} & \text{otherwise} 
\end{cases} \]

0.5 is the threshold defining decision boundary.

We can also use values other than 0.5 as threshold.
Outline

- Perceptron and Perceptron Classifier
- Logistic Regression Classifier
- Neural Networks
  - Neural networks connection with perceptron and logistic regression
Neural Networks

Connection with Logistic Regression and Perceptron:

- $d$ number of real-valued inputs $x^{(1)}, x^{(2)}, \ldots, x^{(d)} \in \mathbb{R}$.
- Boolean output, $y \in \{0, 1\}$.

**Perceptron Model:**

$$y = \begin{cases} 
1 & \text{if } w^T x + b \geq 0 \\
0 & \text{if } w^T x + b < 0 
\end{cases}$$

$$R^d \rightarrow \mathbb{R}$$
Neural Networks

Connection with Logistic Regression and Perceptron:

- $d$ number of real-valued inputs $x^{(1)}, x^{(2)}, \ldots, x^{(d)} \in \mathbb{R}$.
- Boolean output, $y \in \{0, 1\}$.

**Logistic Regression Model:**

Activation function is Logistic/Sigmoid function

$$\frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + b)}}$$
Neural Networks

Connection with Logistic Regression and Perceptron:

**Activation Function**

*Perceptron vs Sigmoid Neuron*

Weighted sum of inputs + bias

\[ w^T x + b \]
Neural Networks

**Neuron Model:**

**Compact Representation:**

\[ g(w^T x + b) \]

\( g \) - activation function.

**More Compact Representation:**

\[ g(w^T x + b) \]

- Neuron model: Characterized by weights, bias and activation function.
- Weights \( w \), bias \( b \) - model parameters
- Activation function \( g \) - hyperparameter
Neural Networks

Neural Networks - Infamous XOR Problem:

- (1969) Minsky and Papert showed that a perceptron cannot classify XOR output.

<table>
<thead>
<tr>
<th>$x_1$</th>
<th>$x_2$</th>
<th>XOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

- Classes are not linearly separable: linear classifier cannot be used.
- We can either transform features or project the data to higher dimensional space.
- We can however build a network of linear classifiers.

Idea: Learn AND and OR boundaries.
Neural Networks

Neural Networks - Infamous XOR Problem:

- This is a neural network; a network of perceptrons, aka multi-layer perceptron (MLP).
Neural Networks

- A neural network is a set of neurons organized in layers.

Each unit in the network is called a neuron and the network of neurons is called **Neural Network**.

- Output is a non-linear function
  - of a linear combination
    - of non-linear functions
      - of a linear combination of inputs

- Given the input and parameters of the neurons, we can determine the output by traversing layers from input to output. This is referred to as **Forward Pass**.
Neural Networks

Example: 3-layer network, 2 hidden layers

- Output is a non-linear function
  - of a linear combination
    - of non-linear functions
      - of linear combinations
        - of non-linear functions
          - of linear combinations of inputs

- We do not count the input layer because there are no parameters associated with it.
- Neural networks with neurons are also referred to as MLPs but we will refer to the network as MLP only when it is constructed using perceptrons.

Feedforward Neural Network: Output from one layer is an input to the next layer.
Neural Networks

What kind of functions can be modeled by a neural network?

Intuition: XOR example

\[ \text{AND} \quad b = 2 \]
\[ \text{OR} \quad b = 1 \]

\[ x^{(1)} \]
\[ x^{(2)} \]
Neural Networks

What kind of functions can be modeled by a neural network?

**Intuition:**  Example (Sigmoid neuron)

- bias=0.5 indicated.
- weight for $x$ is very large.
- weight for $y$ is zero.

- bias=0.5 indicated.
- weight for $y$ is very large.
- weight for $x$ is zero.

Neural Networks

What kind of functions can be modeled by a neural network?

Intuition: Example (Multi layer)

Source: http://neuralnetworksanddeeplearning.com/chap4.html
Neural Networks

What kind of functions can be modeled by a neural network?

Universal Approximation Theorem (Hornik 1991):

“A single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units.”

- The theorem results demonstrates the capability of neural network, but this does not mean there is a learning algorithm that can find the necessary parameter values.

- Since each neuron represents non-linearity, we can keep on increasing the number of neurons in the hidden layer to model the function. But this will also increase the number of parameters defining the model.

- Instead of adding more neurons in the same layer, we prefer to add more hidden layers because non-linear projections of a non-linear projection can model complex functions relatively easy.
- Perceptron and Perceptron Classifier
- Logistic Regression Classifier
- Neural Networks
  - Neural networks connection with perceptron and logistic regression
- Neural networks ‘Forward Pass’
Neural Networks

Neural Networks – Notation:

Single Neuron:

- If we stack $n$ training data in a matrix $X$ of size $d \times n$, that is, $X = [x_1, x_2, \ldots, x_n]$.

- Using $X$ and by defining $1$ a row vector of ones of length $n$, we can define ‘pre-activation’ operation $w^T x + b$ for all inputs compactly, denoted by $z$ as $z = w^T x + b 1_{(1 \times n)}$.

- Using activation function $g$, we obtain $a = g(z)$.

- Activation function is operating on each entry of $z$.

- $a$ - a row vector of length $n$; $i$-th entry represents an output for $i$-th input.
Neural Networks – Notation:

- $L$ - number of layers.
- Number of nodes in the $\ell$-th layer, $m^{[\ell]}$
- $a_i^{[\ell]}$ denotes the output of $i$-th node in the $\ell$-th layer.  
- $a^{[\ell]}$ - vector of outputs of $\ell$-th node.
- $a^{[0]} = x$ input layer.
- $a^{[L]} = y$ output layer.

Example: 3-layer network, 2 hidden layers

- $L = 3$
- $m^{[1]} = 4$, $m^{[2]} = 3$, $m^{[3]} = 1$
Neural Networks – Notation:

- $w_{i}^{[\ell]}$ and $b_{i}^{[\ell]}$ denote the weight and bias associated with the $i$-th node in the $\ell$-th layer respectively.
- $w_{i,j}^{[\ell]}$ denote the weight and bias associated with the $j$-th input of the $i$-th node in the $\ell$-th layer respectively.

Example: 3-layer network, 2 hidden layers

Layer 1 output

\[
\begin{align*}
    a_{1}^{[1]} &= g(z_{1}^{[1]}), & z_{1}^{[1]} &= w_{1}^{[1]T} x + b_{1}^{[1]} \\
    a_{2}^{[1]} &= g(z_{2}^{[1]}), & z_{2}^{[1]} &= w_{2}^{[1]T} x + b_{2}^{[1]} \\
    a_{3}^{[1]} &= g(z_{3}^{[1]}), & z_{3}^{[1]} &= w_{3}^{[1]T} x + b_{3}^{[1]} \\
    a_{4}^{[1]} &= g(z_{4}^{[1]}), & z_{4}^{[1]} &= w_{4}^{[1]T} x + b_{4}^{[1]}
\end{align*}
\]
Neural Networks – Notation:

Layer 1 output

\[
\begin{align*}
    a_1^{[1]} &= g(z_1^{[1]}), \quad z_1^{[1]} = w_1^{[1]T} x + b_1^{[1]} \\
    a_2^{[1]} &= g(z_2^{[1]}), \quad z_2^{[1]} = w_2^{[1]T} x + b_2^{[1]} \\
    a_3^{[1]} &= g(z_3^{[1]}), \quad z_3^{[1]} = w_3^{[1]T} x + b_3^{[1]} \\
    a_4^{[1]} &= g(z_4^{[1]}), \quad z_4^{[1]} = w_4^{[1]T} x + b_4^{[1]}
\end{align*}
\]

\[
\begin{bmatrix}
    w_1^{[1]T} \\
    w_2^{[1]T} \\
    w_3^{[1]T} \\
    w_4^{[1]T}
\end{bmatrix}
\begin{bmatrix}
    b_1^{[1]T} \\
    b_2^{[1]T} \\
    b_3^{[1]T} \\
    b_4^{[1]T}
\end{bmatrix}
\begin{bmatrix}
    z_1^{[1]T} \\
    z_2^{[1]T} \\
    z_3^{[1]T} \\
    z_4^{[1]T}
\end{bmatrix}
\]

\[
\begin{align*}
    a^{[1]} &= g(z^{[1]}), \quad z^{[1]} = W^{[1]} x + b^{[1]} \\
    z^{[1]} &= W^{[1]} a^{[0]} + b^{[1]}
\end{align*}
\]

- \(W^{[1]}\) and \(b^{[1]}\) are the parameters of the first layer.
Neural Networks – Forward Pass:

- \( a^{[1]} = g(z^{[1]}) \), \( z^{[1]} = W^{[1]} x + b^{[1]} \)
- \( z^{[1]} = W^{[1]} a^{[0]} + b^{[1]} \)

- Q. What is the size of \( W^{[1]} \)?
  
  A. No. of nodes × No. of inputs. 4 × 3
  
  No. of nodes × No. nodes in the previous layer.

- Q. Can we write output of second layer using the notation we have defined?

- \( a^{[2]} = g(z^{[2]}) \), \( z^{[2]} = W^{[2]} a^{[1]} + b^{[2]} \)

- \( a^{[3]} = g(z^{[3]}) \), \( z^{[3]} = W^{[3]} a^{[2]} + b^{[3]} \)

- Q. What is the size of \( W^{[2]} \)? 3 × 4
- Q. What is the size of \( W^{[3]} \)? 1 × 3
- \( W^{[\ell]} \) and \( b^{[\ell]} \) are the parameters of the \( \ell \)-th layer.

- Using these equations, we can determine the output given input and parameters of layers (Forward Pass).
Neural Networks – Forward Pass Summary:

\[
a^{[1]} = g(z^{[1]}), \quad z^{[1]} = W^{[1]}x + b^{[1]}
\]
\[
z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}
\]
\[
(4 \times 1) = (4 \times 3)(3 \times 1) + (4 \times 1)
\]

\[
a^{[2]} = g(z^{[2]}), \quad z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}
\]
\[
(3 \times 1) = (3 \times 4)(4 \times 1) + (3 \times 1)
\]

\[
a^{[3]} = g(z^{[3]}), \quad z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}
\]
\[
(1 \times 1) = (1 \times 3)(3 \times 1) + (1 \times 1)
\]

- In general, we have
  \[
a^{[\ell]} = g(z^{[\ell]}), \quad z^{[\ell]} = W^{[\ell]}a^{[\ell-1]} + b^{[\ell]}
  \]
  for \(\ell = 1, 2, \ldots, L\), where \(a^{[0]} = x\).

- How many parameters do we have by the way?

- This formulation is for one input \(x\).

- How can we extend this formulation \(n\) inputs?
Neural Networks

Neural Networks – Forward Pass – Incorporating all Inputs:

\[ a^{[1]} = g(z^{[1]}), \quad z^{[1]} = W^{[1]} x + b^{[1]} \]
\[ z^{[1]} = W^{[1]} a^{[0]} + b^{[1]} \]

\((4 \times 1) = (4 \times 3)(3 \times 1) + (4 \times 1)\)

Recall:

\[ x^{(1)} \]
\[ x^{(2)} \]
\[ \vdots \]
\[ x^{(d)} \]

\[ g(w^T x + b) \]
\[ z = w^T x + b \]
\[ g(z) \]

- For single neuron, we developed the following formulation incorporating all inputs simultaneously.

\[ z = w^T X + b1 \]

\[ a = g(z) \]

- \( a \) - a row vector of length \( n \):
  
  \( i \)-th entry represents an output for \( i \)-th input.

\[ A^{[1]} = g(Z^{[1]}), \quad Z^{[1]} = W^{[1]} X + b^{[1]} \]
\[ Z^{[1]} = W^{[1]} A^{[0]} + b^{[1]} \]

\((4 \times n) = (4 \times 3)(3 \times n) + (4 \times n)\)
Neural Networks

Neural Networks – Forward Pass Summary – All Inputs:

\[ A^{[1]} = g(Z^{[1]}), \quad Z^{[1]} = W^{[1]}X + b^{[1]} \]
\[ Z^{[1]} = W^{[1]}A^{[0]} + b^{[1]} \]
\[ (4 \times n) = (4 \times 3)(3 \times n) + (4 \times n) \]

\[ A^{[2]} = g(Z^{[2]}), \quad Z^{[2]} = W^{[2]}A^{[1]} + b^{[2]} \]
\[ (3 \times n) = (3 \times 4)(4 \times n) + (3 \times n) \]

\[ A^{[3]} = g(Z^{[3]}), \quad Z^{[3]} = W^{[3]}A^{[2]} + b^{[3]} \]
\[ (1 \times n) = (1 \times 3)(3 \times n) + (1 \times n) \]

- In general, we have
  \[ A^{[\ell]} = g(Z^{[\ell]}), \quad Z^{[\ell]} = W^{[\ell]}A^{[\ell-1]} + b^{[\ell]} \]
  \[ \ell = 1, 2, \ldots, L \]
Outline

- Perceptron and Perceptron Classifier
- Logistic Regression Classifier
- Neural Networks
  - Neural networks connection with perceptron and logistic regression
- Neural networks ‘Forward Pass’
- Learning neural network parameters
  - Back Propagation.
Learning Weights:
- Given the training data, we want to learn the weights (weight matrices+bias vectors) for hidden layers and output layer.

Notation revisit:
- $L$ - number of layers.
- Number of nodes in the $\ell$-th layer, $m^{[\ell]}$
- $a_i^{[\ell]}$ denotes the output of $i$-th node in the $\ell$-th layer.
- $a^{[\ell]}$ output of $\ell$-th layer, $a^{[0]} = x$.
- $a^{[L]} = y$ output layer.
- $w_i^{[\ell]}$ and $b_i^{[\ell]}$ denote the weight and bias associated with the $i$-th node in the $\ell$-th layer respectively.
- $w_{i,j}^{[\ell]}$ denotes the weight associated with the $j$-th input of the $i$-th node in the $\ell$-th layer.

Example:
Neural Networks

Learning Weights:

- We assume we have training data $D$ given by

  $$D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\} \subseteq \mathcal{X}^d \times \mathcal{Y}$$

- Consider a network with $d$ nodes (features) at the input layer, 1 output node and any number of hidden layers.

- Define the loss function (for regression problem):

  $$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{n} (\tilde{y}_i - y_i)^2$$

  where $\tilde{y}_i$ denotes the output of the neural network for $i$-th input.

- We can use gradient descent to learn the weight matrices and bias vectors.

- Given our prior knowledge, output $y$ is a composite function of input $x$. Therefore, it is continuous and differentiable and we can use chain rule to compute the gradient.

  We use a method called ‘Back Propagation’ to implement the chain rule for the computation the gradient.
Neural Networks

**Back Propagation – Key Idea:**

- We compute the loss function using forward pass.

![Forward Pass Diagram]

\[ \mathbf{x}_i \xrightarrow{\text{Forward Pass}} \tilde{y}_i \]

\[ L = \frac{1}{2} \sum_{i=1}^{n} (\tilde{y}_i - y_i)^2 \]

The weights are the only parameters that can be modified to make the loss function as low as possible.

**Back Propagation**

- Gradient descent:
  \[ w_{i,j}[\ell] = w_{i,j}[\ell] - \alpha \frac{\partial L}{\partial w_{i,j}[\ell]} \]

- We compute the derivative by propagating the total loss at the output node back into the neural network to determine the contribution of every node in the loss. *(Back Propagation)*
Neural Networks

Back Propagation – Example:
- 2 layer with 2 neurons in the hidden layer, 2 inputs, 2 outputs network.
- Assuming sigmoid as activation function, that is, \( g(z) = \sigma(z) \).

\[
\begin{align*}
    a_1^{[0]} &= x^{(1)} \\
    a_2^{[0]} &= x^{(2)} \\
    a_1^{[1]} &= w_{1,1}^{[1]} a_1^{[0]} + w_{1,2}^{[1]} a_2^{[0]} \\
    a_2^{[1]} &= w_{2,1}^{[1]} a_1^{[0]} + w_{2,2}^{[1]} a_2^{[0]} \\
    a_1^{[2]} &= w_{1,1}^{[2]} a_1^{[1]} + w_{1,2}^{[2]} a_2^{[1]} \\
    a_2^{[2]} &= w_{2,1}^{[2]} a_1^{[1]} + w_{2,2}^{[2]} a_2^{[1]} \\
    y^{(1)} &= \sigma(a_1^{[2]}) \\
    y^{(2)} &= \sigma(a_2^{[2]})
\end{align*}
\]

- Given training data
  \( x^{(1)} = 0.05, \quad x^{(2)} = 0.1, \quad y^{(1)} = 0.01, \quad y^{(2)} = 0.99 \)

- Initial values of weights and biases:
  \( w_{1,1}^{[1]} = 0.15, \quad w_{1,2}^{[1]} = 0.2, \quad w_{2,1}^{[1]} = 0.25, \quad w_{2,2}^{[1]} = 0.3, \quad b_1^{[1]} = 0.35, \quad b_2^{[1]} = 0.35. \)

  \( w_{1,1}^{[2]} = 0.4, \quad w_{1,2}^{[2]} = 0.45, \quad w_{2,1}^{[2]} = 0.5, \quad w_{2,2}^{[2]} = 0.55, \quad b_1^{[1]} = 0.6, \quad b_2^{[1]} = 0.6. \)
Neural Networks

Back Propagation – Example:

- Loss function (noting output is a vector):
  \[ \mathcal{L} = \frac{1}{2} \left\| (\hat{y}^{(1)} - y^{(1)})^2 - (\hat{y}^{(2)} - y^{(2)})^2 \right\|^2 \]
  \[ \mathcal{L} = \frac{1}{2} \left\| (0.01, 0.99) - (0.7514, 0.7729) \right\|^2 = 0.2984 \]

**Forward Pass**

- \( a_1[0] = x(1) \)
- \( a_2[0] = x(2) \)

\[
\begin{align*}
\end{align*}
\]

- \( z_1[1] = w_{1,1}x(1) + w_{1,2}x(2) + b_1[1] = 0.3775, \quad a_1[1] = g(0.3775) = 0.5933 \)
- \( z_2[1] = w_{2,1}x(1) + b_2[1] = 0.3925, \quad a_2[1] = g(0.3925) = 0.5969 \)
- \( z_1[2] = w_1[1]^T x + b_1[2] = 1.106, \quad a_1[2] = g(1.106) = 0.7514 = \hat{y}^{(1)} \)
- \( z_2[2] = w_2[2]^T x + b_2[2] = 1.225, \quad a_2[2] = g(1.225) = 0.7729 = \hat{y}^{(2)} \)

Nothing fancy so far, we have computed the output and loss by traversing neural network. Let’s compute the contribution of loss by each node; back propagate the loss.
Neural Networks

Back Propagation – Example:

\[
\begin{align*}
  a_1^0 &= x(1) \\
  a_2^0 &= x(2) \\
  a_1^1 &= w_{1,1}^1 x(1) \\
  a_2^1 &= w_{2,1}^1 x(2) \\
  a_1^2 &= w_{1,1}^2 a_1^1 \\
  a_2^2 &= w_{2,1}^2 a_2^1 \\
  y^{(1)} &= a_1^2 \\
  y^{(2)} &= a_2^2
\end{align*}
\]

- Consider a case when we want to compute \( \frac{\partial \mathcal{L}}{\partial w_{1,1}^2} \)

- Traverse the path from the loss function back to the weight \( w_{1,1}^2 \):

\[
\begin{align*}
  \mathcal{L} &= \frac{1}{2} \left( (\hat{y}(1) - y^{(1)})^2 - (\hat{y}(2) - y^{(2)})^2 \right) \\
  \hat{y}(1) &= \sigma(z_1^{[2]}) \\
  z_1^{[2]} &= w_{1,1} a_1^1 + w_{1,2} a_2^1 + b_1^{[2]} \\
  \frac{\partial \mathcal{L}}{\partial w_{1,1}^2} &= \sigma(z_1^{[2]}) \left(1 - \sigma(z_1^{[2]}) \right) \frac{\partial z_1^{[2]}}{\partial w_{1,1}^2} \\
  \frac{\partial \hat{y}(1)}{\partial \hat{y}(1)} &= \hat{y}(1) - y^{(1)} = 0.7414 \\
  \frac{\partial \hat{y}(1)}{\partial z_1^{[2]}} &= \sigma(z_1^{[2]}) \left(1 - \sigma(z_1^{[2]}) \right) = 0.1868 \\
  \frac{\partial z_1^{[2]}}{\partial w_{1,1}^2} &= a_1^1 = 0.5933
\end{align*}
\]
Neural Networks

**Back Propagation – Example:**

\[ a_1^{[0]} = x^{(1)} \]
\[ a_2^{[0]} = x^{(2)} \]

- \( a_1^{[1]} = w_{1,1} x^{(1)} + w_{1,2} x^{(2)} \)
- \( a_2^{[1]} = w_{2,1} x^{(1)} + w_{2,2} x^{(2)} \)
- \( a_1^{[2]} = w_{1,1} a_1^{[1]} + w_{1,2} a_2^{[1]} \)
- \( a_2^{[2]} = w_{2,1} a_1^{[1]} + w_{2,2} a_2^{[1]} \)

\[ y^{(1)} = a_1^{[2]} \]
\[ y^{(2)} = a_2^{[2]} \]

\[ \mathcal{L} = \frac{1}{2} \| (\tilde{y}^{(1)} - y^{(1)})^2 - (\tilde{y}^{(2)} - y^{(2)})^2 \|_2^2 \]

- Consider a case when we want to compute \( \frac{\partial \mathcal{L}}{\partial w_{1,1}^{[1]} } \)
- Traverse the path from the loss function back to the weight \( w_{1,1}^{[1]} \). There are two paths from the output to the weight \( w_{1,1}^{[1]} \). In other words, \( w_{1,1}^{[1]} \) is contributing to both the outputs.

\[
\frac{\partial \mathcal{L}}{\partial w_{1,1}^{[1]} } = \frac{\partial \mathcal{L}}{\partial \tilde{y}^{(1)} } \frac{\partial \tilde{y}^{(1)} }{\partial z_1^{[2]} } \frac{\partial z_1^{[2]} }{\partial a_1^{[1]} } \frac{\partial a_1^{[1]} }{\partial z_1^{[1]} } \frac{\partial z_1^{[1]} }{\partial w_{1,1}^{[1]} } + \frac{\partial \mathcal{L}}{\partial \tilde{y}^{(2)} } \frac{\partial \tilde{y}^{(2)} }{\partial z_2^{[2]} } \frac{\partial z_2^{[2]} }{\partial a_2^{[1]} } \frac{\partial a_2^{[1]} }{\partial z_2^{[1]} } \frac{\partial z_2^{[1]} }{\partial w_{1,1}^{[1]} } 
\]

- Looking tedious but the concept is very straightforward. I encourage you to write one partial derivative using the same approach to strengthen the concept.