

Basic MLP with manually-derived Backprop

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1 Introduction

Goal: To design, train and use a simple 3-layer MLP for binary classification of size-2 vectors.

Design: of the form

$$[(layer_size, Activation) \dots]$$

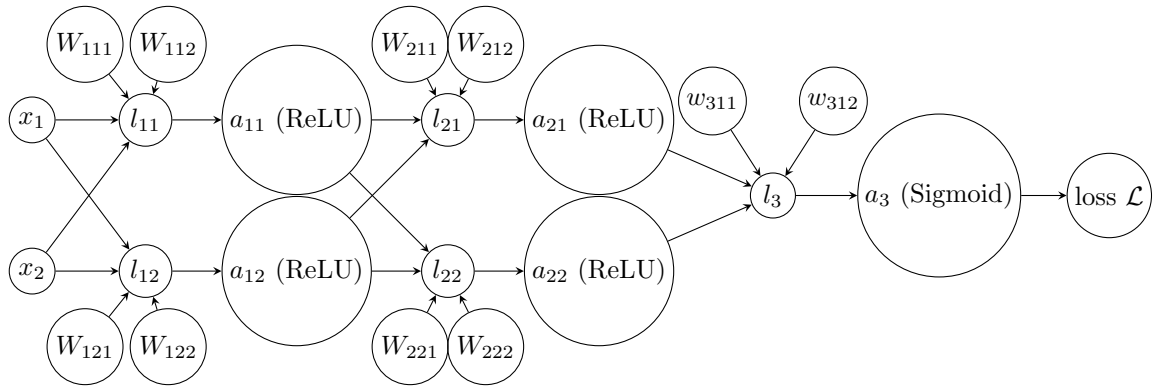
: [(2, ReLU), (2, ReLU), (1, Sigmoid)]

1.1 Diagrams

1.1.1 Vectorized Diagram (Equiv to Roger Grosse' 'Computational Graph')

$$\begin{array}{ccccccc} & \mathbf{W}_1 & & \mathbf{W}_2 & & \mathbf{w}_3 & & t \\ & \searrow & & \searrow & & \searrow & & \searrow \\ \mathbf{x} & \longrightarrow & \mathbf{l}_1 & \longrightarrow & \mathbf{a}_1 & \longrightarrow & \mathbf{l}_2 & \longrightarrow & \mathbf{a}_2 & \longrightarrow & \mathbf{l}_3 & \longrightarrow & \mathbf{a}_3 & \longrightarrow & \mathcal{L} \end{array}$$

1.1.2 Expanded Diagram (Equiv. to Roger Grosse' 'Network Architecture')



1.2 Definitions

1.2.1 Remark on general notation

Since it seems that mathematical notation in this field tends to suffer from overloading, imprecision/lack of specificity, a lack of convention, poor readability, and a generally poor aesthetic/design sense, I am going to try to avoid worsening the situation. So, for the purpose of this work, all non-bold variables denote scalars. A bold lower-case variable denotes a vector, a bold upper-case a Matrix. A non-bold lower-case may denotes either an arbitrary scalar variable or if subscripted typically an element of a vector. A non-bold upper-case, if subscripted, will typically denote a matrix element.

1.2.2 Remark on weight notation

$w_{i,j,k}$ is to say the weight at the i -th layer, j -th neuron, k -th weight. Hence w_{111} is the first weight of the first neuron in the first layer, etc.

1.2.3 Remark on layer notation

This is a sub-case of the weight notation. I.e., L_{ij} is the scalar value of the j -th neuron at the i -th layer, etc.

1.2.4 Neuron firing calculation

This is just a straightforward dot-product. We have:

$$L_{ij} = \mathbf{w}_{ij} \mathbf{x}_i$$

Where \mathbf{x}_i in this case is referring to a more general notion of 'layer input', not necessarily just the first input to the network as in the diagrams above.

1.3 BackPropagation Derivation

Notation for derivative of loss w.r.t. to a function I will be using the following: $\bar{f} = \frac{\partial \mathcal{L}}{\partial f}$. This notation was introduced by Roger Grosse from the University of Toronto.

Pa(x) and Ch(x) these refer to the sets of parent and child vertices of a vertex in a graph.

General Approach Let's label the computational graph nodes as v_1, \dots, v_N with some topological ordering. Then, our general goal for backprop is to compute \bar{v}_i for $i \in 1, \dots, N$. With these, we can trivially calculate the weight updates. We compute a forward pass of the network, then set $v_N = 1$, then, for $i = N - 1, \dots, 1$, we have:

$$\bar{v}_i = \sum_{j \in \text{Ch}(v_i)} \bar{v}_j \frac{\partial v_j}{\partial v_i} \quad (\text{The Backprop Rule}) \quad (1)$$

1.3.1 Applying the backprop rule

Loss and final activation Then, going backwards through the 'computational graph', starting at the end:

$$\begin{aligned}
\bar{\mathcal{L}} &= 1 \\
\bar{a}_3 &= \bar{\mathcal{L}} \frac{\partial \mathcal{L}}{\partial a_3} \\
\bar{a}_3 &= (1) \frac{\partial \mathcal{L}}{\partial a_3} \\
\bar{a}_3 &= \frac{\partial \mathcal{L}}{\partial a_3} \\
\bar{a}_3 &= \frac{\partial}{\partial a_3} \frac{1}{2} (a_3 - t)^2 \\
\bar{a}_3 &= (a_3 - t) \frac{\partial}{\partial a_3} (a_3 - t) \\
\bar{a}_3 &= (a_3 - t)(1) \\
\bar{a}_3 &= (a_3 - t)
\end{aligned} \tag{2}$$

Final layer *N.B.* I use σ to denote the sigmoid function here, not an activation function.

$$\begin{aligned}
\bar{l}_3 &= \bar{a}_3 \frac{\partial a_3}{\partial l_3} \\
\bar{l}_3 &= \bar{a}_3 \frac{\partial}{\partial l_3} \sigma(l_3) \\
\bar{l}_3 &= \bar{a}_3 \sigma(l_3)(1 - \sigma(l_3))
\end{aligned} \tag{4}$$

Final layer weights

$$\begin{aligned}
\overline{w_{31i}} &= \bar{l}_3 \frac{\partial}{\partial w_{31i}} l_3 \\
\overline{w_{31i}} &= \bar{l}_3 \frac{\partial}{\partial w_{31i}} \sum_j w_{31j} a_{2j} \\
\overline{w_{31i}} &= \bar{l}_3 a_{2i}
\end{aligned} \tag{5}$$

Second layer activation

$$\begin{aligned}
\overline{a_{2i}} &= \bar{l}_3 \frac{\partial}{\partial a_{2i}} l_3 \\
\overline{a_{2i}} &= \bar{l}_3 \frac{\partial}{\partial a_{2i}} \sum_j w_{31j} a_{2j} \\
\overline{a_{2i}} &= \bar{l}_3 w_{31i}
\end{aligned} \tag{6}$$

Second layer

$$\begin{aligned}\overline{l_{2i}} &= \overline{a_{2i}} \frac{\partial}{\partial l_{2i}} a_{2i} \\ \overline{l_{2i}} &= \overline{a_{2i}} \frac{\partial}{\partial l_{2i}} \text{ReLU}(l_{2i})\end{aligned}$$

Note that $d/dx(\text{ReLU}(x))$ is the heaviside step function $\theta(x)$:

$$\begin{aligned}\begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \\ \overline{l_{2i}} = \overline{a_{2i}} \quad \theta(l_{2i}) \cdot (1) \\ \overline{l_{2i}} = \overline{a_{2i}} \quad \theta(l_{2i})\end{aligned}\tag{7}$$

Second layer weights

$$\begin{aligned}\overline{W_{2ij}} &= \overline{l_{2i}} \frac{\partial}{\partial W_{2ij}} l_{2i} \\ \overline{W_{2ij}} &= \overline{l_{2i}} \frac{\partial}{\partial W_{2ij}} \sum_k W_{2ik} a_{1k} \\ \overline{W_{2ij}} &= \overline{l_{2i}} a_{1j}\end{aligned}\tag{8}$$

Input layer activation

$$\begin{aligned}\overline{a_{1i}} &= \overline{l_{21}} \frac{\partial}{\partial a_{1i}} l_{21} + \overline{l_{22}} \frac{\partial}{\partial a_{1i}} l_{22} \\ \overline{a_{1i}} &= \overline{l_{21}} \frac{\partial}{\partial a_{1i}} \sum_j W_{21j} a_{1j} + \overline{l_{22}} \frac{\partial}{\partial a_{1i}} \sum_j W_{22j} a_{1j} \\ \overline{a_{1i}} &= \overline{l_{21}} W_{21i} + \overline{l_{22}} W_{22i}\end{aligned}\tag{9}$$

Input layer

$$\begin{aligned}\overline{l_{1i}} &= \overline{a_{1i}} \frac{\partial}{\partial l_{1i}} a_{1i} \\ \overline{l_{1i}} &= \overline{a_{1i}} \frac{\partial}{\partial l_{1i}} \text{ReLU}(l_{1i}) \\ \overline{l_{1i}} &= \overline{a_{1i}} \quad \theta(l_{1i}) \cdot (1) \\ \overline{l_{1i}} &= \overline{a_{1i}} \quad \theta(l_{1i})\end{aligned}\tag{10}$$

Input layer weights

$$\begin{aligned}
\overline{W_{1ij}} &= \overline{l_{1i}} \frac{\partial}{\partial W_{1ij}} l_{1i} \\
\overline{W_{1ij}} &= \overline{l_{1i}} \frac{\partial}{\partial W_{1ij}} \sum_k W_{1ik} x_{1k} \\
\overline{W_{1ij}} &= \overline{l_{1i}} x_{1j}
\end{aligned} \tag{11}$$

Notes to self Grosse follows a per-element approach first, then somehow transformed those results into a vectorized form involving (in some cases) re-arranged multiplications and matrix transpose. I am somewhat confused/overwhelmed by this.

1.3.2 Vectorized derivation:

1.3.3 Forward pass vectorized:

$$\begin{aligned}
\mathbf{L}_1 &= \mathbf{w}_1 \cdot \mathbf{x} \\
\mathbf{a}_1 &= \text{ReLU}(\mathbf{L}_1) \\
\mathbf{L}_2 &= \mathbf{w}_2 \cdot \mathbf{a}_1 \\
\mathbf{a}_2 &= \text{ReLU}(\mathbf{L}_2) \\
L_3 &= \mathbf{w}_3 \cdot \mathbf{a}_2 \\
a_3 &= \sigma(L_3) \\
\mathcal{L} &= \frac{1}{2}(a_3 - t)^2
\end{aligned}$$

1.3.4 Backpropagation vectorized:

$$\begin{aligned}
\overline{\mathcal{L}} &= 1 \\
\overline{a_3} &= \overline{\mathcal{L}}(a_3 - t) \\
\overline{a_3} &= (a_3 - t) \\
\overline{L_3} &= \overline{a_3} \times \frac{\partial}{\partial L_3} a_3 \\
\overline{L_3} &= \overline{a_3} \times \frac{\partial}{\partial L_3} \sigma(L_3) \\
\overline{L_3} &= \overline{a_3} \times \sigma'(L_3) \\
\overline{\mathbf{w}_3} &= \overline{L_3} \frac{\partial}{\partial \mathbf{w}_3} L_3 \\
\overline{\mathbf{w}_3} &= \overline{L_3} \frac{\partial}{\partial \mathbf{w}_3} \mathbf{w}_3 \cdot \mathbf{a}_2
\end{aligned} \tag{12}$$

$$\begin{aligned}
\overline{\mathbf{w}}_3 &= \overline{L}_3 \left[\frac{\partial}{\partial w_{311}} (w_{311}a_{21} + w_{312}a_{22}) \right] \\
&\quad \overline{\mathbf{w}}_3 = \overline{L}_3 \begin{bmatrix} a_{21} \\ a_{22} \end{bmatrix} \\
&\quad \overline{\mathbf{w}}_3 = \overline{L}_3 \mathbf{a}_2
\end{aligned} \tag{14}$$

$$\begin{aligned}
\overline{\mathbf{a}}_2 &= \overline{L}_3 \frac{\partial}{\partial \mathbf{a}_2} L_3 \\
\overline{\mathbf{a}}_2 &= \overline{L}_3 \frac{\partial}{\partial \mathbf{a}_2} \mathbf{w}_3 \cdot \mathbf{a}_2 \\
\overline{\mathbf{a}}_2 &= \overline{L}_3 \left[\frac{\partial}{\partial a_{21}} (w_{311}a_{21} + w_{312}a_{22}) \right] \\
&\quad \overline{\mathbf{a}}_2 = \overline{L}_3 \begin{bmatrix} w_{311} \\ w_{312} \end{bmatrix} \\
&\quad \overline{\mathbf{a}}_2 = \overline{L}_3 \mathbf{w}_3^T
\end{aligned} \tag{15}$$

$$\begin{aligned}
\overline{l}_2 &= \overline{a}_2 \frac{\partial}{\partial l_2} \mathbf{a}_2 \\
\overline{l}_2 &= \overline{a}_2 \frac{\partial}{\partial l_2} \text{ReLU}(l_2) \\
\overline{l}_2 &= \overline{a}_2 \theta(l_2) \cdot 1 \\
&\quad \overline{l}_2 = \overline{a}_2 \theta(l_2) \\
&\quad \overline{\mathbf{W}}_2 = \overline{l}_2 \frac{\partial}{\partial \mathbf{W}_2} l_2
\end{aligned} \tag{16}$$

1.4 Misc. Remarks

1.4.1 Rounding: Training vs Inference

Since we aim to train a binary classifier, the `round()` would be necessary for the correct output range. However since `round()` is not differentiable, we omit it during training, calculating fractional losses instead. We only include `round()` during inference.

1.4.2 2023-10-18 Remaining points of confusion

How does one go about, concretely, on an element-by-element level, determining say the matrix equivalent of derivative of a function applied to a matrix? Is the derivative applied element-wise to the existing matrix, yielding a matrix of the same dimension as the original? Then we need to have a clean notation for that without getting confusing/ambiguous. I find some of the notational conventions here unclear and confusing. The current approach is vague and imprecise, which I find bothersome.

1.4.3 2023-10-19 Remaining questions

- What is the meaning of \circ in the context of these vectorized equations? What is the difference between \circ and \cdot ? Answer: According to ChatGPT, it is the composition of the linear transformations represented by the matrices. Apparently ChatGPT can also be coaxed into thinking it's the same as matrix multiplication, i.e., $A \circ B = AB$. OK, so if one looks at [https://math.libretexts.org/Bookshelves/Linear_Algebra/Interactive_Linear_Algebra_\(Margalit_and_Rabinoff\)/03%3A_Linear_Transformations_and_Matrix_Algebra/3.04%3A_Matrix_Multiplication#:~:text=As%20we%20will%20see%2C%20composition,of%20transformations%20and%20of%20matrices](https://math.libretexts.org/Bookshelves/Linear_Algebra/Interactive_Linear_Algebra_(Margalit_and_Rabinoff)/03%3A_Linear_Transformations_and_Matrix_Algebra/3.04%3A_Matrix_Multiplication#:~:text=As%20we%20will%20see%2C%20composition,of%20transformations%20and%20of%20matrices). It does seem like it really IS matrix multiplication, but then WHY bother to use this symbol? I am somewhat confused but am still feeling reassured that I am justified in assuming it's equiv. to matrix multiplication.
- Why are some of the matrices in these vectorized backprops transposed? Examples from Roger Grosse:

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$$\overline{\mathbf{W}^{(2)}} = \mathbf{\bar{y}} \mathbf{h}^T$$

- This would be so much easier if they stated the dimensions of the various matrices/vectors in the equations
- Other questions: What does it mean to take for example: $\frac{\partial}{\partial \mathbf{w}_3}(\mathbf{w}_3 \cdot \mathbf{a}_2)$? Answer: There are two observations. One, that in general, for $\mathbf{x} \in \mathbb{R}^n, f(\mathbf{x}) : \mathbb{R}^n \mapsto \mathbb{R}$, we have that $\frac{\partial f}{\partial \mathbf{x}} = [\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots]$ Also, recall that in our MLP: $\mathbf{w}_3 = [w_{311}, w_{312}]$ and $\mathbf{a}_2 = [a_{21}, a_{22}]$ so $\mathbf{w}_3 \cdot \mathbf{a}_2 = w_{311}a_{21} + w_{312}a_{22}$, so $\frac{\partial \mathbf{w}_3 \cdot \mathbf{a}_2}{\partial \mathbf{w}_3} = [\frac{\partial}{\partial w_{311}}(w_{311}a_{21} + w_{312}a_{22}), \frac{\partial}{\partial w_{312}}(w_{311}a_{21} + w_{312}a_{22})]$ so $\frac{\partial \mathbf{w}_3 \cdot \mathbf{a}_2}{\partial \mathbf{w}_3} = [a_{21} + \frac{\partial}{\partial w_{311}}(w_{312}a_{22}), \frac{\partial}{\partial w_{312}}(w_{311}a_{21}) + a_{22}]$ so $\frac{\partial \mathbf{w}_3 \cdot \mathbf{a}_2}{\partial \mathbf{w}_3} = [a_{21} + 0, 0 + a_{22}]$ so $\frac{\partial \mathbf{w}_3 \cdot \mathbf{a}_2}{\partial \mathbf{w}_3} = [a_{21}, a_{22}]$ so $\frac{\partial \mathbf{w}_3 \cdot \mathbf{a}_2}{\partial \mathbf{w}_3} = \mathbf{a}_2$

1.4.4 2023-10-22 Remaining questions

- what is the derivative of an $n \times m$ vector/matrix with respect to another matrix of the same dimension? ChatGPT: in general, the derivative of one vector w.r.t. another is called the Jacobian. The generalized answer for derivative of a matrix w.r.t another is still unanswered.