Inf2b - Learning

Lecture 14: Multi-layer neural networks (1)

Hiroshi Shimodaira
(Credit: Iain Murray and Steve Renals)

Centre for Speech Technology Research (CSTR)
School of Informatics
University of Edinburgh

http://www.inf.ed.ac.uk/teaching/courses/inf2b/
https://piazza.com/ed.ac.uk/spring2020/infr08028
Office hours: Wednesdays at 14:00-15:00 in IF-3.04

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Today's Schedule

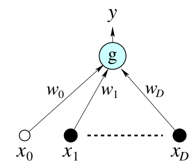
1. Single-layer network with a single output node (recap)
2. Single-layer network with multiple output nodes
3. Multi-layer neural network
4. Activation functions

Single-layer network with a single output node (recap)

- Activation function:

$$y = g(a) = g\left(\sum_{i=0}^{D} w_i x_i\right)$$

$$g(a) = \frac{1}{1+\exp(-a)}$$



- Training set : $\mathcal{D} = \{(\mathbf{x}_n, t_n)\}_{n=1}^{N}$
  where $t_n \in \{0,1\}$
- Error function:

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}(y_n - t_n)^2$$

- Optimisation problem (training)

$$\min_{\boldsymbol{w}} E(\boldsymbol{w})$$

Training of single layer neural network

- Optimisation problem: $\min_{\boldsymbol{w}} E(\boldsymbol{w})$
- No analytic solution (no closed form)
- Employ an iterative method (requires initial values)
  e.g. Gradient descent (steepest descent), Newton's method, Conjugate gradient methods
- Gradient descent
  (scalar rep.)

$$w_i^{(\text{new})} \leftarrow w_i - \eta\frac{\partial}{\partial w_i}E(\boldsymbol{w}), \qquad (\eta > 0)$$

  (vector rep.)

$$\boldsymbol{w}^{(\text{new})} \leftarrow \boldsymbol{w} - \eta\nabla_{\boldsymbol{w}}E(\boldsymbol{w}), \qquad (\eta > 0)$$

- Online/stochastic gradient descent (cf. Batch training)
  Update the weights one pattern at a time. (See Note 11)

Training of the single-layer neural network

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}(y_n - t_n)^2 = \frac{1}{2}\sum_{n=1}^{N}(g(a_n) - t_n)^2$$

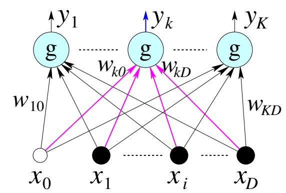
where $y_n = g(a_n)$, $a_n = \sum_{i=0}^{D} w_i x_{ni}$, $\frac{\partial a_n}{\partial w_i} = x_{ni}$

$$\frac{\partial E(\boldsymbol{w})}{\partial w_i} = \frac{\partial E(\boldsymbol{w})}{\partial y_n}\frac{\partial y_n}{\partial a_n}\frac{\partial a_n}{\partial w_i}$$

$$= \sum_{n=1}^{N}(y_n - t_n)\frac{\partial g(a_n)}{\partial a_n}\frac{\partial a_n}{\partial w_i}$$

$$= \sum_{n=1}^{N}(y_n - t_n)\, g'(a_n)\, x_{ni}$$

Single-layer network with multiple output nodes



- K output nodes: $y_1, \ldots, y_K$.
- For $\mathbf{x}_n = (x_{n0}, \ldots, x_{nD})^T$,

$$y_{nk} = g\left(\sum_{i=0}^{D} w_{ki}\, x_{ni}\right) = g(a_{nk})$$

$$a_{nk} = \sum_{i=0}^{D} w_{ki}\, x_{ni}$$

Single-layer network with multiple output nodes

- Training set : $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{t}_1), \ldots, (\mathbf{x}_N, \mathbf{t}_N)\}$
  where $\mathbf{t}_n = (t_{n1}, \ldots, t_{nK})$ and $t_{nk} \in \{0,1\}$
- Error function:

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}\|\mathbf{y}_n - \mathbf{t}_n\|^2 = \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

$$= \sum_{n=1}^{N} E_n, \quad \text{where } E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

- Training by the gradient descent:

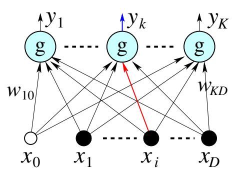
$$w_{ki} \leftarrow w_{ki} - \eta\frac{\partial E}{\partial w_{ki}}, \qquad (\eta > 0)$$

The derivatives of the error function (single-layer)

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

$$y_{nk} = g(a_{nk})$$

$$a_{nk} = \sum_{i=0}^{D} w_{ki} x_{ni}$$



$$\frac{\partial E_n}{\partial w_{ki}} = \frac{\partial E_n}{\partial y_{nk}}\frac{\partial y_{nk}}{\partial a_{nk}}\frac{\partial a_{nk}}{\partial w_{ki}}$$

$$= (y_{nk} - t_{nk})\, g'(a_{nk})\, x_{ni}$$

Multi-layer neural networks

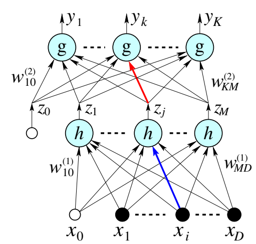
Multi-layer perceptron (MLP)

- Hidden-to-output weights:

$$w_{kj}^{(2)} \leftarrow w_{kj}^{(2)} - \eta\frac{\partial E}{\partial w_{kj}^{(2)}}$$

- Input-to-hidden weights:

$$w_{ji}^{(1)} \leftarrow w_{ji}^{(1)} - \eta\frac{\partial E}{\partial w_{ji}^{(1)}}$$



Training of MLP

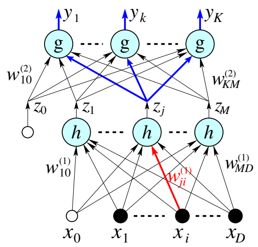
- 1940s Warren McCulloch and Walter Pitts : 'threshold logic'
  Donald Hebb : 'Hebbian learning'
- 1957 Frank Rosenblatt : 'Perceptron'
- 1969 Marvin Minsky and Seymour Papert : limitations of neural networks
- 1980 Kunihiro Fukushima: 'Neocognitoron'
- 1986 D. Rumelhart, G. Hinton, and R. Williams, "Learning representations by back-propagating errors" (1974, Paul Werbos)

The derivatives of the error function (two-layers)

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk}-t_{nk})^2$$

$$y_{nk} = g(a_{nk}), \quad a_{nk} = \sum_{j=1}^{M} w_{kj}^{(2)} z_{nj}$$

$$z_{nj} = h(b_{nj}), \quad b_{nj} = \sum_{i=0}^{D} w_{ji}^{(1)} x_{ni}$$



$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \frac{\partial E_n}{\partial y_{nk}}\frac{\partial y_{nk}}{\partial a_{nk}}\frac{\partial a_{nk}}{\partial w_{kj}^{(2)}}$$

$$= (y_{nk}-t_{nk})\, g'(a_{nk})\, z_{nj}$$

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}}\frac{\partial z_{nj}}{\partial b_{nj}}\frac{\partial b_{nj}}{\partial w_{ji}^{(1)}} = \left(\sum_{k=1}^{K}(y_{nk}-t_{nk})\frac{\partial y_{nk}}{\partial z_{nj}}\right) h'(b_{nj})\, x_{ni}$$

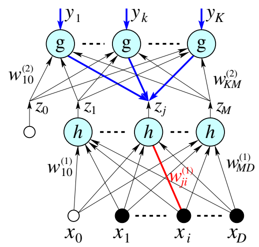
$$= \left(\sum_{k=1}^{K}(y_{nk}-t_{nk}) g'(a_{nk}) w_{kj}^{(2)}\right) h'(b_{nj})\, x_{ni}$$

Error back propagation

$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \frac{\partial E_n}{\partial y_{nk}}\frac{\partial y_{nk}}{\partial a_{nk}}\frac{\partial a_{nk}}{\partial w_{kj}^{(2)}}$$

$$= (y_{nk}-t_{nk})\, g'(a_{nk})\, z_{nj}$$

$$= \delta_{nk}^{(2)} z_{nj}, \quad \delta_{nk}^{(2)} = \frac{\partial E_n}{\partial a_{nk}}$$

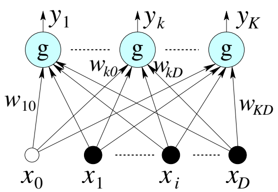


$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}}\frac{\partial z_{nj}}{\partial b_{nj}}\frac{\partial b_{nj}}{\partial w_{ji}^{(1)}}$$

$$= \left(\sum_{k=1}^{K}(y_{nk}-t_{nk}) g'(a_{nk}) w_{kj}^{(2)}\right) h'(b_{nj})\, x_{ni}$$

$$= \left(\sum_{k=1}^{K}\delta_{nk}^{(2)} w_{kj}^{(2)}\right) h'(b_{nj})\, x_{ni}$$

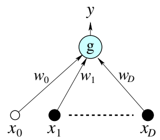
Notes on Activation functions



- Interpretation of output values
- Normalisation of the output values
- Other activation functions

Output of logistic sigmoid activation function

- Consider a single-layer network with a single output node logistic sigmoid activation function:



$$y = g(a) = \frac{1}{1+\exp(-a)} = g\left(\sum_{i=0}^{D} w_i x_i\right)$$

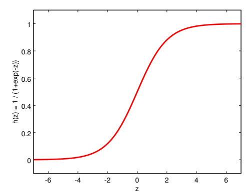
$$= \frac{1}{1+\exp\left(-\sum_{i=0}^{D} w_i x_i\right)}$$

- Consider a two class problem, with classes C_1 and C_2. The posterior probability of C_1:

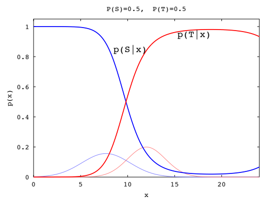
$$P(C_1|\mathbf{x}) = \frac{p(\mathbf{x}|C_1)\,P(C_1)}{p(\mathbf{x})} = \frac{p(\mathbf{x}|C_1)\,P(C_1)}{p(\mathbf{x}|C_1)\,P(C_1) + p(\mathbf{x}|C_2)\,P(C_2)}$$

$$= \frac{1}{1+\frac{p(\mathbf{x}|C_2)\,P(C_2)}{p(\mathbf{x}|C_1)\,P(C_1)}} = \frac{1}{1+\exp\left(-\ln\frac{p(\mathbf{x}|C_1)\,P(C_1)}{p(\mathbf{x}|C_2)\,P(C_2)}\right)}$$

Approximation of posterior probabilities



Logistic sigmoid function $g(a) = \dfrac{1}{1+\exp(-a)}$



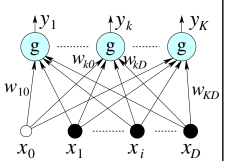
Posterior probabilities of two classes with Gaussian distributions:

Normalisation of output nodes

- Outputs with sigmoid activation funtion:

$$\sum_{k=1}^{K} y_k \neq 1$$

$$y_k = g(a_k) = \frac{1}{1+\exp(-a_k)}, \quad a_k = \sum_{i=0}^{D} w_{ki} x_i$$



- Softmax activation function for $g()$:

$$y_k = \frac{\exp(a_k)}{\sum_{\ell=1}^{K}\exp(a_\ell)}$$

- Properties of the softmax function
  - (i) $0 \le y_k \le 1$
  - (ii) $\sum_{k=1}^{K} y_k = 1$
  - (iii) differentiable
  - (iv) $y_k \approx P(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)P(C_k)}{\sum_{\ell=1}^{K} p(\mathbf{x}|C_\ell)P(C_\ell)}$

Some questions on activation functions

- Is the logistic sigmoid function necessary for single-layer single-output-node network?
  - No, in terms of classification. (we can replace it with $g(a) = a$)
- What benefits are there in using the logistic sigmoid function?

Summary

- Training of single-layer network
- Training of multi-layer network with 'error back propagation'
- Activation functions
  - Approximation of posterior probabilities
    - Sigmoid function (for single output node)
    - Softmax function (for multiple output nodes)
- A very good reference: http://neuralnetworksanddeeplearning.com/