Machine Learning - Theoretical exercise 5

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Problem 1

Let φ be a linear function used as the activation function for the two-layer network. As φ is linear, we have $\varphi(u) = ku$, with $k \in \mathbb{R}$. We first compute the outputs at the first layer.

$$\begin{aligned} \boldsymbol{y}^{(1)} &= \varphi\left(\boldsymbol{\Theta}^{(1)}\boldsymbol{x}\right) \\ &= k\boldsymbol{\Theta}^{(1)}\boldsymbol{x} \end{aligned}$$

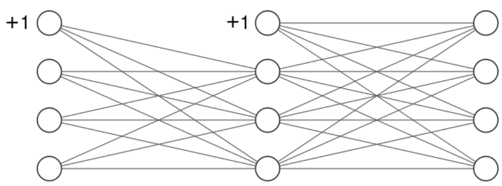
We can now use this result for computing the outputs at the second layer.

$$\begin{aligned} \boldsymbol{y}^{(2)} &= \varphi\left(\boldsymbol{\Theta}^{(2)}\boldsymbol{y}^{(1)}\right) \\ &= \varphi\left(\boldsymbol{\Theta}^{(2)}k\boldsymbol{\Theta}^{(1)}\boldsymbol{x}\right) \\ &= k^2\boldsymbol{\Theta}^{(2)}\boldsymbol{\Theta}^{(1)}\boldsymbol{x} \end{aligned}$$

We see that this result is equivalent to a single layer network having $k^2\boldsymbol{\Theta}^{(2)}\boldsymbol{\Theta}^{(1)}$ as its weight matrix and constant activation function.

Problem 2

a) The network has the following structure. The +1 neurons indicate the bias units.



b) Normalizing the training vectors gives us the following normalized dataset.

$$x_1 = \begin{bmatrix} 1 \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix} \; x_2 = \begin{bmatrix} 1 \\ \frac{1}{4} \\ 0 \end{bmatrix} \; x_3 = \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{bmatrix} \; x_4 = \begin{bmatrix} \frac{1}{2} \\ 0 \\ 0 \end{bmatrix}$$

c) Let σ be the activation function used in the network. We could compute the consecutive outputs by performing a matrix multiplication and then a matrix addition.

$$\boldsymbol{y} = \sigma(\boldsymbol{\Theta}\boldsymbol{x} + \boldsymbol{b})$$

but it is easier to incorporate the bias to our weight matrix, and prepend a unit component to each of our training vectors, as this allows us to perform a single matrix multiplication. In the following, this augmented weight matrix will be denoted $\boldsymbol{\Theta}$. The first column of $\boldsymbol{\Theta}$ corresponds to the bias weights, and the remaining columns to the given $\boldsymbol{\theta}$ values. The normalized training vectors are prepended with a unit row, corresponding to the bias component. We denote an augmented vector with the hat notation $\boldsymbol{x} \to \hat{\boldsymbol{x}}$.

We first compute the output at the first hidden layer.

$$\begin{aligned}
\boldsymbol{y}_1^{(1)} &= \sigma\left(\boldsymbol{\Theta}^{(1)}\hat{\boldsymbol{x}}_1\right) \\
&= \sigma\left(\begin{bmatrix} 0.5 & 0 & -0.5 & 0.5 \\ -0.5 & 0.5 & -0.5 & 0 \\ 0.5 & -0.5 & 0 & 0.5 \end{bmatrix}\begin{bmatrix} 1 \\ 1 \\ 0.25 \\ 0.25 \end{bmatrix}\right) \\
&= \sigma\left(\begin{bmatrix} 0.5 \\ -0.125 \\ 0.125 \end{bmatrix}\right) \\
&= \begin{bmatrix} 0.378 \\ 0.531 \\ 0.469 \end{bmatrix}
\end{aligned}$$

We then use this result to compute the output at the output layer.

$$\begin{aligned}
\boldsymbol{y}_1^{(2)} &= \sigma\left(\boldsymbol{\Theta}^{(2)}\hat{\boldsymbol{y}}_1^{(1)}\right) \\
&= \sigma\left(\begin{bmatrix} -0.5 & 0.5 & -0.5 & 0.5 \\ 0.5 & 0 & -0.5 & 0.5 \\ -0.5 & -0.5 & 0.5 & 0 \\ 0.5 & 0.5 & 0 & -0.5 \end{bmatrix}\begin{bmatrix} 1 \\ 0.378 \\ 0.531 \\ 0.469 \end{bmatrix}\right) \\
&= \sigma\left(\begin{bmatrix} -0.342 \\ 0.469 \\ -0.423 \\ 0.454 \end{bmatrix}\right) \\
&= \begin{bmatrix} 0.585 \\ 0.385 \\ 0.604 \\ 0.388 \end{bmatrix}
\end{aligned}$$

We can now compute the loss for this training sample.

$$\begin{aligned}
J(\boldsymbol{\theta}) &= \frac{1}{2}\left\|\boldsymbol{y}_1^{(2)} - \boldsymbol{y}_1\right\|^2 \\
&= \frac{1}{2}\left\|\begin{bmatrix} -0.415 \\ 0.385 \\ 0.604 \\ 0.388 \end{bmatrix}\right\|^2 \\
&= 0.418
\end{aligned}$$

d) We now use the backpropagation algorithm to update the weights matrices, using a learning rate of $\mu = 1$. For the following computations, we will need the derivative of the activation function.

$$\sigma(u) = \frac{1}{1+e^u} \implies \sigma'(u) = -\frac{e^u}{(1+e^u)^2} = \sigma(u)(\sigma(u)-1)$$

We start by computing the gradients for both layers.

$$\begin{aligned}
\delta^{(2)} &= \left(\boldsymbol{y}_1^{(2)} - \boldsymbol{y}_1\right) \circ \sigma'\left(\boldsymbol{\Theta}^{(2)}\boldsymbol{y}_\mathbf{1}^{(\mathbf{1})}\right) \\
&= \begin{bmatrix} -0.415 \\ 0.385 \\ 0.604 \\ 0.388 \end{bmatrix} \circ \sigma'\left(\begin{bmatrix} -0.342 \\ 0.469 \\ -0.423 \\ 0.454 \end{bmatrix}\right) \\
&= \begin{bmatrix} -0.415 \\ 0.385 \\ 0.604 \\ 0.388 \end{bmatrix} \circ \begin{bmatrix} -0.243 \\ -0.237 \\ -0.239 \\ -0.238 \end{bmatrix} \\
&= \begin{bmatrix} 0.100 \\ -0.091 \\ -0.144 \\ -0.092 \end{bmatrix}
\end{aligned}$$

$$\begin{aligned}
\delta^{(1)} &= \boldsymbol{\Theta}^{(2)}\delta^{(2)} \circ \sigma'\left(\boldsymbol{\Theta}^{(1)}\boldsymbol{x}_\mathbf{1}\right) \\
&= \begin{bmatrix} -0.5 & 0.5 & -0.5 & 0.5 \\ 0.5 & 0 & -0.5 & 0.5 \\ -0.5 & -0.5 & 0.5 & 0 \\ 0.5 & 0.5 & 0 & -0.5 \end{bmatrix} \begin{bmatrix} 0.100 \\ -0.091 \\ -0.144 \\ -0.092 \end{bmatrix} \circ \sigma'\left(\begin{bmatrix} 0.5 & 0 & -0.5 & 0.5 \\ -0.5 & 0.5 & -0.5 & 0 \\ 0.5 & -0.5 & 0 & 0.5 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0.25 \\ 0.25 \end{bmatrix}\right) \\
&= \begin{bmatrix} -0.070 \\ 0.077 \\ -0.077 \\ 0.051 \end{bmatrix} \circ \begin{bmatrix} -0.235 \\ -0.249 \\ -0.249 \end{bmatrix}
\end{aligned}$$

As we can see, the dimensions do not seem to match for taking the Hadamard product between $\boldsymbol{\Theta}^{(2)}\delta^{(2)}$ and $\sigma'\left(\boldsymbol{\Theta}^{(1)}\boldsymbol{x}_\mathbf{1}\right)$. That's because the gradient of the bias unit does not get backpropagated, as shown in the network structure graph. Therefore, we should not consider the first component of $\boldsymbol{\Theta}^{(2)}\delta^{(2)}$.

$$\begin{aligned}
\delta^{(1)} &= \begin{bmatrix} 0.077 \\ -0.077 \\ 0.051 \end{bmatrix} \circ \begin{bmatrix} -0.235 \\ -0.249 \\ -0.249 \end{bmatrix} \\
&= \begin{bmatrix} -0.018 \\ 0.019 \\ -0.013 \end{bmatrix}
\end{aligned}$$

We now use the gradients to compute the weights update for each layer.

$$\begin{aligned}
\Delta\boldsymbol{\Theta}^{(2)} &= -\mu\delta^{(2)}\boldsymbol{y}_1^{(1)T} \\
&= -\begin{bmatrix} 0.100 \\ -0.091 \\ -0.144 \\ -0.092 \end{bmatrix} \begin{bmatrix} 1 & 0.378 & 0.531 & 0.469 \end{bmatrix} \\
&= \begin{bmatrix} -0.101 & -0.038 & -0.054 & -0.047 \\ 0.091 & 0.034 & 0.048 & 0.043 \\ 0.144 & 0.055 & 0.077 & 0.068 \\ 0.092 & 0.035 & 0.049 & 0.043 \end{bmatrix}
\end{aligned}$$

$$
\begin{aligned}
\Delta\boldsymbol{\Theta}^{(1)} &= -\mu\delta^{(1)}\boldsymbol{x}_1^{(1)T} \\
&= -\begin{bmatrix} -0.018 \\ 0.019 \\ -0.013 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0.25 & 0.25 \end{bmatrix} \\
&= \begin{bmatrix} 0.018 & 0.018 & 0.004 & 0.004 \\ -0.019 & -0.019 & -0.005 & -0.005 \\ 0.013 & 0.013 & 0.003 & 0.003 \end{bmatrix}
\end{aligned}
$$

Finally, we update the weights matrices.

$$
\begin{aligned}
\boldsymbol{\Theta}^{(2)} &= \boldsymbol{\Theta}^{(2)} + \Delta\boldsymbol{\Theta}^{(2)} \\
&= \begin{bmatrix} -0.601 & 0.462 & -0.554 & 0.453 \\ 0.591 & 0.034 & -0.452 & 0.543 \\ -0.356 & -0.445 & 0.577 & 0.068 \\ 0.592 & 0.535 & 0.049 & -0.457 \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{\Theta}^{(1)} &= \boldsymbol{\Theta}^{(1)} + \Delta\boldsymbol{\Theta}^{(1)} \\
&= \begin{bmatrix} 0.518 & 0.018 & -0.496 & 0.504 \\ -0.519 & 0.481 & -0.505 & -0.005 \\ 0.513 & -0.487 & 0.003 & 0.503 \end{bmatrix}
\end{aligned}
$$