Problem Solutions

e-Chapter 7

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Problem 7.1

To solve this problem, we first begin by separating the positive decision region into two components: the lower one corresponding to $x_2 \in [-1, 1]$ and the upper one corresponding to $x_2 \in [1, 2]$. To define the decision region, we need 7 perceptrons, namely

$$h_1(x) = \operatorname{sign}(x_2 - 2), \ h_2(x) = \operatorname{sign}(x_2 - 1), \ h_3(x) = \operatorname{sign}(x_2 + 1),$$

for the horizontal lines, and

$$h_4(x) = \operatorname{sign}(x_1 + 2), \ h_5(x) = \operatorname{sign}(x_1 + 1), \ h_6(x) = \operatorname{sign}(x_1 - 1), \ h_7(x) = \operatorname{sign}(x_1 - 2)$$

for the vertical lines. We are now able to define the lower decision region by $\overline{h_2}h_3h_4\overline{h_7}$, and the upper decision region by $\overline{h_1}h_2h_5\overline{h_6}$, which means that the total decision region is defined by

$$f = \overline{h_2}h_3h_4\overline{h_7} + \overline{h_1}h_2h_5\overline{h_6}$$

which actually characterizes a 3-layer perceptron.

Problem 7.2

(a) Let x and x' be two points from the same region. If we consider a set of M hyperplanes defined by $\{x: w_i^T x = 0\}$, we have that

$$(\operatorname{sign}(w_1^T x), \cdots, \operatorname{sign}(w_M^T x)) = (\operatorname{sign}(w_1^T x'), \cdots, \operatorname{sign}(w_M^T x'));$$

or put more simply that $\operatorname{sign}(w_i^T x) = \operatorname{sign}(w_i^T x') = s_i$ for $i = 1, \dots, M$ where $s_i = \pm 1$. We begin by the case where $s_i = 1$. Here, we know that $w_i^T x > 0$ and $w_i^T x' > 0$, consequently we have that, for $\lambda \in [0, 1]$,

$$w_i^T(\lambda x + (1 - \lambda)x') = \lambda w_i^T x + (1 - \lambda)w_i^T x' > 0$$

and

$$\operatorname{sign}(w_i^T(\lambda x + (1 - \lambda)x')) = 1.$$

Now, we consider the case where $s_i = -1$. Here, we know that $w_i^T x < 0$ and $w_i^T x' < 0$, consequently we have that, for $\lambda \in [0,1]$,

$$w_i^T(\lambda x + (1 - \lambda)x') = \lambda w_i^T x + (1 - \lambda)w_i^T x' < 0$$

and

$$\operatorname{sign}(w_i^T(\lambda x + (1 - \lambda)x')) = -1.$$

So, in conclusion, the region is actually convex.

(b) A region is defined as the following set

$$\{x : (\operatorname{sign}(w_1^T x), \dots, \operatorname{sign}(w_M^T x)) = (s_1, \dots, s_M); s_i \in \{-1, 1\}\};$$

thus a region is characterized by a particular M-uple (s_1, \dots, s_M) . Since there are at most 2^M of such M-uples, we have at most 2^M different regions.

(c) Let B(N,d) be the maximum number of regions created by M hyperplanes in d-dimensional space. Now, consider adding an (M+1)th hyperplane; this hyperplane can obviously be viewed as a (d-1)-dimensional

space, so if we project the initial M hyperplanes into this space, we obtain M hyperplanes in a (d-1)-dimensional space. These hyperplanes can create at most B(M,d-1) regions in this space, and for each of these regions, we get two regions in the original d-dimensional space. Thus, this means that the (M+1)th hyperplane intersects at most B(M,d-1) of the regions created by the M hyperplanes in the d-dimensional space, and so

$$B(M+1,d) \le B(M,d) + B(M,d-1).$$

Now, we will prove that

$$B(M,d) \le \sum_{i=0}^{d} {M \choose i}$$

by induction. We begin by evaluating the boundary conditions, we have

$$B(M,1) = M + 1 \le \sum_{i=0}^{1} {M \choose i} = {M \choose 0} + {M \choose 1} = M + 1$$

for all M, and

$$B(1,d) = 2 \le \sum_{i=0}^{d} {1 \choose i} = {1 \choose 0} + {1 \choose 1} = 2$$

for all d. Now, we assume the statement is true for $M = M_0$ and all d, we will prove that the statement is still true for $M = M_0 + 1$ and all d. We have that

$$B(M_{0} + 1, d) \leq B(M_{0}, d) + B(M_{0}, d - 1)$$

$$\leq \sum_{i=0}^{d} {M_{0} \choose i} + \sum_{i=0}^{d-1} {M_{0} \choose i}$$

$$= {M_{0} \choose 0} + \sum_{i=1}^{d} {M_{0} \choose i} + \sum_{i=1}^{d} {M_{0} \choose i - 1}$$

$$= 1 + \sum_{i=1}^{d} \left[{M_{0} \choose i} + {M_{0} \choose i - 1} \right]$$

$$= {M_{0} + 1 \choose i}$$

$$= \sum_{i=0}^{d} {M_{0} + 1 \choose i}.$$

We have thus proved the induction step, so the statement is true for all M and d.

Problem 7.3

We begin by proving the following equivalence relation

$$h_m(x) = c_m \Leftrightarrow h_m^{c_m}(x) = +1.$$

The condition is necessary because if $c_m = +1$, we have

$$h_m^{c_m}(x) = h_m(x) = c_m = +1;$$

and if $c_m = -1$, we have

$$h_m^{c_m}(x) = \overline{h}_m(x) = \overline{c}_m = +1.$$

Now the condition is also sufficient because if $c_m = +1$, we have

$$+1 = h_m^{c_m}(x) = h_m(x),$$

which means that $h_m(x) = +1 = c_m$; and if $c_m = -1$, we have

$$+1 = h_m^{c_m}(x) = \overline{h}_m(x),$$

which implies that $h_m(x) = -1 = c_m$.

Now we are able to write that

$$x \in r$$

$$\Leftrightarrow (h_1(x), \dots, h_M(x)) = (c_1, \dots, c_M)$$

$$\Leftrightarrow h_m^{c_m}(x) = +1, \forall m$$

$$\Leftrightarrow \prod_{m=1}^M h_m^{c_m}(x) = +1$$

$$\Leftrightarrow t_r(x) = +1.$$

The above relation also implies that

$$x \notin r \Leftrightarrow t_r(x) = -1.$$

Now if x is in a positive region (f(x) = +1), we know that there exists i such that $x \in r_i$, and consequently that $t_{r_i}(x) = +1$ which means that

$$t_{r_1}(x) + \cdots + t_{r_k}(x) = +1 = f(x).$$

And if x is in a negative region (f(x) = -1), we know that $x \notin r_i$ for all i, so $t_{r_i}(x) = -1$ for all i which means that

$$t_{r_1}(x) + \cdots + t_{r_k}(x) = -1 = f(x).$$

Problem 7.4

Since $f = t_{r_1} + \cdots + t_{r_k}$, we may write that

$$f = \text{sign}(k - \frac{1}{2} + \sum_{i=1}^{k} t_{r_i}),$$

which characterizes the penultimate layer of our perceptron. For the layer before, we have that $t_{r_i} = h_1^{c_1^{(i)}} \cdots h_M^{c_M^{(i)}}$, and consequently

$$t_{r_i} = \text{sign}(-M + \frac{1}{2} + \sum_{m=1}^{M} h_m^{c_m^{(i)}});$$

moreover, the previous layer may be characterized with

$$h_m^{c_m^{(i)}} = \operatorname{sign}(c_m^{(i)} w_m^T x).$$

Putting all this together, we obtain the following characterization of a 3-layer perceptron

$$f = \text{sign}(k - \frac{1}{2} + \sum_{i=1}^{k} \text{sign}(-M + \frac{1}{2} + \sum_{m=1}^{M} \text{sign}(c_m^{(i)} w_m^T x)))$$

whose structure is given by [d, kM, k, 1].

Problem 7.5

First, we decompose the unit hypercube $[0,1]^d$ into $1/\epsilon^d$ ϵ -hypercubes (hypercube whose sides have length equal to ϵ), thus we get a grid-like structure of our unit hypercube. Now, if we consider a decision region (which may be composed by disconnected regions) whose boundary surfaces are smooth, this decision region partition the unit hypercube into two regions: one labelled +1 and one labelled -1. We now have k_{ϵ} ϵ -hypercubes labelled +1 which are formed by 2d hyperplanes each defined by $h_m^{(i)} = \text{sign}(w_m^{(i),T}x)$ where $m = 1, \dots, 2d$ and $i = 1, \dots, k_{\epsilon}$. So, the first layer whose task is to activate the hyperplanes involved in the positive ϵ -hypercubes is characterized by

$$h_m^{(i)} = \operatorname{sign}(w_m^{(i),T} x).$$

Now to activate the positive ϵ -hypercubes H_i themselves we characterize the second layer by

$$t_{H_i} = (h_1^{(i)})^{c_1^{(i)}} \cdots (h_{2d}^{(i)})^{c_{2d}^{(i)}},$$

where the $c_m^{(i)}$ are defined as in Problem 7.3 and 7.4; or

$$t_{H_i} = \text{sign}(-2d + \frac{1}{2} + \sum_{m=1}^{2d} (h_m^{(i)})^{c_m^{(i)}}).$$

And finally to activate all the positive ϵ -hypercubes, we define the MLP output h by

$$h = t_{H_1} + \cdots + t_{H_{k_s}};$$

or

$$h = \operatorname{sign}(k_{\epsilon} - \frac{1}{2} + \sum_{i=1}^{k_{\epsilon}} t_{H_i}).$$

Putting all this together, we obtain the following characterization of a 3-layer perceptron

$$h = \operatorname{sign}(k_{\epsilon} - \frac{1}{2} + \sum_{i=1}^{k_{\epsilon}} \operatorname{sign}(-2d + \frac{1}{2} + \sum_{m=1}^{2d} \operatorname{sign}(c_m^{(i)} w_m^{(i),T} x))).$$

Now, it remains to see that the above MLP can aribtrarily closely approximate the initial positive decision region D_{+} (and consequently the negative decision region also); to do so, we first note that

$$Vol(H_i) = \epsilon^d \to 0 \text{ and } k_{\epsilon} \to \infty$$

when $\epsilon \to 0$. So, the ϵ -hypercubes can be made arbitrarily small, which obviously means that the total volume of the positive ϵ -hypercubes can be made arbitrarily close to the volume of the positive decision region (because of its smoothness). Mathematically, we may write that

$$\operatorname{Vol}(H_1 \cup \cdots \cup H_{k_{\epsilon}}) = \sum_{i=1}^{k_{\epsilon}} \epsilon^d \to \operatorname{Vol}(D_+)$$

when $\epsilon \to 0$. This means that the region where our 3-layer perceptron will output +1 (resp. -1) converges to the positive (resp. negative) decision region in our unit hypercube.

Problem 7.6

For a specific layer l, if we replace the weight $w_{ij}^{(l)}$ with $w_{ij}^{(l)} + \epsilon$, we need to recompute the corresponding node output of that layer and also the node outputs for the subsequent layers (which are the ones numbered from l+1 to L). Consequently, for each weight $w_{ij}^{(l)}$, we have

$$\sum_{k=l+1}^{L} d^{(l)} (d^{(l-1)} + 1) + 1 + \sum_{k=l+1}^{L} d^{(l)}$$

multiplications and θ -evaluations respectively; this means that the computational complexity of obtaining the partial derivatives is overall equal to

$$2\sum_{l=1}^{L} d^{(l)}(d^{(l-1)}+1) \left(\sum_{k=l+1}^{L} d^{(l)}(d^{(l-1)}+1) + 1 + \sum_{k=l+1}^{L} d^{(l)}\right)$$

$$\leq 2|W| \left(\sum_{k=1}^{L} d^{(l)}(d^{(l-1)}+1) + 1 + \sum_{k=1}^{L} \underbrace{d^{(l)}}_{\leq d^{(l)}(d^{(l-1)}+1)}\right)$$

$$\leq 2|W|(2|W|+1) = O(|W|^{2})$$

since we need to compute the derivatives corresponding to $w_{ij}^{(l)} + \epsilon$ and also to $w_{ij}^{(l)} - \epsilon$.

Problem 7.7

(a) We know that

$$E_{in} = \frac{1}{N} \sum_{i=1}^{N} ||y_i - \hat{y}_i||^2,$$

and also that

$$(Y - \hat{Y})(Y - \hat{Y})^T = \begin{pmatrix} y_1^T - \hat{y}_1^T \\ \vdots \\ y_N^T - \hat{y}_N^T \end{pmatrix} (y_1 - \hat{y}_1, \dots, y_N - \hat{y}_N) = \begin{pmatrix} ||y_1 - \hat{y}_1||^2 & * & * \\ * & \ddots & * \\ * & * & ||y_N - \hat{y}_N||^2 \end{pmatrix}.$$

Consequently, we get that

$$E_{in} = \frac{1}{N} \operatorname{trace}((Y - \hat{Y})(Y - \hat{Y})^{T}).$$

(b) We may write that

$$E_{in} = \frac{1}{N} \operatorname{trace}(YY^T - ZVY^Y - YV^TZ^T + ZVV^TZ^T)$$
$$= \frac{1}{N} \operatorname{trace}(YY^T - 2ZVY^T + ZVV^TZ^T),$$

since $trace(A) = trace(A^T)$. We are now ready to compute the derivatives, we have

$$\frac{\partial E_{in}}{\partial V} = \frac{1}{N} \left(-2 \underbrace{\frac{\partial \operatorname{trace}(ZVY^T)}{\partial V}}_{=Z^TY} + \underbrace{\frac{\partial \operatorname{trace}(ZVV^TZ^T)}{\partial V}}_{=Z^TZV + Z^TZV = 2Z^TZV} \right) \\
= \frac{1}{N} (2Z^TZV - 2Z^TY),$$

because of the following identities

$$\frac{\partial \operatorname{trace}(AXB)}{\partial X} = A^T B^T \text{ and } \frac{\partial \operatorname{trace}(AXX^TB)}{\partial X} = BAX + A^T B^T X.$$

We also have

$$\begin{split} E_{in} &= \frac{1}{N} \mathrm{trace}(YY^T - 2(V_0 + \theta(XW)V_1)Y^T + (V_0 + \theta(XW)V_1)(V_0^T + V_1^T\theta(XW)^T) \\ &= \frac{1}{N} \mathrm{trace}(YY^T - 2V_0Y^T - 2\theta(XW)V_1Y^T + V_0V_0^T + V_0V_1^T\theta(XW)^T + \theta(XW)V_1V_0^T + \theta(XW)V_1V_1^T\theta(XW)^T) \\ &= \frac{1}{N} \mathrm{trace}(YY^T - 2V_0Y^T - 2\theta(XW)V_1Y^T + V_0V_0^T + 2\theta(XW)V_1V_0^T + V_1V_1^T\theta(XW)^T\theta(XW)), \end{split}$$

since the trace can be permuted in a cycle and $trace(A) = trace(A^T)$. The other derivative may be written as

$$\frac{\partial E_{in}}{\partial W} = \frac{1}{N} \left(-2 \frac{\partial \operatorname{trace}(\theta(XW)V_1Y^T)}{\partial W} + 2 \frac{\partial \operatorname{trace}(\theta(XW)V_1V_0^T)}{\partial W} + \frac{\partial \operatorname{trace}(V_1V_1^T\theta(XW)^T\theta(XW))}{\partial W} \right)
= \frac{1}{N} \left(-2X^T\theta'(XW) \otimes YV_1^T + 2X^T\theta'(XW) \otimes V_0V_1^T + X^T(\theta'(XW) \otimes [\theta(XW)2V_1V_1^T]) \right)
= 2X^T[\theta'(XW) \otimes (-YV_1^T + V_0V_1^T + \theta(XW)V_1V_1^T)]$$

because of the following identities

$$\frac{\partial \mathrm{trace}(\theta(BX)A)}{\partial X} = B^T \theta'(BX) \otimes A^T \text{ and } \frac{\partial \mathrm{trace}(A\theta(BX)^T \theta(BX))}{\partial X} = B^T [\theta'(BX) \otimes (\theta(BX)(A + A^T))].$$

Problem 7.8

(a) By hypothesis, we know that $\{\eta_1, \eta_2, \eta_3\}$ with $\eta_1 < \eta_2 < \eta_3$ is an U-arrangement which means that

$$E(\eta_2) < \min\{E(\eta_1), E(\eta_3)\}.$$

Since $E(\eta)$ is a quadratic curve, we know that it is decreasing (resp. increasing) to the left (resp. right) of its minimum $\bar{\eta}$. So if we assume that $\bar{\eta} < \eta_1$, we get that $E(\eta_1) \leq E(\eta_2) \leq E(\eta_3)$ which is impossible by definition of an U-arrangement; and if we assume that $\bar{\eta} > \eta_3$, we get that $E(\eta_1) \geq E(\eta_2) \geq E(\eta_3)$ which is also impossible by definition of an U-arrangement. Consequently, we have $\bar{\eta} \in [\eta_1, \eta_3]$.

(b) First, we solve the linear system in a, b, and c below

$$\begin{cases} E(\eta_1) &= a\eta_1^2 + b\eta_1 + c = e_1 \\ E(\eta_2) &= a\eta_2^2 + b\eta_2 + c = e_2 \\ E(\eta_3) &= a\eta_3^2 + b\eta_3 + c = e_3 \end{cases}.$$

Let D be the determinant of the system, which is

$$D = \left| \begin{array}{ccc} \eta_1^2 & \eta_1 & 1 \\ \eta_2^2 & \eta_2 & 1 \\ \eta_3^2 & \eta_3 & 1 \end{array} \right|,$$

where $D \neq 0$ since $\eta_1 < \eta_2 < \eta_3$; now we easily get that

$$a = \begin{vmatrix} e_1 & \eta_1 & 1 \\ e_2 & \eta_2 & 1 \\ e_3 & \eta_3 & 1 \end{vmatrix} / D = \frac{(e_1 - e_2)(\eta_1 - \eta_3) - (e_1 - e_3)(\eta_1 - \eta_2)}{D}$$

and

$$b = \begin{vmatrix} \eta_1^2 & e_1 & 1 \\ \eta_2^2 & e_2 & 1 \\ \eta_3^2 & e_3 & 1 \end{vmatrix} / D = \frac{-(e_1 - e_2)(\eta_1^2 - \eta_3^2) + (e_1 - e_3)(\eta_1^2 - \eta_2^2)}{D}.$$

Since the minimum of such a quadratic function is given by -b/2a, we finally get

$$\bar{\eta} = \frac{1}{2} \left[\frac{(e_1 - e_2)(\eta_1^2 - \eta_3^2) - (e_1 - e_3)(\eta_1^2 - \eta_2^2)}{(e_1 - e_2)(\eta_1 - \eta_3) - (e_1 - e_3)(\eta_1 - \eta_2)} \right].$$

- (c) We enumerate the four cases below.
 - 1. If $\bar{\eta} < \eta_2$:
 - If $E(\bar{\eta}) < E(\eta_2)$, then $\{\eta_1, \bar{\eta}, \eta_2\}$ is a new U-arrangement.
 - If $E(\bar{\eta}) > E(\eta_2)$, then $\{\bar{\eta}, \eta_2, \eta_3\}$ is a new U-arrangement.
 - 2. If $\bar{\eta} > \eta_2$:
 - If $E(\bar{\eta}) < E(\eta_2)$, then $\{\eta_2, \bar{\eta}, \eta_3\}$ is a new U-arrangement.
 - If $E(\bar{\eta}) > E(\eta_2)$, then $\{\eta_1, \eta_2, \bar{\eta}\}$ is a new U-arrangement.
- (d) If $\bar{\eta} = \eta_2$, by continuity we are always able to find another η'_2 close to η_2 such that

$$E(\eta_2') < \min\{E(\eta_1), E(\eta_3)\}.$$

In this case, we can use this new η'_2 in place of η_2 and proceed with the algorithm.