CSCE 790 Neural Networks and Their Applications Homework 2 Report

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Part A

Rumelhart, D.E., Hinton, G.E. and Williams, R.J., 1986. Learning representations by back- propagating errors. Nature, 323(6088), pp.533-536.

This paper is the seminal work that brought back-propagation (a.k.a. automatic differentiation) into the mainstream in the context of neural network training. To summarize the algorithm described in the paper -

1. For a set a of training inputs and labels, do forward computation to get a prediction. Make sure to save all the intermediate computations.
2. Calculate the difference between true labels vs the predictions using some metric. This is the error.
3. Calculate derivative of the error with respect to the prediction. From this, gradually calculate derivatives of the inner layers of the network using chain rule.
4. The key observation is that, the gradient of a weight in a particular layer is a linear function of the inputs from inner layer and the back-propagated gradient from outer layer.
5. Using functional dependency relation of neuron's output to it's input, the gradient chain can be linked all the way to the network input.
6. Iteratively adjust all weights in the opposite direction of their gradients until convergence.

LeCun, Y.A., Bottou, L., Orr, G.B. and Müller, K.R., 2012. Efficient backprop. In Neural networks: Tricks of the trade (pp. 9-48). Springer, Berlin, Heidelberg.

This paper describes some heuristics and tricks to improve performance of standard back-propagation. Most of the techniques described here is still widely used and is pretty relevant.

1. In section `4.1` The authors present stochastic, batch and mini-batch approaches to gradient descent. They go-through pros and cons of all three methods.
2. Section `4.2` focuses on importance of sample randomization. With randomized input order, the chance of a network falling into a local optima is greatly reduced.
3. Section `4.3` describes data normalization. The authors suggests the input samples to be normalized close to zero. Also, they recommend to scale different components of the input vector to have identical covariance.
4. In section `4.6`, the authors describe a particular approach to weight initialization. They recommend to sample from a uniform distribution with zero mean.
5. Section `4.7` discusses learning rates and momentum.

The paper also goes over ineffectiveness of some classical optimization algorithms in the context of training a neural network.

Part B

Section 1 and 2

I have implemented a general framework for simple multi-layer perceptrons, along with hand-rolled back-propagation, using numpy. The network class `MLP`, along with some routines for training is implemented inside the network.py file. `MLP` class can be invoked with different a sequence of layer specifications to configure network topology and complexity. The file also contains two simple neural networks as test cases.

Initially I implemented the back-propagation algorithm using various matrix operations offered in numpy. Later, I found einstein-summation notation to be simpler and re-implemented some parts using this generalized operation.

The single layer network of section 1 is implemented in one_layer_classifier.py.

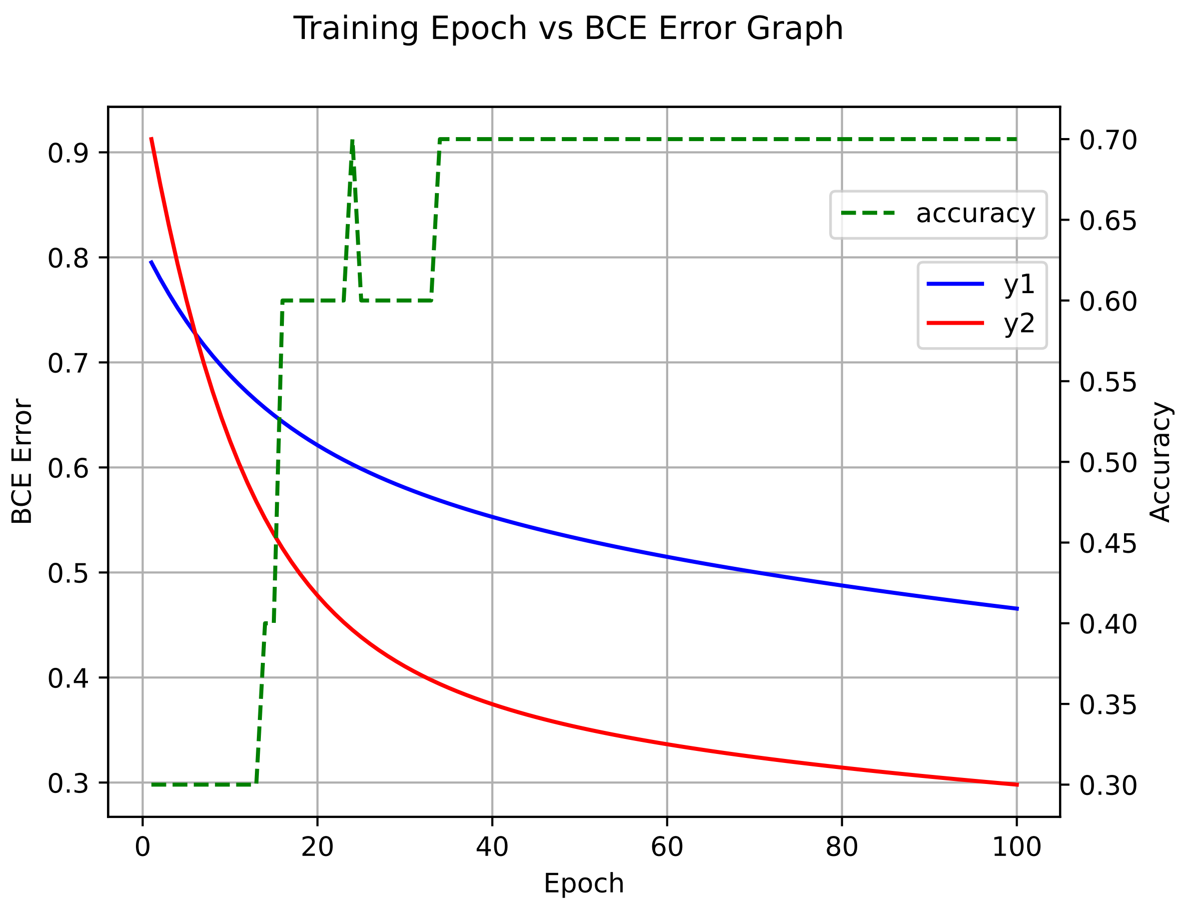
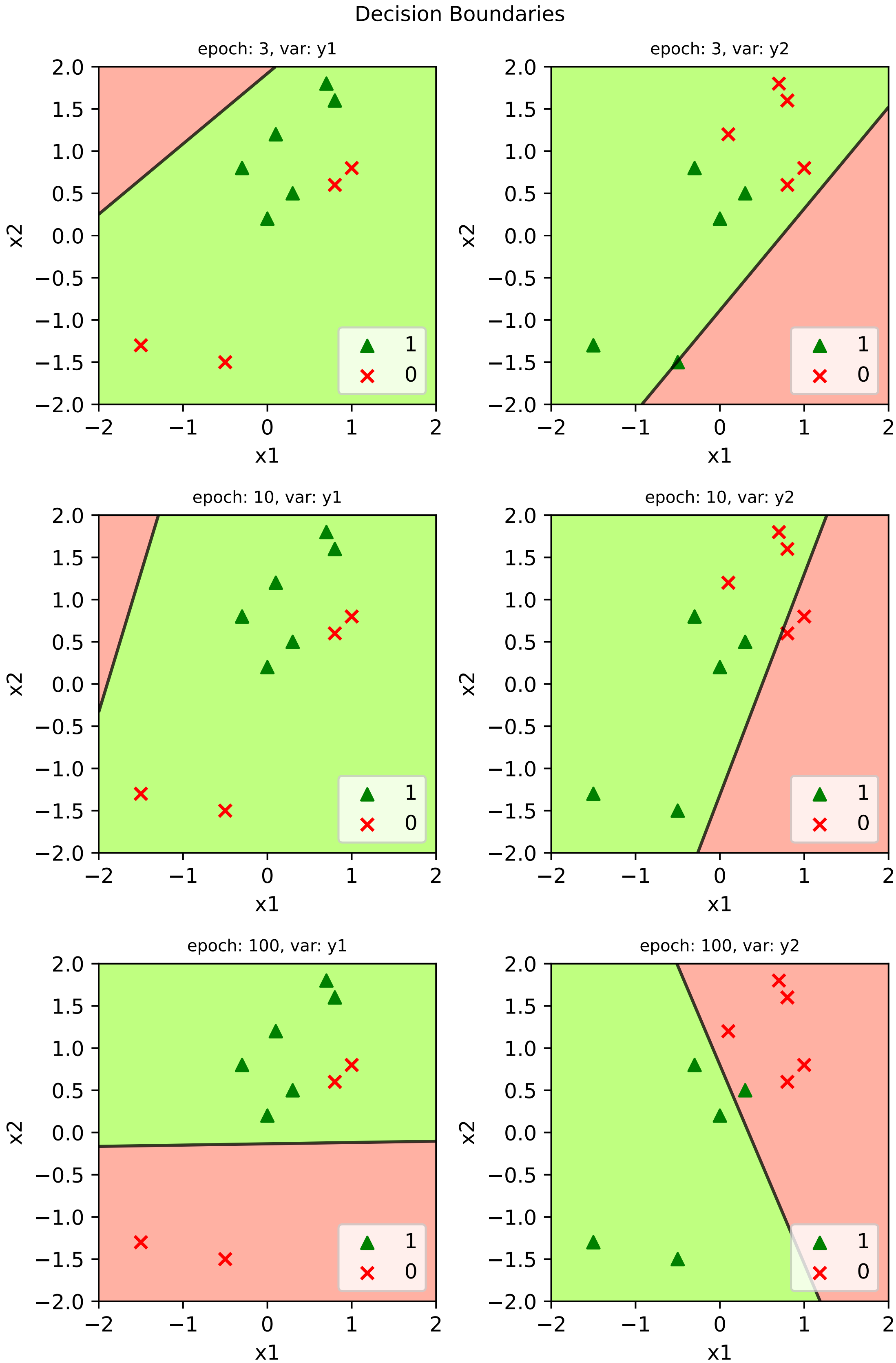


Figure 1: Training error vs epoch number for one-layer classifier


Decision Boundaries
epoch: 3, var: y1
epoch: 3, var: y2
epoch: 10, var: y1
epoch: 10, var: y2
epoch: 100, var: y1
epoch: 100, var: y2
x1
x2
1
0

The double layer regression network in implemented in two_layer_regression.py.

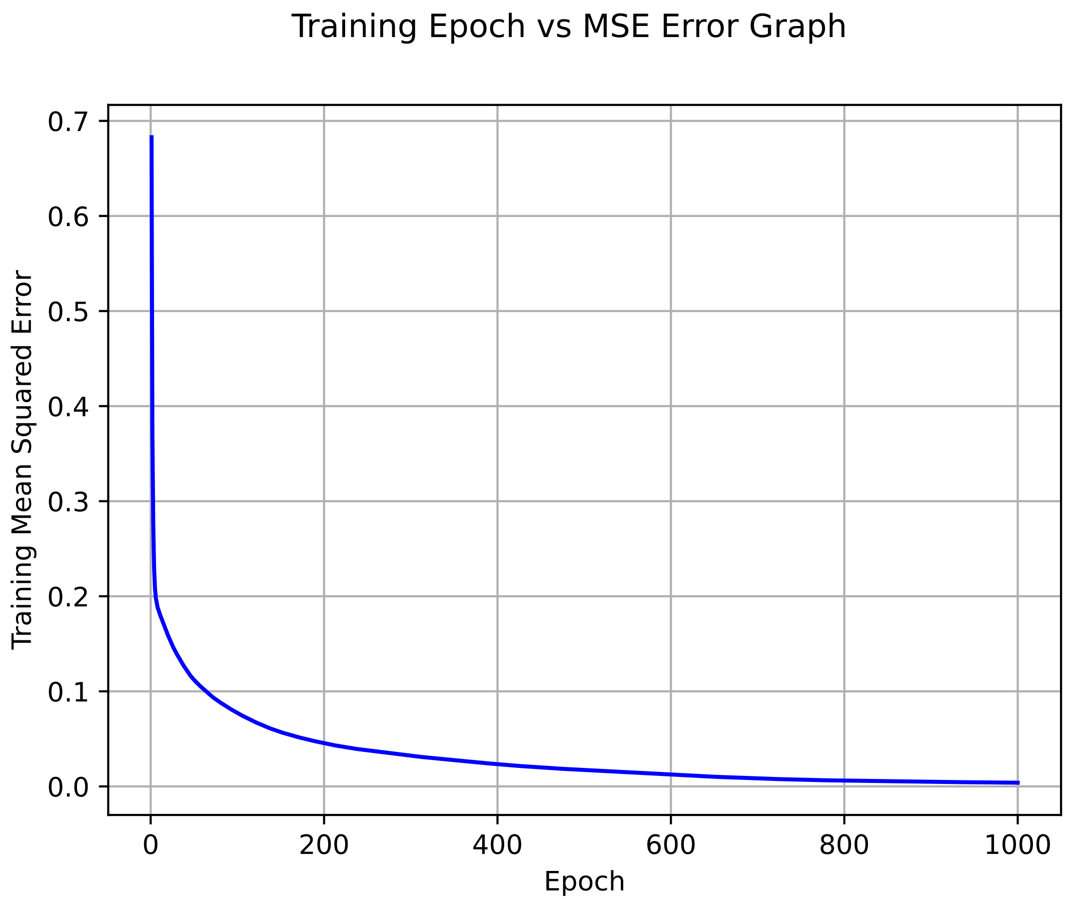


Figure 2: Training error vs epoch number for two-layer regressor

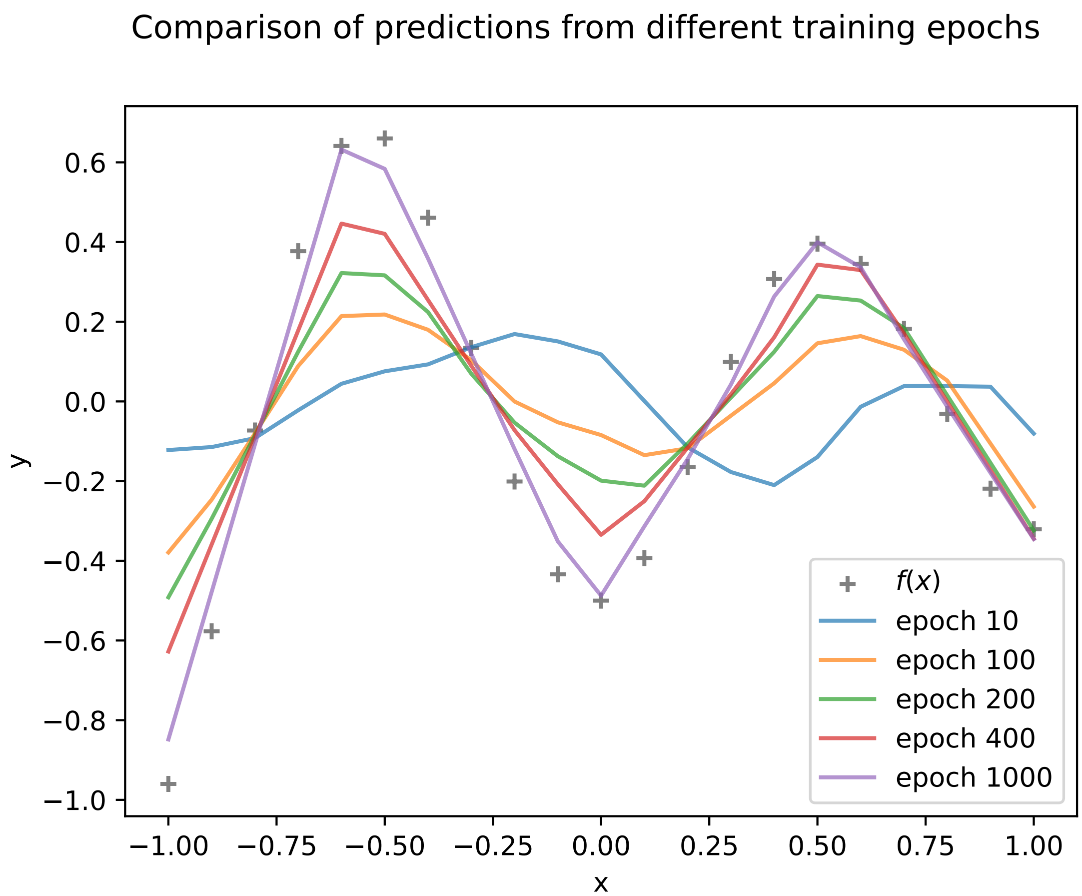


Figure 3: f(x) vs x and NN vs x for two-layer regressor

Section 3

The article describes creating an standard multi-head attention transformer for sequence to sequence mapping. The task was to map a randomly generated sequence of size $(64, 100)$ to another randomly generated sequence of size $(64, 100)$. The proposed model uses a 8-head, 512 neuron-wide attention mechanism. The whole model employs 6 encoder and 6 decoder stages.

Both the source and the target vocabulary was 5000. Verbatim copy of the code is available here. The training session standard output is available here.

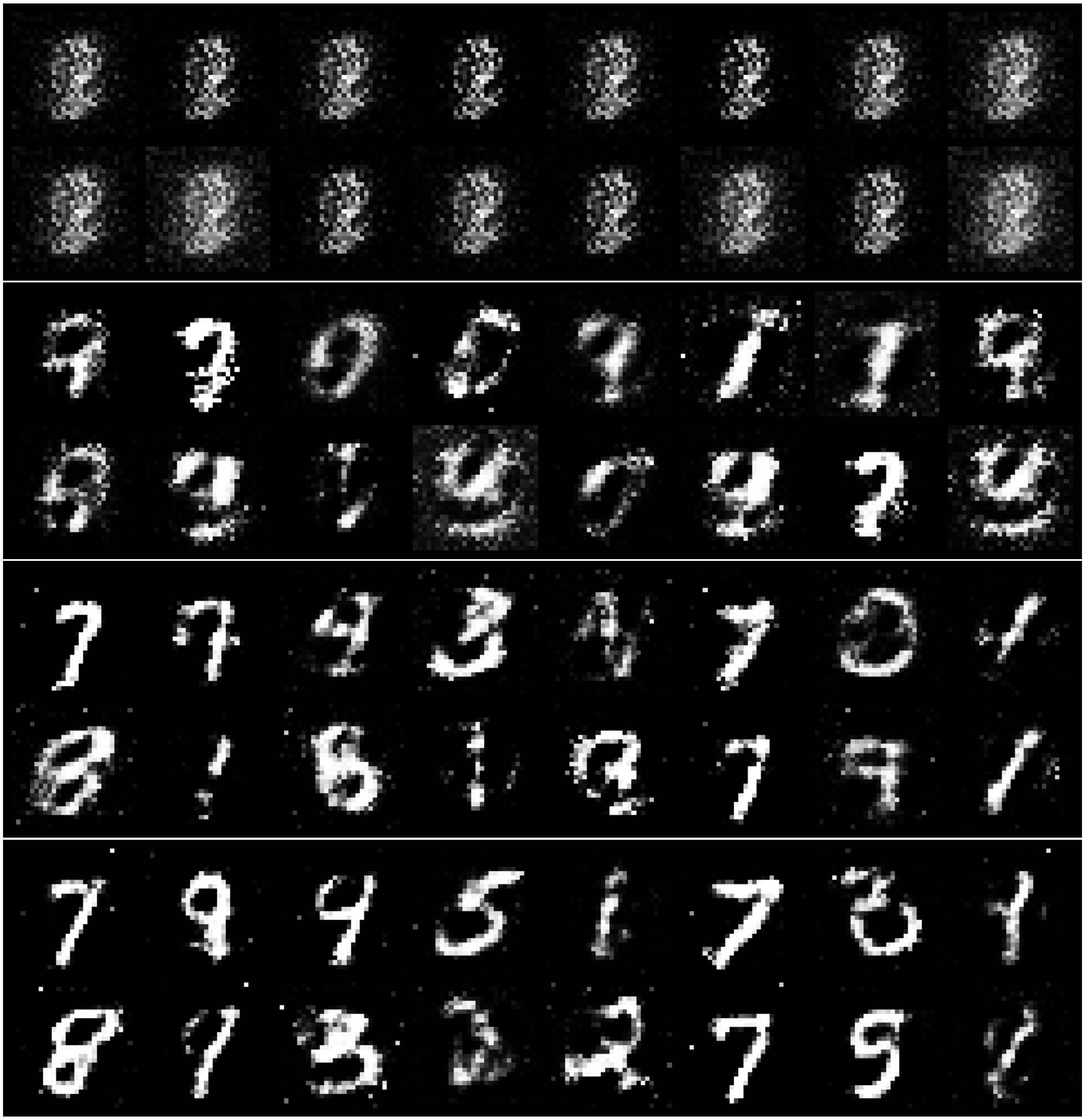
Section 4

This article describes generative adversarial networks(GAN) in detail. All the code used in the article is available here. I simply cloned the repository and ran the jupyter notebooks in my local machine to generate the results.

Vanilla GAN was relatively inexpensive to compute compared to DCGAN. VGAN ran for full 200 epochs. I had to forcefully stop training for DCGAN at 50 epochs. Samples generated by

DCGAN were much more visually pleasant.

Generated samples by Vanilla GAN after training for 0, 10, 25 and 50 epochs:



Generated samples by DCGAN after training for 0, 10, 25 and 50 epochs:

Part C

Let us define the symbols for the 2-layer feed-forward NN,

$$
\begin{aligned}
i &= \text{The network input size} \\
h &= \text{Number of neurons in first(hidden) layer} \\
o &= \text{Number of neurons in second(output) layer} \\
{}^{h\times i}W_1 &= \text{Weight matrix of size (h}\times\text{i) for hidden layer} \\
{}^{h\times 1}b_1 &= \text{Bias vector of size (h}\times\text{1) for hidden layer} \\
{}^{o\times h}W_2 &= \text{Weight matrix of size (o}\times\text{h) for output layer} \\
{}^{o\times 1}b_2 &= \text{Bias vector of size (o}\times\text{1) for output layer} \\
{}^{o\times 1}E' &= \text{The gradient of the loss function as a matrix of size (o}\times\text{1)} \\
{}^{i\times 1}X_1 &= \text{Input vector of size (i}\times\text{1)} \\
{}^{o\times 1}Y_2 &= \text{Output vector of size (o}\times\text{1)}
\end{aligned}
$$

For clarity, let's brake-up the forward computation into steps.

$$
\begin{aligned}
{}^{h\times 1}Z_1 &= {}^{h\times i}W_1 . {}^{i\times 1}X_1 + {}^{h\times 1}b_1 \qquad \text{Hidden layer (linear)} \\
{}^{h\times 1}Y_1 &= tanh({}^{h\times 1}Z_1) \qquad \text{Hidden layer (activation)} \\
{}^{o\times h}Z_2 &= {}^{o\times h}W_2 . {}^{h\times 1}Y_1 + {}^{o\times 1}b_2 \qquad \text{Output layer (linear)} \\
{}^{o\times 1}Y_2 &= tanh({}^{o\times 1}Z_2) \qquad \text{Output layer(activation)}
\end{aligned}
$$

Using chain rule, the gradient of the error w.r.t. W_2 is,

$$
\begin{aligned}
\frac{\mathrm{d}E}{\mathrm{d}W_2} &= \frac{\partial E}{\partial Y_2}.\frac{\partial Y_2}{\partial Z_2}.\frac{\partial Z_2}{\partial W_2} \\
&= E'.\frac{\partial tanh(Z_2)}{\partial Z_2}.\frac{\partial (W_2.Y_1 + b_2)}{\partial W_2} \\
&= E'.(1 - tanh^2(Z_2)).(Y_1 + 0) \quad ; \frac{\mathrm{d}tanh(x)}{\mathrm{d}x} = 1 - tanh^2(x) \\
&= E'.(1 - tanh^2(Z_2)).Y_1
\end{aligned}
$$

With matrix sizes and operations specified,

$$
{}^{o\times h}\frac{\mathrm{d}E}{\mathrm{d}W_2} = \left[{}^{o\times 1}E' \odot {}^{o\times 1}(1 - tanh^2(Z_2))\right] \otimes {}^{h\times 1}Y_1 \quad ; \otimes = \text{outer product}, \odot = \text{hadamard product}
$$

Similarly, we can derive the gradient of the bias b_2,

$$ {}^{o\times 1}\frac{\mathrm{d}E}{\mathrm{d}b_2} = {}^{o\times 1}E' \odot {}^{o\times 1}(1 - tanh^2(Z_2)) $$

For the hidden layer, the gradient of the error w.r.t. W_1 is,

$$ \begin{aligned} \frac{\mathrm{d}E}{\mathrm{d}W_1} &= \frac{\partial E}{\partial Y_2}.\frac{\partial Y_2}{\partial Z_2}.\frac{\partial Z_2}{\partial Y_1}.\frac{\partial Y_1}{\partial Z_1}.\frac{\partial Z_1}{\partial W_1} \\ &= E'.(1 - tanh^2(Z_2)).(W_2 + 0).(1 - tanh^2(Z_1)).(X_1 + 0) \\ &= E'.(1 - tanh^2(Z_2)).W_2.(1 - tanh^2(Z_1)).X_1 \end{aligned} $$

With matrix sizes and operations specified,

$$ {}^{h\times i}\frac{\mathrm{d}E}{\mathrm{d}W_1} = \left[\left[{}^{h\times o}{W_2}^T \left[{}^{o\times 1}E' \odot {}^{o\times 1}(1 - tanh^2(Z_2))\right]\right] \odot {}^{h\times 1}(1 - tanh^2(Z_1))\right] \otimes {}^{i\times 1}X_1 $$

For bias b_1,

$$ {}^{h\times 1}\frac{\mathrm{d}E}{\mathrm{d}b_1} = \left[{}^{h\times o}{W_2}^T \left[{}^{o\times 1}E' \odot {}^{o\times 1}(1 - tanh^2(Z_2))\right]\right] \odot {}^{h\times 1}(1 - tanh^2(Z_1)) $$