Exercise sheet 2

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Exercise 2.1

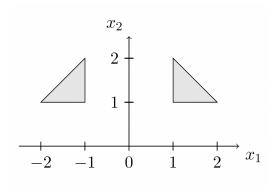


Figure 1: Visualization of the problem

We design a 3-layer perceptron using hard-threshold (Heaviside) activations to output y = 1 if and only if the input point $x = (x_1, x_2)$ lies in one of two shaded triangles, and y = 0 otherwise.

Since the input is bidimensional, the input layer will feature 2 nodes. In the following subsections we deal with the 2 hidden layers and the final output layer.

Layer 1: Half-space Detectors (8 Units)

Each unit computes

$$h_i^{(1)} = \theta(w_i^{(1)T}x + b_i^{(1)}), \quad \theta(u) = \begin{cases} 1, & u \ge 0, \\ 0, & u < 0. \end{cases}$$

Where $w_i^{(1)T}$ is a column 2-dimensional vector and x is the row 2-dimensional vector described above. We chose to use 8 nodes for the first hidden layer, the weights and biases implement the following linear inequalities:

| Unit | $w_i^{(1)}$ | $b_i^{(1)}$ | Inequality |
|------|-------------|-------------|--|
| 1 | [1,0] | +2 | $x_1 + 2 \ge 0 \iff x_1 \ge -2$ |
| 2 | [-1, 0] | -1 | $-x_1 - 1 \ge 0 \iff x_1 \le -1$ |
| 3 | [0, 1] | -1 | $x_2 - 1 \ge 0 \iff x_2 \ge 1$ |
| 4 | [1, -1] | +3 | $x_1 - x_2 + 3 \ge 0 \iff x_2 \le x_1 + 3$ |
| 5 | [1,0] | -1 | $x_1 - 1 \ge 0 \iff x_1 \ge 1$ |
| 6 | [-1, 0] | +2 | $-x_1 + 2 \ge 0 \iff x_1 \le 2$ |
| 7 | [0, 1] | -1 | $x_2 - 1 \ge 0 \iff x_2 \ge 1$ |
| 8 | [-1, -1] | +3 | $-x_1 - x_2 + 3 \ge 0 \iff x_2 \le -x_1 + 3$ |

Table 1: Layer 1 implements four boundary tests for each of the two triangles.

Units 1–4 carve the left triangle; units 5–8 carve the right triangle.

Layer 2: Triangle Indicators (2 Units)

In the second hidden layer we combine ("AND") the four half-space tests for each triangle by a single linear threshold unit. Denote by $h^{(1)} = (h_1^{(1)}, \dots, h_8^{(1)})^T$ the outputs of Layer 1. We set:

$$h_1^{(2)} = \theta \left(h_1^{(1)} + h_2^{(1)} + h_3^{(1)} + h_4^{(1)} - 3.5 \right),$$

$$h_2^{(2)} = \theta \left(h_5^{(1)} + h_6^{(1)} + h_7^{(1)} + h_8^{(1)} - 3.5 \right).$$

where θ was defined in the previous layer.

Interpretation of the threshold:

Each sum $S_j = \sum_{i \in I_j} h_i^{(1)}$ for j = 1, 2 can only take integer values 0, 1, 2, 3, 4. By choosing the bias $b_j^{(2)} = -3.5$, the argument of ϕ is

$$S_j - 3.5 \ge 0 \iff S_j \ge 3.5 \iff S_j = 4.$$

Thus $h_j^{(2)} = 1$ if and only if *all four* relevant half-space tests are satisfied simultaneously—i.e. the point lies inside (or on the boundary of) the corresponding triangle.

This can also be visualized in matrix form. Let:

$$W^{(2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}, \quad b^{(2)} = \begin{pmatrix} -3.5 \\ -3.5 \end{pmatrix}.$$

Then

$$h^{(2)} = \phi(W^{(2)} h^{(1)} + b^{(2)}) \implies h_j^{(2)} = 1 \iff \sum_{i \in I_j} h_i^{(1)} = 4, \quad j = 1, 2.$$

Layer 3: OR Operation (1 Unit)

We "OR" the two triangle indicators:

$$y = \phi (h_1^{(2)} + h_2^{(2)} - 0.5),$$

which yields y = 1 if either $h_1^{(2)} = 1$ or $h_2^{(2)} = 1$. In weights:

$$W^{(3)} = [1 \ 1], \quad b^{(3)} = -0.5.$$

This network classifies exactly the two shaded triangles.

Exercise 2.2: Equivalent Networks

Proof that any multi-layer perceptron with identity activations collapses to a single layer

Setup. Label the layers by k = 1, 2, ..., L. Let the input be $x \in \mathbb{R}^n$, and the final output $y \in \mathbb{R}^m$. Since the activation function is the identity,

$$\phi(u) = u,$$

each layer computes an affine map

$$h^{(k)} = W^{(k)} h^{(k-1)} + b^{(k)}, \qquad h^{(0)} = x,$$

and the network output is

$$y = h^{(L)} = W^{(L)} h^{(L-1)} + b^{(L)}.$$

Folding in layers. We now show by repeated substitution that every bias term $b^{(k)}$ is carried forward through all higher-numbered weight matrices. Starting from

$$y = W^{(L)} h^{(L-1)} + b^{(L)},$$

and using $h^{(L-1)} = W^{(L-1)} h^{(L-2)} + b^{(L-1)}$, we get

$$\begin{split} y &= W^{(L)} \big(W^{(L-1)} \, h^{(L-2)} + b^{(L-1)} \big) + b^{(L)} \\ &= \big(W^{(L)} W^{(L-1)} \big) \, h^{(L-2)} + \underbrace{W^{(L)} \, b^{(L-1)}}_{\text{bias from layer } L-1} + b^{(L)}. \end{split}$$

Next, substitute $h^{(L-2)} = W^{(L-2)} h^{(L-3)} + b^{(L-2)}$ to carry forward $b^{(L-2)}$:

$$y = W^{(L)}W^{(L-1)}W^{(L-2)}h^{(L-3)} + W^{(L)}W^{(L-1)}b^{(L-2)} + W^{(L)}b^{(L-1)} + b^{(L)}.$$

and so on down to layer 1. After folding in all layers $k = L - 1, L - 2, \dots, 1$, we arrive at

$$y = \underbrace{W^{(L)}W^{(L-1)}\cdots W^{(1)}}_{W_{\text{total}}} x + \sum_{k=1}^{L} \left(\underbrace{W^{(L)}W^{(L-1)}\cdots W^{(k+1)}}_{\text{propagate }b^{(k)} \text{ forward}}\right) b^{(k)}.$$

Here by convention the empty product for k = L is the identity:

$$\prod_{j=L}^{L+1} W^{(j)} = I.$$

Thus defining

$$W_{\text{total}} = W^{(L)} W^{(L-1)} \cdots W^{(1)}, \quad b_{\text{total}} = \sum_{k=1}^{L} \left(\prod_{j=L}^{k+1} W^{(j)} \right) b^{(k)},$$

we obtain the single-layer form

$$y = W_{\text{total}} x + b_{\text{total}}.$$

Conclusion. Since each layer with identity activation is affine, and the composition of affine maps is affine, the entire L-layer network is equivalent to a single affine transformation $x \mapsto W_{\text{total}}x + b_{\text{total}}$. Hence no hidden layer increases expressivity beyond that of a single layer.

(b) Construction of an equivalent single-layer perceptron

The given network has one hidden layer of size 3 and an output layer of size 2, with identity activations:

$$h^{(1)} = W^{(1)}x + b^{(1)}, y = W^{(2)}h^{(1)} + b^{(2)}.$$

By the result of part (a), the two layers collapse to one affine map

$$y = W_{\text{total}} x + b_{\text{total}},$$

where

$$W_{\text{total}} = W^{(2)} W^{(1)}, \qquad b_{\text{total}} = W^{(2)} b^{(1)} + b^{(2)}.$$

Substitute the given matrices

$$W^{(1)} = \begin{pmatrix} 1 & 2 & -2 \\ -1 & -1 & 2 \\ 3 & 2 & 3 \end{pmatrix}, \quad b^{(1)} = \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}, \quad W^{(2)} = \begin{pmatrix} 2 & -1 & -1 \\ 1 & 2 & 3 \end{pmatrix}, \quad b^{(2)} = \begin{pmatrix} 1 \\ -2 \end{pmatrix}.$$

Then

$$W_{\text{total}} = W^{(2)}W^{(1)} = \begin{pmatrix} 2 & -1 & -1 \\ 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} 1 & 2 & -2 \\ -1 & -1 & 2 \\ 3 & 2 & 3 \end{pmatrix} = \begin{pmatrix} 0 & 3 & -9 \\ 8 & 6 & 11 \end{pmatrix},$$

$$b_{\text{total}} = W^{(2)} b^{(1)} + b^{(2)} = \begin{pmatrix} 2 & -1 & -1 \\ 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix} + \begin{pmatrix} 1 \\ -2 \end{pmatrix} = \begin{pmatrix} -5 \\ 7 \end{pmatrix} + \begin{pmatrix} 1 \\ -2 \end{pmatrix} = \begin{pmatrix} -4 \\ 5 \end{pmatrix}.$$

Hence the equivalent single-layer perceptron is

$$y = \begin{pmatrix} 0 & 3 & -9 \\ 8 & 6 & 11 \end{pmatrix} x + \begin{pmatrix} -4 \\ 5 \end{pmatrix}.$$

As required.

Exercise 2.3: Matrix-valued functions and gradients

Let $X = R^{n \times n}$ be the vector space of real $n \times n$ matrices. We equip X with the *Frobenius inner product*, defined entry-wise by

$$\langle A, B \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij} = tr(A B^{T}).$$

Here tr(M) denotes the trace of M, i.e. the sum of its diagonal entries. Indeed,

$$tr(A B^T) = \sum_{i=1}^{n} (A B^T)_{ii} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij},$$

which shows that $tr(AB^T)$ coincides with the standard dot-product of the n^2 entries of A and B.

For a (possibly matrix-valued) function $f: X \to Y$, its Fréchet derivative $f(A): X \to Y$ at A is the unique linear map satisfying

$$f(A + H) = f(A) + df(A)[H] + o(||H||).$$

When Y = R, the gradient $\nabla f(A) \in X$ is defined implicitly by

$$df(A)[H] = \langle \nabla f(A), H \rangle$$
 for all $H \in X$.

(a) Function:

$$f(A) = A : B = \langle A, B \rangle, B \in X$$
 fixed.

Derivation: For a small perturbation H,

$$f(A+H) = tr\big((A+H)B^T\big) = tr(AB^T) + tr(HB^T) = f(A) + tr(HB^T).$$

Hence the linear part is

$$df(A)[H] = tr(HB^T) = \langle H, B \rangle,$$

and by the Riesz representation the gradient is $\nabla f(A) = B$.

(b) Function:

$$f(A) = B A$$
, $B \in X$ fixed.

Derivation: Since f is itself matrix-valued, we perturb by H and get

$$f(A + H) - f(A) = B(A + H) - BA = BH.$$

No higher-order terms appear, so the Fréchet derivative is the linear map

$$df(A)[H] = B H.$$

(c) Function:

$$f(A) = A^2 = A \cdot A.$$

Derivation: Perturbing A by H gives

$$(A+H)^2 - A^2 = AH + HA + H^2.$$

The term H^2 is o(||H||), so the Fréchet derivative is

$$df(A)[H] = AH + HA.$$

(d) Function:

$$f(A) = A : A = \langle A, A \rangle = tr(A A^T).$$

Derivation: Under $A \mapsto A + H$,

$$f(A+H)-f(A) = tr\big((A+H)(A+H)^T\big) - tr(AA^T) = tr(AH^T + HA^T) + tr(HH^T).$$

The last term is o(||H||), so

$$df(A)[H] = tr(AH^T) + tr(HA^T) = \langle H, A \rangle + \langle A, H \rangle = 2 \langle H, A \rangle.$$

Thus by the Riesz representation the gradient is $\nabla f(A) = 2A$.