On Gradient

Giulio Galvan

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Abstract

1 How to compute gradient

1.1 Backpropagation

First of all we need to define a loss function over the training data, so we define a dataset D as

$$D \triangleq \{x^{(i)} \in \mathbb{R}^p, y^{(i)} \in \mathbb{R}^q, i \in [1, N]\} \tag{1}$$

and the loss function $L_D : \mathbb{R}^U \to \mathbb{R}_{\geq 0}$ over D as

$$L_D(w) \triangleq \frac{1}{N} \sum_{i=1}^{N} L_i(w) \tag{2}$$

where $w \in \mathbb{R}^U$ represents all the weights of the net and L_i is an arbitrary loss function for the ith example.

The network is composed of several layers as show in figure 1, each layer is composed of several neuron defined, as show in figure 2, by

$$a_l \triangleq \sum_j w_{lj} \phi_j \tag{3}$$

$$\phi_l \triangleq \sigma(a_l) \tag{4}$$

where w_{lj} is the weight of the connection between neuron j and neuron l and σ is the non linear activation function.

So we can compute partial derivatives with respect to a single weight w_{lj}, using simply the chain rule, as

$$\frac{\partial L}{\partial w_{lj}} = \frac{\partial L}{\partial a_l} \cdot \frac{\partial a_l}{\partial w_{lj}} = \delta_l \cdot \phi_j$$

where we put

$$\delta_l \triangleq \frac{\partial L}{\partial a_l} \tag{5}$$
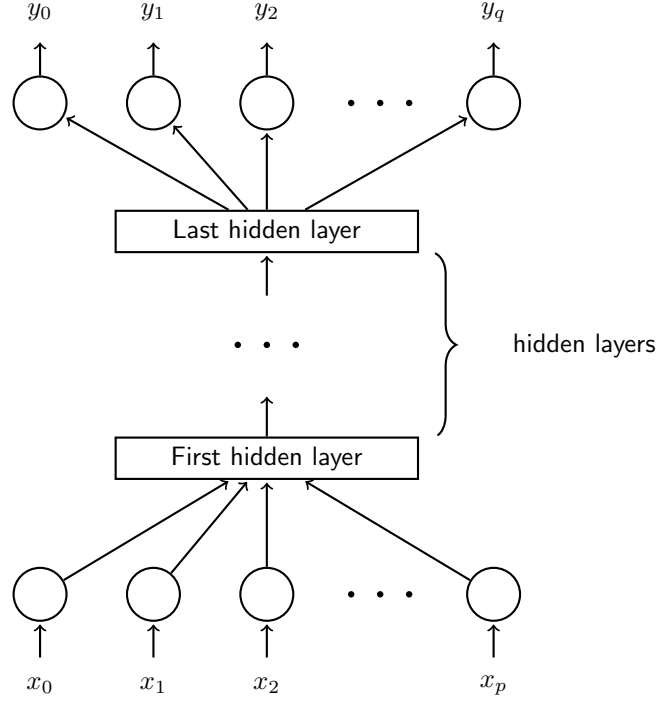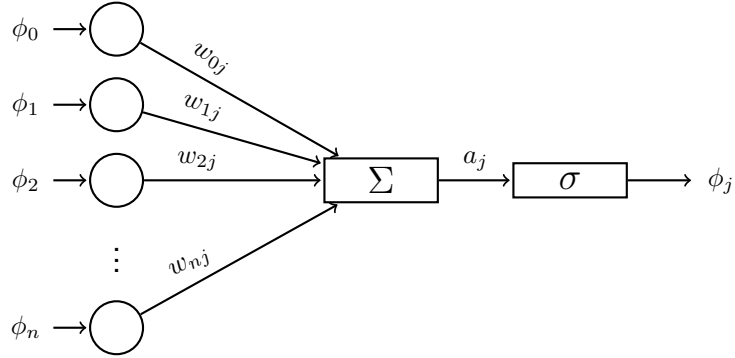
Figure 1: Feed forward neural network model

Figure 2: Neuron model

So we can easily compute $\delta_u = \frac{\partial L^{(i)}}{\partial a_u}$ for each output unit u once we choose a differentiable loss function; note that we don't need the weights for such a computation.

Let $P(l)$ be the set of parents of neuron l, formally:

$$P(l) = \{k : \exists \text{ a link between } l \text{ and } k \text{ with weight } w_{lk}\} \tag{6}$$

Again, simply using the chain rule, we can write, for each non output unit l:

$$\delta_l = \sum_{k \in P(l)} \frac{\partial L^{(i)}}{\partial a_k} \cdot \frac{\partial a_k}{\partial a_l} = \sum_{k \in P(l)} \delta_k \cdot \frac{\partial a_k}{\partial \phi_l} \cdot \frac{\partial \phi_l}{\partial a_l} = \sum_{k \in P(l)} \delta_k \cdot w_{kl} \cdot \sigma'(a_l) \qquad (7)$$

For output units instead we can compute $\delta_u = \frac{\partial L^{(i)}}{\partial a_u}$ directly once we define the loss function.

1.2   Backpropagation matrix notation

Here we rewrite the previously derived equations in matrix notation. Let us define the weight matrix for the ith layer as the $p(i) \times p(i-1)$ matrix whose elements $w_{l,k}$ are the weights of the arcs which link neuron k from level $i-1$ to neuron l from level i, where $p(i)$ is the number of neuron layer i is composed of.

$$\boldsymbol{a}_{i+1} \triangleq W_{i+1} \cdot \boldsymbol{\phi}_i \tag{8}$$

$$\boldsymbol{\phi}_{i+1} \triangleq \sigma(\boldsymbol{a}_{i+1}) \tag{9}$$

$$\boldsymbol{\phi}_1 \triangleq \boldsymbol{x} \tag{10}$$

where $\sigma(\cdot)$ is the non-linear activation function and it's applied element by element. We can rewrite equation 7 in matrix notation as:

$$\frac{\partial L}{\partial W_i} = \frac{\partial L}{\partial \boldsymbol{a}_i} \cdot \frac{\partial \boldsymbol{a}_i}{\partial W_i}^T = \Delta_i \cdot \boldsymbol{\phi}_{i-1}^T \tag{11}$$

where

$$\Delta_i \triangleq \frac{\partial L}{\partial \boldsymbol{a}_i} \tag{12}$$

$$\Delta_i = W_{i+1}^T \cdot \Delta_{i+1} \circ \sigma(\Delta_i) \tag{13}$$

References