PRML 5.[1,2,5-8,18]

1. EX 5.1 answer here.

Let a_k^s to be activation for the neural network whose activation function in the hidden layer is sigmoid function. Denote parameters in this neural network as $w_{kj}^{(2s)}, w_{k0}^{(2s)}, w_{ji}^{(1s)}, w_{j0}^{(1s)}$. Let a_k^t to be activation for the neural network whose activation function in the hidden layer is tanh function. Denote parameters in this neural network as $w_{kj}^{(2t)}, w_{k0}^{(2t)}, w_{ji}^{(1t)}, w_{j0}^{(1t)}$.

According to Ex 3.1, $tanh(a) = 2\sigma(2a) - 1$. Then,

$$\begin{split} a_k^t &= \sum_{j=1}^M w_{kj}^{(2t)} tanh(\sum_{i=1}^D w_{ji}^{(1t)} x_i + w_{j0}^{(1t)}) + w_{k0}^{(2t)} \\ &= \sum_{j=1}^M w_{kj}^{(2t)} (2\sigma(2(\sum_{i=1}^D w_{ji}^{(1t)} x_i + w_{j0}^{(1t)})) - 1) + w_{k0}^{(2t)} \ (substitute \ tanh(a) = 2\sigma(2a) - 1) \\ &= \sum_{j=1}^M 2w_{kj}^{(2t)} \sigma(2(\sum_{i=1}^D w_{ji}^{(1t)} x_i + w_{j0}^{(1t)})) - \sum_{j=1}^M w_{kj}^{(2t)} + w_{k0}^{(2t)} \ (simplify \ the \ function \ outside \ \sigma) \\ &= \sum_{j=1}^M 2w_{kj}^{(2t)} \sigma(\sum_{i=1}^D 2w_{ji}^{(1t)} x_i + 2w_{j0}^{(1t)})) - \sum_{j=1}^M w_{kj}^{(2t)} + w_{k0}^{(2t)} \ (simplify \ the \ \sigma \ function) \end{split}$$

$$a_k^s = \sum_{j=1}^M w_{kj}^{(2s)} \sigma(\sum_{i=1}^D w_{ji}^{(1s)} x_i + w_{j0}^{(1s)}) + w_{k0}^{(2s)}$$

To make two networks equivalent, $a_k^t = a_k^s$. Therefore, $\sum_{j=1}^M w_{kj}^{(2s)} \sigma(\sum_{i=1}^D w_{ji}^{(1s)} x_i + w_{j0}^{(1s)}) + w_{k0}^{(2s)} = \sum_{j=1}^M 2w_{kj}^{(2t)} \sigma(\sum_{i=1}^D 2w_{ji}^{(1t)} x_i + 2w_{j0}^{(1t)})) - \sum_{j=1}^M w_{kj}^{(2t)} + w_{k0}^{(2t)}$

Then, through linear transformation, we make $w_{kj}^{(2s)}=2w_{kj}^{(2t)},~w_{k0}^{(2s)}=-\sum_{j=1}^{M}w_{kj}^{(2t)}+w_{k0}^{(2t)},~w_{ji}^{(1s)}=2w_{ji}^{(1t)},~\text{and}~w_{j0}^{(1s)}=2w_{j0}^{(1t)}.$

2. Ex 5.2 answer here

The likelihood function under the conditional distribution for a multioutput neural network is $\prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, w), \beta^{-1}I)$. To maximize this function is equivalent to minimize the negative log of it, which is

$$-ln(\prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, w), \beta^{-1}I)) = -\sum_{n=1}^{N} ln(\mathcal{N}(t_n|y(x_n, w)) \ (basic log operation)$$

$$= \frac{1}{2} \sum_{n=1}^{N} (t_n - y(x_n, w))^T (\beta I)(t_n - y(x_n, w)) - \frac{NK}{2} ln(\beta) + const$$

$$(According to (5.13))$$

$$(const is a value that is independent of w and \beta)$$

$$= \frac{\beta}{2} \sum_{n=1}^{N} (t_n - y(x_n, w))^T I(t_n - y(x_n, w)) - \frac{NK}{2} ln(\beta) + const$$

$$(take \ \beta \ out, \ since \ it \ is \ independent \ of \ n)$$

$$= \frac{\beta}{2} \sum_{n=1}^{N} (t_n - y(x_n, w))^T (t_n - y(x_n, w)) - \frac{NK}{2} ln(\beta) + const$$

$$(since \ I \ is \ identity \ matrix)$$

$$= \frac{\beta}{2} \sum_{n=1}^{N} ||t_n - y(x_n, w)^T||^2 - \frac{NK}{2} ln(\beta) + const$$

$$(since \ w^T w = ||w||^2)$$

The first term of this function is (5.11). Therefore, to minimize the negative log of (5.16) is to minimize (5.11). Hence, maximize (5.16) is equivalent to minimize (5.11).

3. Ex 5.5 answer here.

Taking the negative log of the likelihood is

$$E(w) = -\ln\left(\prod_{n=1}^{N}\prod_{k=1}^{K}y_{nk}(x_n, w)^{t_n k}[1 - y_{nk}(x_n, w)^{1-t_n k}]\right) (plug in (5.22))$$

$$= -\sum_{n=1}^{N}\ln\left(\prod_{k=1}^{K}y_{nk}(x_n, w)^{t_n k}[1 - y_{nk}(x_n, w)]^{1-t_n k}\right) (basic log operation)$$

$$= -\sum_{n=1}^{N}\sum_{k=1}^{K}y_{nk}\ln((x_n, w)^{t_n k}[1 - y_{nk}(x_n, w)]^{1-t_n k}) (basic log operation)$$

$$= -\sum_{n=1}^{N}\sum_{k=1}^{K}\ln(y_{nk}(x_n, w)^{t_n k}) + \ln([1 - y_{nk}(x_n, w)]^{1-t_n k}) (basic log operation)$$

$$= -\sum_{n=1}^{N}\sum_{k=1}^{K}(t_n k)\ln(y_{nk}(x_n, w)) + (1 - t_n k)\ln([1 - y_{nk}(x_n, w)]) (basic log operation)$$

$$= -\sum_{n=1}^{N}\sum_{k=1}^{K}(t_n k)\ln(y_{nk}) + (1 - t_n k)\ln((1 - y_{nk})) (Let y_{nk} = y_{nk}(x_n, w))$$

$$= -\sum_{n=1}^{N}\sum_{k=1}^{K}(t_n k)\ln(y_{nk})$$

$$(since t_{nk} \in \{0, 1\} and y_{nk} = p(t_{nk} = 1|x), I get rid of the last term)$$

Therefore, maximizing likelihood for a multiclass neural network model in which the network outputs have the interpretation $y_k(x, w) = p(t_k = 1|x)$ is equivalent to the minimization of the corss-entropy error function (5.24).

4. Ex 5.6 answer here

Since
$$y_n = \sigma(a_n) = \frac{1}{1 + e^{-a_n}}, \ \frac{\partial y_n}{\partial a_n} = \frac{0 - 1(-e^{a_n})}{(1 + e^{-a_n})^2} = \frac{e^{a_n}}{(1 + e^{-a_n})^2} = \frac{1}{1 + e^{a_n}} \frac{e^{a_n}}{1 + e^{a_n}} = y_n(1 - y_n)$$

$$\begin{split} \frac{\partial E(w)}{\partial a_n} &= \frac{\partial - (t_k ln(y_k) + (1-t_k) ln(1-y_k))}{\partial a_k} \\ &(plug\ in E(w) = -\sum_{n=1}^N (t_n ln(y_n) + (1-t_n) ln(1-y_n))) \\ &((t_k ln(y_k) + (1-t_k) ln(1-y_k)\ is\ the\ only\ term\ that\ depends\ on\ a_k) \\ &= -\frac{t_k ln(y_k) + (1-t_k) ln(1-y_k)}{\partial a_k}\ (take\ summation\ out) \\ &= -(\frac{t_k}{y_k} \frac{\partial y_k}{\partial a_k} - \frac{1-t_k}{1-y_k} \frac{\partial y_k}{\partial a_k})\ (chain\ rule) \\ &= -(\frac{\partial y_k}{\partial a_k} \frac{t_k(1-y_k) - (1-t_k)y_k}{y_k(1-y_k)}) \\ &= -(\frac{\partial y_k}{\partial a_k} \frac{t_k-y_k}{y_k(1-y_k)}) \\ &= -(y_k(1-y_k) \frac{t_k-y_k}{y_k(1-y_k)})\ (plug\ in\ \frac{\partial y_k}{\partial a_k} = y_k(1-y_k)) \\ &= -(t_k-y_k) \\ &= y_k-t_k \end{split}$$

5. Ex 5.7 answer here

According to previous HW (4.17), $\frac{\partial y_k}{\partial a_j} = y_k(I_{kj} - y_j)$.

$$\begin{split} \frac{\partial E(w)}{\partial a_{j}} &= \frac{\partial - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} ln(y_{k}(x_{n}, w))}{\partial a_{j}} \ (plug \ in \ E(w) = - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} ln(y_{k})(x_{n}, w)) \\ &= - \sum_{n=1}^{N} \sum_{k=1}^{K} \frac{\partial t_{kn} ln(y_{k}(x_{n}, w))}{\partial a_{j}} \ (take \ summations \ out) \\ &= - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} \frac{1}{y_{k}(x_{n}, w)} \frac{\partial y_{k}(x_{n}, w)}{\partial a_{j}} \ (chain \ rule) \\ &= - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} \frac{1}{y_{kn}} \frac{\partial y_{kn}}{\partial a_{j}} \ (denote \ y_{k}(x_{n}, w) \ as \ y_{kn}) \\ &= - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} \frac{1}{y_{kn}} y_{kn} (I_{kj} - y_{jn}) \ (plug \ in \frac{\partial y_{k}}{\partial a_{j}} = y_{k} (I_{kj} - y_{j})) \\ &= - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} I_{kj} - t_{kn} y_{jn} \\ &= - \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} I_{kj} + \sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} y_{jn} \\ &= - \sum_{n=1}^{N} t_{jn} + \sum_{n=1}^{N} y_{jn} \ (I_{kj} = 1, \ only \ when \ k = j. \ Otherwise, \ I_{kj} = 0. \sum_{k=1}^{K} t_{kn} = 1) \\ &= \sum_{n=1}^{N} (y_{jn} - t_{jn}) \end{split}$$

6. Ex 5.8 answer here

According to (5.59), $tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$.

Then.

$$\begin{split} d\frac{tanh(a)}{da} &= \frac{d\frac{e^a - e^{-a}}{e^a + e^{-a}}}{da} \; (plug \; intanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}) \\ &= \frac{(e^a + e^{-a})(e^a + e^{-a}) - (e^a - e^{-a})(e^a - e^{-a})}{(e^a + e^{-a})^2} \; (division \; rule) \\ &= \frac{(e^a + e^{-a})^2}{(e^a + e^{-a})^2} - \frac{(e^a - e^{-a})^2}{(e^a + e^{-a})^2} \\ &= 1 - tanh(a)^2 \; (plug \; in \; tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}) \end{split}$$

7. Ex 5.18

Suppose the extra parameters corresponding to skip-layer connections that go directly from the inputs to the outputs is given by the matrix s_{ij} . Introducing skip layer weights s_{ij} into the two-layer network of the form shown in Fig. 5.1 would only affect the forward propagation equation Eq. (5.64):

$$y_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + \sum_{i=1}^{D} s_{ki} x_i$$

Then,
$$\frac{\partial y_k}{\partial s_{ki}} = \frac{\partial \sum_{j=1}^M w_{kj}^{(2)} z_j + \sum_{i=1}^D s_{ki} x_i}{\partial s_{ki}} = x_i$$

According to Eq. (5.61), $E_n = \frac{1}{2} \sum_{k=1}^K (y_k - t_k)^2$. Therefore, $\frac{\partial E_n}{\partial y_k} = \frac{1}{2} 2(y_k - t_k)$ (chain rule and $y_k = a_k$ due to linear activation function)

$$= y_k - t_k = \delta_k$$
 (definition of δ_k in Eq.(5.65)).

$$\frac{\partial E_n}{\partial s_{ki}} = \frac{\partial E_n}{\partial y_k} \frac{\partial y_k}{\partial s_{ki}} \quad (chain \ rule)$$

$$= \delta_k x_i \quad (substitute \ \frac{\partial y_k}{\partial s_{ki}} = x_i, \ and \ \frac{\partial E_n}{\partial y_k} = \delta_k)$$