Christoph Windheuser, July 14, 2021

Supervised Learning

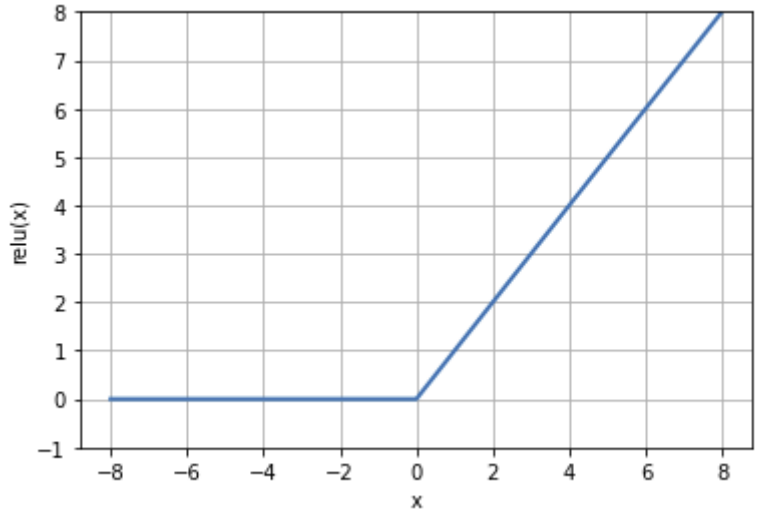
Definition of *Supervised Learning*:
(Goodfellow et.al. Deep Learning Book, p. 105)

Supervised learning involves observing several examples $X = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\}$ of a random vector $\mathbf{x}$ and associated values $Y = \{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(m)}\}$ of a random vector $\mathbf{y}$, and learning to predict $\mathbf{y}$ from $\mathbf{x}$, usually by estimating $p(\mathbf{y}|\mathbf{x})$.

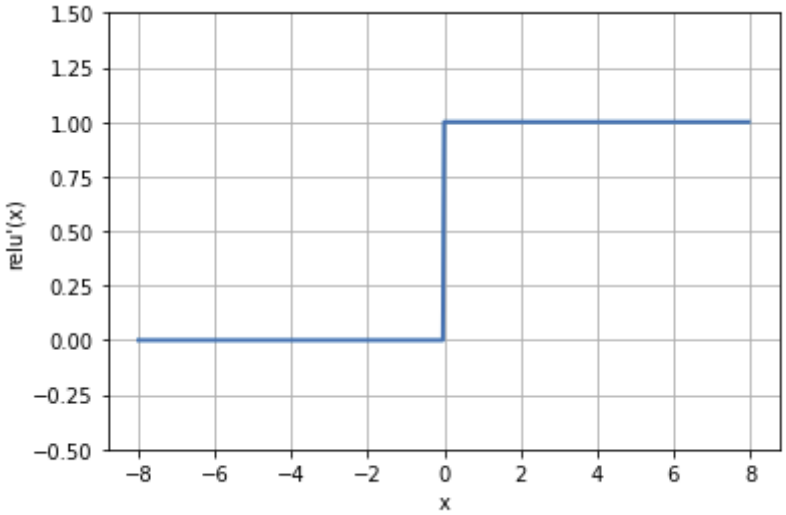
Activation Function for Hidden Units

The most widely used activation function in modern feedforward neural networks for hidden units is the *"Rectified Linear Unit"* or *RELU-function*. It is piecewise linear and has a non-linear point at 0. The function is easy to implement and very efficient. It is defined:

$$f_{RELU}(x) = \max\{0, x\} \tag{1}$$



The derivative of the RELU-function is defined 0 for $x <= 0$ and 1 for $x > 0$.



Activation Function for the Output Units - the Softmax Function

(Goodfellow et.al. Deep Learning Book, p. 183)

If the feedforward network is trained as a classifier to present the probability distribution over n different classes, the most used activation function of the output units is the *softmax function*.

For a feedforward network working as a classifier, we have to produce a vector $\mathbf{y}$ with $y_i = P(y = i|\mathbf{x})$ as the probability that the input vector $\mathbf{x}$ belongs to category i. To ensure that the output vector $\mathbf{y}$ is a valid probability distribution, all y_i of vector $\mathbf{y}$ must be between 0 and 1 and must sum up to 1. The softmax function ensures this:

$$softmax(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{n} \exp(z_j)} \tag{2}$$

z_i is the output of a linear layer as the output layer:

$$\mathbf{z} = \mathbf{W}^T \mathbf{h} + \mathbf{b} \tag{3}$$

When the network is trained to minimize the log likelihood, the output unit y_i approximates the conditional probability of class i given input pattern $\mathbf{x}$:

$$y_i = P(y = i|\mathbf{x}) \tag{4}$$

Cost Function

In order to train the desired behavior of a machine learning model with a set of parameters θ it is important to define the right *cost function*, as the gradient descent algorithm will minimize this function. The cost function $J(\theta)$ computes a *cost value* c dependent on the model parameters θ:

$$J(\theta) = c \tag{5}$$

Modern Feed-Forward Neural Networks are trained using the maximum likelihood function, which means that the cost function is the negative log-likelihood (NLL) or equivalently the cross-entropy between the training data distribution and the model distribution.

For multilayer perceptron classifier the negative conditional log-likelihood (NLL) as our cost function $J(\theta)$ of a set of parameter θ is defined as:

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} - \log p(\mathbf{y}^{(i)}|\mathbf{x}^{(i)}; \theta) \tag{6}$$

If we replace $p(\mathbf{y}^{(i)}|\mathbf{x}^{(i)})$ by the softmax function (2), we get:

$$\begin{aligned} J(\theta) &= \frac{1}{m} \sum_{i=1}^{m} \left(- \log \frac{\exp(z_i)}{\sum_{j=1}^{n} \exp(z_j)} \right) \\ &= -\frac{1}{m} \sum_{i=1}^{m} \left(\log \exp(z_i) - \log \sum_{j=1}^{n} \exp(z_j) \right) \\ &= -\frac{1}{m} \sum_{i=1}^{m} \left(z_i - \log \sum_{j=1}^{n} \exp(z_j) \right) \end{aligned} \tag{7}$$

Minimizing the NLL cost function $J(\theta)$ means to maximize z_i (the output of unit i) and to minimize the term $\log \sum_{j=1}^{n} \exp(z_j)$ which means to minimize all other output units $j \neq i$. This demonstrates the discriminative power of the maximum likelihood estimation algorithm.

Gradient Descent

Learning of a parameterized model is to optimize the parameters of the model in a way to minimize a *cost function* (also called *objective function, loss function* or *error function*).

As typically the optimal values of the parameters cannot be calculated directly, an iterative optimization approach is used.

If we assume that $J(\theta)$ is the cost function providing a cost value c for a parameter set θ. We want to find the optimal value for θ so that $J(\theta)$ is minimal. We use the derivative $J'(\theta)$ which gives us the slope at point θ. If the slope $J'(\theta) > 0$, decreasing θ will decrease $J(\theta)$. If the slope $J'(\theta) < 0$, increasing θ will decrease $J(\theta)$. By iteratively calculating new values for θ with:

$$\theta^{new} = \theta - \epsilon J'(\theta) \tag{8}$$

we can find at least a local minimum for $J(\theta)$ if ϵ is small enough. ϵ is called the *learning rate* and is a positive small number (usually $\epsilon << 1$).

As θ is an n-dimensional vector, the derivative is also a vector called the *gradient* $\nabla_\theta J(\theta)$. Element i of the gradient is the partial derivative of J with respect to θ_i. The iterative process of formula (8) is written:

$$\theta^{new} = \theta - \epsilon \nabla_\theta J(\theta) \tag{9}$$

This iterative technique is called *gradient descent* and is generally attributed to *Augustin-Louis Cauchy*, who first suggested it in 1847.

Optimizing the cost function with gradient descent

The gradient of the cost function of (6) is defined as:

$$\nabla_\theta J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \nabla_\theta \log p(\mathbf{y}^{(i)} | \mathbf{x}^{(i)}; \theta) \tag{10}$$

For every parameter θ_i the gradient $\nabla_{\theta i} J(\theta)$ has to be calculated:

$$\nabla_{\theta i} J(\theta) = \frac{\partial J(\theta)}{\partial \theta_i} \tag{11}$$

And the parameter θ_i is then changed by:

$$\theta_i^{new} = \theta_i - \epsilon \nabla_{\theta i} J(\theta) \tag{12}$$

Stochastic Gradient Descent (SGD)

(Goodfellow et.al. Deep Learning Book, p. 150)

Nearly all *deep learning* algorithms are working with a particular version of gradient descent: *stochastic gradient descent (SGD)*.

We have a set of several examples $X = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\}$ and $Y = \{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(m)}\}$ of a random vector $\mathbf{x}$ and an associated value or vector $\mathbf{y}$, and we are going to learn to predict $\mathbf{y}$ from $\mathbf{x}$ with gradient descent. We define the negative conditional log-likelihood (NLL) as our cost function $J(\theta)$ of a set of parameter θ:

$$J(\theta) = E_{x,y \sim \hat{P}_{data}} [L(\mathbf{x}, \mathbf{y}, \theta)] = \frac{1}{m} \sum_{i=1}^{m} L(\mathbf{x}^{(i)}, y^{(i)}, \theta) \tag{13}$$

L is the per-example loss:

$$L(\mathbf{x}, \mathbf{y}, \theta) = -\log p(\mathbf{y}|\mathbf{x}, \theta) \tag{14}$$

For this additive cost function, the gradient descent requires the computing of all per-example losses:

$$\nabla_\theta J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \nabla_\theta L(\mathbf{x}^{(i)}, y^{(i)}, \theta) \tag{15}$$

When the training size m is large, this is computational expensive or even impractical.

The idea of stochastic gradient descent is to see the gradient as an *expectation* (like in formula (13)). This expectation can can be approximately estimated using a smaller set of examples, a *minibatch* of examples $B_X = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m')}\}$ and $B_Y = \{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(m')}\}$ drawn uniformly from the training set. The size of the minibatch m' is typically chosen to be a small number ranging between 1 and a few hundred.

The estimate of the gradient $\mathbf{g}$ is calculated:

$$\mathbf{g} = \frac{1}{m'} \nabla_\theta \sum_{i=1}^{m'} L(\mathbf{x}^{(i)}, y^{(i)}, \theta) \tag{16}$$

using examples $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$ from the minibatch B_X and B_Y. Analog to formula (9) the parameters θ are changed along the negative estimate of the gradient $\mathbf{g}$ multiplied by the learning rate ϵ:

$$\theta^{new} = \theta - \epsilon\, \mathbf{g} \tag{17}$$

Weight Initialization

Before starting the learning algorithm, it is important to initialize the weights with small random values.

Label Smoothing

Label Smoothing Regularization (LSR) is a technique to regularize a classifier during training and was introduced by Christian Szegedy et. al. in the 2015 paper *Rethinking the Inception Architecture for Computer Vision* (link).

In a Multilayer Neural Network classifier, the activation of the output layer is usually calculated with the *softmax function* (see formula (2)) and the network is trained with the negative log-likelihood (NLL) against the *one-hot* labels of the training set. This encourages the network to maximize the output of the correct unit and to bring all other units to an output of zero or very close to zero. The behavior can lead to over-fitting and a weaker generalization of the network, as the networks becomes too confident about its predictions.

Szegedy et. al. propose to smooth the hard one-hot distribution of the labels by adding an additional distribution: For a label y the original desired output of the network is: $q(y|x) = 1$ and $q(k|x) = 0$ for all $k \neq y$. We can say that $q(k|x) = \delta_{k,y}$ where $\delta_{k,y}$ is the *Dirac delta* with $\delta_{k,y} = 1$ if $k = y$ and o for all $k \neq y$.

Szegedy et. al. are proposing a new label distribution $q'(k|x)$ with:

$$q'(k|x) = (1 - \epsilon)\delta_{k,y} + \epsilon u(k) \tag{18}$$

which is a mixture of the original distribution $q(k|x)$ and a fixed distribution $u(k)$. The paper proposes a simple uniform distribution $u(k) = 1/K$, K is the number different labels. The paper describes ImageNet experiments with $K = 1000$ classes and $\epsilon = 0.1$. They reported an consistent improvement of about 0.2% by Label Smoothing Regularization.

Links

- Original paper by Christian Szegedy et. al. (2015)
- How to implement Label Smoothing in TensorFlow or PyTorch (StackOverflow)