Chapter 12

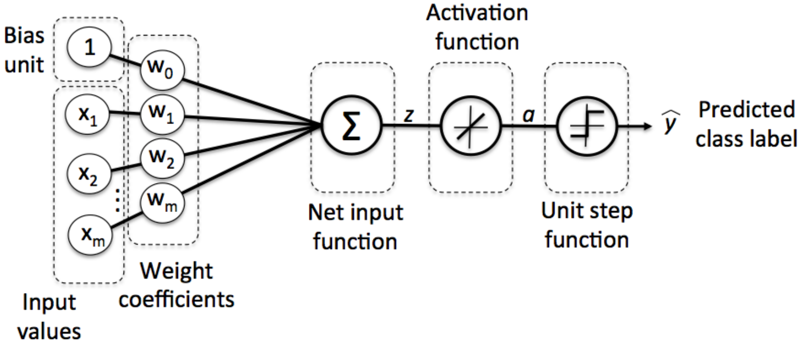
Artificial Neural Networks

August 15, 2016

Deep learning

- Big in ML
- Set of algorithms to train neural networks
- Python libraries available
- Outline
  - Forward propagation in ANNs
  - Backpropagation to learn the parameters
  - Debugging ANNs
  - Alternative architectures (CNN, RNN)

Single neuron review



Adaline review

- Perceptron
  - Update all weights, then recompute $\hat{y}$
  - Weight update done after seeing each sample

$$\Delta w_j = \eta \left(y^{(i)} - \hat{y}^{(i)} \right) x_j^{(i)}$$

- Adaline
  - Weight update done after entire training set has been seen
  - In every epoch, update all weights as follows:

$$\mathbf{w} := \mathbf{w} + \Delta \mathbf{w}, \quad \text{where } \Delta \mathbf{w} = -\eta \nabla J(\mathbf{w})$$

  - I.e. compute the gradient based on all samples in the training set (this is known as batch gradient descent)
  - SGD updates after seeing n samples
  - Mini-batch: middle ground bewteen SGD and batch GD

Weight update details

Partial derivative for each weight w_j in the weight vector $\mathbf{w}$:

$$\frac{\partial}{\partial w_j} J(\mathbf{w}) = \sum_i \left(y^{(i)} - a^{(i)}\right) x_j^{(i)}$$

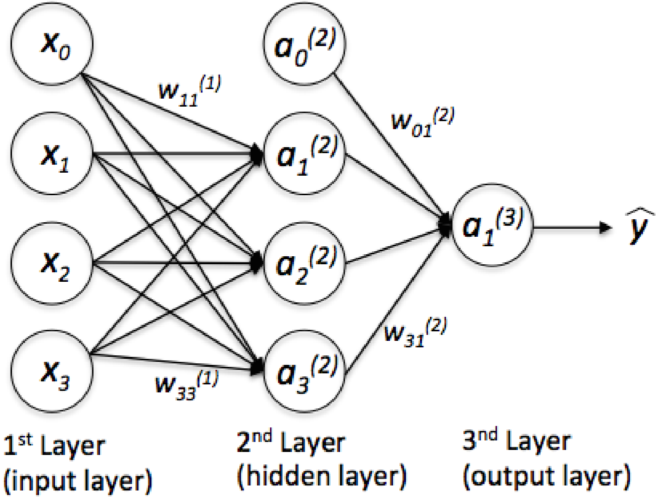
Here $y^{(i)}$ is the target class label of a particular sample $x^{(i)}$, and $a^{(i)}$ is the *activation* of the neuron, which is a linear function in the case of Adaline: Remember that we defined the *activation function* $\phi(\cdot)$ as follows:

$$\phi(z) = z = a$$

Here, the net input z is a linear combination of the weights that are connecting the input to the output layer:

$$z = \sum_j w_j x_j = \mathbf{w}^T \mathbf{x}$$

Multi-layer feedforward neural network



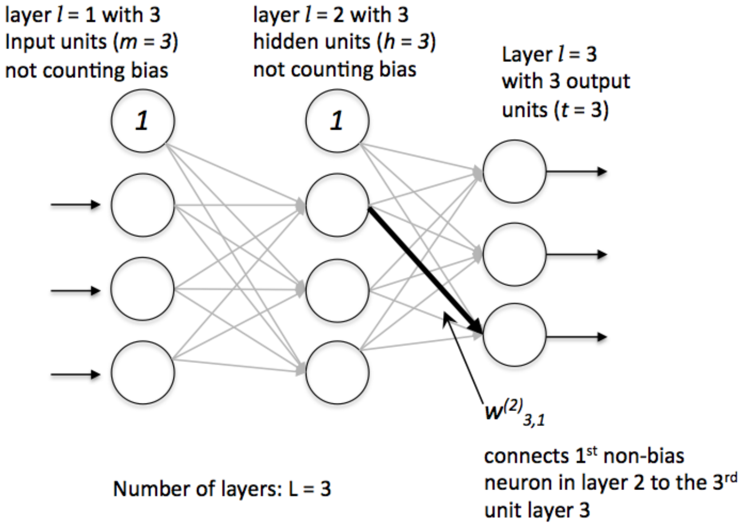
Notation

- We denote the ith activation unit in the lth layer as $a_i^{(l)}$
- The activation units $a_0^{(1)}$ and $a_0^{(2)}$ are the *bias units*, respectively, which we set equal to 1
- The activation of the units in the input layer:

$$\mathbf{a}^{(i)} = \begin{bmatrix} a_0^{(1)} \\ a_1^{(1)} \\ \vdots \\ a_m^{(1)} \end{bmatrix} = \begin{bmatrix} 1 \\ x_1^{(i)} \\ \vdots \\ x_m^{(i)} \end{bmatrix}$$

- The connection between the kth unit in layer l to the jth unit in layer $l+1$ written as $w_{j,k}^{(l)}$

Notation summary



MLP learning procedure

1. Starting at the input layer, forward propagate $\mathbf{x^{(i)}}$
2. Calculate the error that we will want to minimize
3. Find its derivative with respect to each weight
4. Update the weights

Forward propagation

1. Assume, input has m dimensions
2. Compute the net input $a_1^{(2)}$ for unit 1 in the hidden layer:

$$z_1^{(2)} = a_0^{(1)} w_{1,0}^{(1)} + a_1^{(1)} w_{1,1}^{(1)} + \cdots + a_m^{(1)} w_{l,m}^{(1)}$$

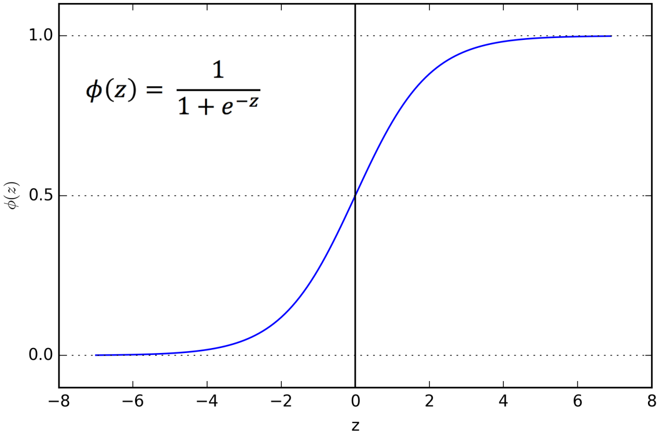
3. Compute the activation for unit 1 in the hidden layer:

$$a_1^{(2)} = \phi\left(z_1^{(2)}\right)$$

4. Here $\phi(\cdot)$ is the activation function
5. Logistic sigmoid is often used:

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

Sigmoid function



Vectorized notation

- Write activation in a matrix form
- Readability + more efficient code
- Net inputs for the hidden layer:

$$\mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{a}^{(1)}$$

- Dimensions (ignoring bias units for simplicity)

$$[h \times 1] = [h \times m][m \times 1]$$

- Activations for the hidden layer:

$$\mathbf{a}^{(2)} = \phi\left(\mathbf{z}^{(2)}\right)$$

Matrix notation

- Generalize computation to all n samples in the training set

$$\mathbf{Z}^{(2)} = \mathbf{W}^{(1)} \left[\mathbf{A}^{(1)}\right]^T$$

- Matrix dimensions

$$[h \times n] = [h \times m][n \times m]^T$$

- Activation matrix

$$\mathbf{A}^{(2)} = \phi\left(\mathbf{Z}^{(2)}\right)$$

- Now activation of the output layer

$$\mathbf{Z}^{(3)} = \mathbf{W}^{(2)} \mathbf{A}^{(2)}$$

- Matrix dimensions

$$[t \times n] = [t \times h][h \times n]$$

- Output of the network

$$\mathbf{A}^{(3)} = \phi\left(\mathbf{Z}^{(3)}\right), \ \mathbf{A}^{(3)} \in \mathbb{R}^{t \times n}.$$

Cost function

The logistic Cost function is the same we used for logistic regression:

$$J(\mathbf{w}) = -\sum_{i=1}^{n} y^{(i)} \log\left(a^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - a^{(i)}\right)$$

Here, $a^{(i)}$ is the sigmoid activation of the ith unit $a^{(i)} = \phi\left(z^{(i)}\right)$.
Regularization:

$$L2 = \lambda \|\mathbf{w}\|_2^2 = \lambda \sum_{j=1}^{m} w_j^2$$

$$J(\mathbf{w}) = -\left[\sum_{i=1}^{n} y^{(i)} \log\left(a^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - a^{(i)}\right)\right] + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

Cost function for all units in output layer

The activation of the third layer and the target class could be:

$$a^{(3)} = \begin{bmatrix} 0.1 \\ 0.9 \\ \vdots \\ 0.3 \end{bmatrix}, \ \mathbf{y} = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

So, we need to generalize the logistic cost function to all activation units j in our network. The cost function (without the regularization term) becomes:

$$J(\mathbf{w}) = -\sum_{i=1}^{n}\sum_{j=1}^{t} y_j^{(i)} \log(a_j^{(i)}) + (1 - y_j^{(i)}) \log(1 - a_j^{(i)})$$

Superscript i is the index of a particular sample in training set

Cost function for the entire network

Sum all the weights in the entire network in the regularization term:

$$J(\mathbf{w}) = -\left[\sum_{i=1}^{n}\sum_{j=1}^{m} y_j^{(i)} \log\left(\phi\left(z_j^{(i)}\right)\right) + \left(1 - y_j^{(i)}\right) \log\left(1 - \phi\left(z_j^{(i)}\right)\right)\right] +$$

$$+\frac{\lambda}{2}\sum_{l=1}^{L-1}\sum_{i=1}^{u_l}\sum_{j=1}^{u_{l+1}}\left(w_{j,i}^{(l)}\right)^2$$

The following expression represents the L2-penalty term:

$$\frac{\lambda}{2}\sum_{l=1}^{L-1}\sum_{i=1}^{u_l}\sum_{j=1}^{u_{l+1}}\left(w_{j,i}^{(l)}\right)^2$$

Minimizing the cost function

We want to minimize the cost function $J(\mathbf{w})$, so we calculate the partial derivative with respect to each weight for every layer in the network:

$$\frac{\partial J(\mathbf{W})}{\partial w_{j,i}^{(l)}}$$