

Notes on Neural Networks

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Introduction

TBD

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Chapter 1

Neural network basics

1.1 Logistic regression

Lets consider a simple example of logistic regression that can be used for classification task. I.e. it will provide **yes** or **no** answer on a question about input data.

Suppose our input data are represented as the following vector

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

The result is a scalar $y \in \{1, 0\}$

In the model of supervised learning we have a set of m samples that are used for learning process:

$$\begin{aligned} \vec{x}^{(1)} &\rightarrow y^{(1)}, \\ \vec{x}^{(2)} &\rightarrow y^{(2)}, \\ &\vdots \\ \vec{x}^{(m)} &\rightarrow y^{(m)} \end{aligned}$$

We want to construct a function \mathcal{Y} such that

$$\mathcal{Y}(\vec{x}^{(i)}) = y^{(i)}$$

for all $i \in \{1, \dots, m\}$. Taking into consideration that the result is a binary function, we can interpret \mathcal{Y} as a probability that the outcome will be 1, i.e.

$$\mathcal{Y}(\vec{x}) = p(y = 1 | \vec{x}) \tag{1.1}$$

from eq. (1.1) we can derive

$$\begin{aligned} p(y = 1 | \vec{x}) &= \mathcal{Y}(\vec{x}), \\ p(y = 0 | \vec{x}) &= 1 - p(y = 1 | \vec{x}) = \\ &= 1 - \mathcal{Y}(\vec{x}) \end{aligned}$$

Thus we can conclude that

$$\begin{aligned} p(y | \vec{x}) &= p(y = 1 | \vec{x})^y \cdot p(y = 0 | \vec{x})^{1-y} = \\ &= \mathcal{Y}(\vec{x})^y \cdot (1 - \mathcal{Y}(\vec{x}))^{1-y} \end{aligned} \quad (1.2)$$

For any test input $\vec{x}^{(i)} \rightarrow y^{(i)}$ we want to maximize the probability eq. (1.2). Taking into consideration that $p \geq 0$ and \log is a monotonic function [3] then we can conclude that we want to maximize $\log p$ or

$$\log p = y \cdot \log(\mathcal{Y}(\vec{x})) + (1 - y) \log(1 - \mathcal{Y}(\vec{x})) \quad (1.3)$$

Instead of maximizing $\log p$ eq. (1.3) we can minimize $-\log p$. Thus we will want to minimize the following cost function

$$\mathcal{L} = -y \cdot \log(\mathcal{Y}(\vec{x})) - (1 - y) \log(1 - \mathcal{Y}(\vec{x})) \quad (1.4)$$

That is similar to Shannon entropy [2].

We want to minimize eq. (1.4) for each test input i.e.

$$\mathcal{L}^{(i)} = -y^{(i)} \cdot \log(\mathcal{Y}(\vec{x}^{(i)})) - (1 - y^{(i)}) \log(1 - \mathcal{Y}(\vec{x}^{(i)})) \quad (1.5)$$

The eq. (1.5) can be combined into total cost function as follows

$$\mathcal{L} = -\frac{1}{m} \sum_{i=1}^m [y^{(i)} \cdot \log(\mathcal{Y}(\vec{x}^{(i)})) + (1 - y^{(i)}) \log(1 - \mathcal{Y}(\vec{x}^{(i)}))] \quad (1.6)$$

we have not spoke about \mathcal{Y} so far. Lets assume a linear dependency for it. it will consists of 2 functions: \mathcal{Z} and σ . The first one is the \mathcal{Z} that can be defined as follows

$$\mathcal{Z} = \vec{\omega}^T \vec{x} + b, \quad (1.7)$$

where

$$\vec{\omega} = \begin{bmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_n \end{bmatrix}$$

i.e. the vector of the same dimension as \vec{x} . The equation eq. (1.7) can be rewritten as follows

$$\mathcal{Z} = \sum_{j=1} \omega_j x_j + b$$

and can be considered as a linear form on x_j . The eq. (1.7) cannot be interpret as a probability and we need a special function apply on it that is monotonic [3] and has its value between 0 and 1. The sigmoid function is our choice:

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

Combining all together we can write

$$\mathcal{Y}(\vec{\omega}, b, \vec{x}) = \sigma(\vec{\omega}^T \vec{x} + b) \quad (1.8)$$

The form eq. (1.8) is useful for computational purposes as soon as modern computer uses SIMD (single instruction multiple data) instruction set that allows to implement vector operations extremely efficient.

We have parameters $\omega_1, \dots, \omega_n, b$ as unknown in eq. (1.8). We want to find them by finding a minimum for cost function eq. (1.6).

Contrary to eq. (1.8), our cost function is a function of unknown parameters only:

$$\begin{aligned} \mathcal{L}(\omega_1, \dots, \omega_n, b) = & -\frac{1}{m} \sum_{i=1}^m [y^{(i)} \cdot \log(\mathcal{Y}(\omega_1, \dots, \omega_n, b, \vec{x}^{(i)})) + \\ & + (1 - y^{(i)}) \log(1 - \mathcal{Y}(\omega_1, \dots, \omega_n, b, \vec{x}^{(i)}))] \end{aligned} \quad (1.9)$$

For finding a minimum of $\mathcal{L}(\omega_1, \dots, \omega_n, b)$ we can start with any point, for instance $\omega_j = 0, \forall j$ and $b = 0$ as well. Then we should move in the direction opposite to gradient:

$$\begin{aligned} \omega_j^{(k)} &= \omega_j^{(k-1)} - \alpha \frac{\partial \mathcal{L}}{\partial \omega_j}(\omega_1^{(k-1)}, \dots, \omega_n^{(k-1)}, b^{(k-1)}), \\ b^{(k)} &= b^{(k-1)} - \alpha \frac{\partial \mathcal{L}}{\partial b}(\omega_1^{(k-1)}, \dots, \omega_n^{(k-1)}, b^{(k-1)}) \end{aligned}$$

where α is a parameter that relegates how fast we move to the minimum, k is the iteration counter.

Thus to find the final formula we have to calculate the derivatives. Lets

rewrite our cost function eq. (1.9) for the easiest calculations

$$\begin{aligned}
\mathcal{L}(\omega_1, \dots, \omega_n, b) &= \\
&= -\frac{1}{m} \sum_{i=1}^m [y^{(i)} \cdot \log(\mathcal{Y}(\omega_1, \dots, \omega_n, b, \vec{x}^{(i)})) + \\
&\quad + (1 - y^{(i)}) \log(1 - \mathcal{Y}(\omega_1, \dots, \omega_n, b, \vec{x}^{(i)}))] = \\
&= -\frac{1}{m} \sum_{i=1}^m \left[y^{(i)} \log \left[\sigma \left(\sum_{j=1}^n \omega_j x_j^{(i)} + b \right) \right] + \right. \\
&\quad \left. + (1 - y^{(i)}) \log \left[1 - \sigma \left(\sum_{j=1}^n \omega_j x_j^{(i)} + b \right) \right] \right]
\end{aligned}$$

For instance

$$\frac{\partial \mathcal{L}}{\partial \omega_j} = -\frac{1}{m} \sum_{i=1}^m \left[y^{(i)} \frac{1}{\sigma} \frac{d\sigma}{dz} \frac{\partial z}{\partial \omega_j} - (1 - y^{(i)}) \frac{1}{1 - \sigma} \frac{d\sigma}{dz} \frac{\partial z}{\partial \omega_j} \right]$$

where we used

$$(\log(f))' = \frac{f'}{f}$$

and used z as

$$z = \sum_{j=1}^n \omega_j x_j^{(i)} + b$$

i.e.

$$\frac{\partial z}{\partial \omega_j} = x_j^{(i)}$$

from the other side

$$\begin{aligned}
\frac{d\sigma}{dz} &= -\frac{1}{(1 + e^{-z})^2} \cdot (-e^{-z}) = \\
&= \frac{1}{(1 + e^{-z})^2} \left(1 - \frac{1}{1 + e^{-z}} \right) (1 + e^{-z}) = \\
&= \frac{1}{1 + e^{-z}} \left(1 - \frac{1}{1 + e^{-z}} \right) = \sigma(z) (1 - \sigma(z)).
\end{aligned}$$

Thus

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \omega_j} &= -\frac{1}{m} \sum_{i=1}^m \left[y^{(i)} x_j^{(i)} (1 - \sigma(z)) - (1 - y^{(i)}) x_j^{(i)} \sigma(z) \right] = \\
&= -\frac{1}{m} \sum_{i=1}^m \left[y^{(i)} x_j^{(i)} - \sigma(z) y^{(i)} x_j^{(i)} - x_j^{(i)} \sigma(z) + y^{(i)} x_j^{(i)} \sigma(z) \right] = \\
&= -\frac{1}{m} \sum_{i=1}^m \left[y^{(i)} x_j^{(i)} - x_j^{(i)} \sigma(z) \right] = -\frac{1}{m} \sum_{i=1}^m x_j^{(i)} [y^{(i)} - \sigma(z)] = \\
&= \frac{1}{m} \sum_{i=1}^m x_j^{(i)} [\sigma(z) - y^{(i)}]
\end{aligned}$$

where

$$\sigma(z) = \sigma(\vec{\omega}^T \vec{x}^{(i)} + b).$$

For derivative by b we have

$$\frac{\partial \sigma}{\partial b} = 1,$$

thus

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{1}{m} \sum_{i=1}^m [\sigma(z) - y^{(i)}]$$

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