Introduction to Artificial Intelligence (CS470): Assignment 1

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1 Multi-Layer Perceptron (MLP)

1.1 A forward pass: compute a SoftMax loss

Let $\mathbf{x} \in \mathbb{R}^{n \times d}$ be the input matrix with n batch size and d input size.

The hidden layer uses weights $\mathbf{w}^{(1)}$ and biases $\mathbf{b}^{(1)}$

The output layer uses weights $\mathbf{w}^{(2)}$ and biases $\mathbf{b}^{(2)}$

The output of the network is a matrix $\mathbf{y}^{(2)} \in \mathbb{R}^{n \times \mathbf{l}_2}$.

To introduce nonlinearity, we apply the Rectified Linear Unit (ReLU) activation function:

$$\sigma(\mathbf{x}) = \max(0, \mathbf{x})$$

Then, the forward pass equations for the network can be written as:

$$\mathbf{y}^{(1)} = \mathbf{x}\mathbf{w}^{(1)} + \mathbf{b}^{(1)}$$
, where $\mathbf{y}^{(1)} \in R^{n \times \mathbf{l}_1}$, $\mathbf{w}^{(1)} \in R^{d \times \mathbf{l}_1}$, $\mathbf{b}^{(1)} \in R^{\mathbf{l}_1}$

$$\mathbf{h}^{(1)} = \sigma(\mathbf{y}^{(1)}) = \max(0, \mathbf{y}^{(1)}), \text{ where } \mathbf{h}^{(1)} \in \mathbb{R}^{n \times \mathbf{l}_1}$$

$$\mathbf{v}^{(2)} = \mathbf{h}^{(1)} \mathbf{w}^{(2)} + \mathbf{b}^{(2)}$$
, where $\mathbf{v}^{(2)} \in R^{n \times l_2}$, $\mathbf{w}^{(1)} \in R^{l_1 \times l_2}$, $\mathbf{b}^{(2)} \in R^{l_2}$

$$\hat{\mathbf{y}}^{(2)} = softmax(\mathbf{y}^{(2)}), \text{ where } \hat{\mathbf{y}}^{(2)} \in \mathbb{R}^{n \times l_2}$$

To compute the softmax loss, we need to first apply the softmax on the output layer $\hat{\mathbf{y}}^{(2)}$. We recall that softmax is apply on each row vectors of index i of the matrix:

softmax(
$$\mathbf{x}$$
)_i = $\frac{e^{x_i}}{\sum_{i=1}^{l_2} e^{x_i}}$, $i = 1, ..., n$

The softmax loss, also known as the cross-entropy loss is computed this way:

$$L_i(\hat{\mathbf{y}}_i^{(2)}, \mathbf{t}) = -\frac{1}{l_2} \sum_{j=1}^{l_2} t_j \log(\hat{\mathbf{y}}_{i,j}^{(2)}), \text{ where } \mathbf{t} \text{ is the target vector}$$

The final loss is the mean over the softmax loss of all sample :

$$\mathcal{L} = -\frac{1}{n} \sum_{i} L_{i}$$

```
def forward_pass(self, x, w1, b1, w2, b2):
1
2
        y1 = x.dot(w1) + b1
        if self.activation_method == 0:
          # ReLU
6
         h1 = np.where(y1 > 0, y1, 0)
        elif self.activation_method == 1:
          # Leaky ReLU
9
          h1 = np.where(y1 > 0, y1, self.leaky_relu_c*y1)
10
        elif self.activation_method == 2:
11
          # SWISH
          h1 = y1 * sigmoid(y1)
13
        else:
14
            h1 = self.selu_lambda * np.where(y1 > 0, y1, self.selu_alpha * (np.exp(y1) - 1))
15
16
        y2 = h1.dot(w2) + b2
17
```

```
def softmax_loss(self, x, y):
        #...
2
        loss = 0
3
        epsilon = 1e-15
        n = x.shape[0]
5
        exp = np.exp(x)
        softmax = exp / np.sum(exp,axis=1,keepdims=True)
9
        for i in range(n):
            loss += -np.log(softmax[i, y[i]]+epsilon)
11
        loss = (-loss/n)
12
13
        dx = softmax
        dx[np.arange(n), y] = 1
15
        dx /= n
16
```

1.2 A backward pass: compute gradients

To compute the backward propagation we use the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(1)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{y}^{(2)}} \frac{\partial \mathbf{y}^{(2)}}{\partial \mathbf{h}^{(1)}} \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{y}^{(1)}} \frac{\partial \mathbf{y}^{(1)}}{\partial \mathbf{W}^{(1)}}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{(1)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{y}^{(2)}} \frac{\partial \mathbf{y}^{(2)}}{\partial \mathbf{h}^{(1)}} \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{y}^{(1)}} \frac{\partial \mathbf{y}^{(1)}}{\partial \mathbf{b}^{(1)}}$$

First let's compute $\frac{\partial \hat{\mathbf{y}}^{(2)}}{\mathbf{y}^{(2)}}$

Each element
$$i,j$$
 of the matrix $\frac{\partial \hat{\mathbf{y}}^{(2)}}{\mathbf{y}^{(2)}}$ is equal to $\frac{\partial \hat{\mathbf{y}}_i^{(2)}}{\partial \mathbf{y}_i^{(2)}}$

Let p_i be the i^{th} element of the softmax output vector $\hat{\mathbf{y}}^{(2)}$, and let y_j be the j^{th} element of the input vector $\mathbf{y}^{(2)}$:

First we know that

$$\frac{\partial e^{y_i}}{\partial y_j} = \begin{cases} e^{y_i} & \text{if } i = j\\ 0 & \text{otherwise} \end{cases}$$

$$\frac{\partial}{\partial y_j} \sum_{k=1}^{l_2} e^{y_k} = e^{y_j}$$

So when i = j, we have:

$$\begin{split} \frac{\partial p_i}{\partial y_j} &= \frac{\partial}{\partial y_j} \frac{e^{y_i}}{\sum_{k=1}^{l_2} e^{y_k}} \\ &= \frac{e^{y_j} \sum_{k=1}^{l_2} e^{y_k} - e^{y_i} e^{y_j}}{\left(\sum_{k=1}^{l_2} e^{y_k}\right)^2} \\ &= \frac{e^{y_j}}{\sum_{k=1}^{l_2} e^{y_k}} \left(\frac{\sum_{k=1}^{l_2} e^{y_k}}{\sum_{k=1}^{l_2} e^{y_k}} - \frac{e^{y_i}}{\sum_{k=1}^{l_2} e^{y_k}}\right) \\ &= p_i (1 - p_j) \end{split}$$

When $i \neq j$, we have:

$$\begin{split} \frac{\partial p_i}{\partial y_j} &= \frac{\partial}{\partial y_j} \frac{e^{y_i}}{\sum_{k=1}^{l_2} e^{y_k}} \\ &= -\frac{e^{y_i} e^{y_j}}{\left(\sum_{k=1}^{l_2} e^{y_k}\right)^2} \\ &= -\frac{e^{y_i}}{\sum_{k=1}^{l_2} e^{y_k}} \cdot \frac{e^{y_j}}{\sum_{k=1}^{l_2} e^{y_k}} \\ &= -p_i p_i \end{split}$$

Now we can compute $\frac{\partial \mathcal{L}}{\partial \mathbf{y}^{(2)}}$

$$\begin{split} Li &= -\sum_j t_j \log(p_j) \\ \frac{\partial Li}{\partial y_i} &= -\sum_j t_j \frac{\partial \log(p_j)}{\partial y_i} \\ &= -\sum_j t_j \frac{1}{p_j} \frac{\partial p_j}{\partial y_i} \\ &= -t_i \frac{p_i}{p_i} (1-p_i) - \sum_{j \neq i} t_j \frac{1}{p_j} (-p_j p_i), \text{ from the previous computation} \\ &= -t_i + t_i p_i + \sum_{j \neq i} t_j p_i \\ &= -t_i + p_i (ti + \sum_{j \neq i} t_j) \\ &= p_i - t_i, \text{ because } (t_i + \sum_{j \neq i} t_j) = 1 \text{ , since } \mathbf{t} \text{ is a one-hot encoded vector} \end{split}$$

So finally,

$$\frac{\partial \mathcal{L}}{\partial \mathbf{y}^{(2)}} = \frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t})$$

We compute the others derivative of the chain rule which are straight-forwards,

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{v}^{(2)}} \frac{\partial \mathbf{y}^{(2)}}{\mathbf{W}^{(2)}} = \frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{h}^{(1)}$$
(1)

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{(2)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{v}^{(2)}} \frac{\partial \mathbf{y}^{(2)}}{\mathbf{b}^{(2)}} = \frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \cdot \mathbf{1}$$
(2)

$$\overline{\mathbf{y}^{(1)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{y}^{(1)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{y}^{(2)}} \frac{\partial \mathbf{y}^{(2)}}{\mathbf{h}^{(1)}} \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{y}^{(1)}} = \frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{W}^{(2)} \sigma'(\mathbf{y}^{(1)})$$
(3)

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(1)}} = \overline{\mathbf{y}^{(1)}} \frac{\partial \mathbf{y}^{(1)}}{\partial \mathbf{W}^{(1)}} = \frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{W}^{(2)} \sigma'(\mathbf{y}^{(1)}) \mathbf{x}$$
(4)

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{(1)}} = \overline{\mathbf{y}^{(1)}} \frac{\partial \mathbf{y}^{(1)}}{\partial \mathbf{b}^{(1)}} = \frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{W}^{(2)} \sigma'(\mathbf{y}^{(1)}) \cdot \mathbf{1}$$
(5)

$$\sigma'(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{otherwise} \end{cases}$$
 (6)

```
def backward_pass(self, dY2_dLoss, x, w1, y1, h1, w2):
2
        #without regularization
        dY2_dw2 = h1.T
        dY2_dh1 = dY2_dLoss.dot(w2.T)
6
        grads['w2'] = dY2_dw2.dot(dY2_dLoss)
        grads['b2'] = dY2_dLoss.sum(axis=0)
10
        if self.activation_method == 0:
11
          # ReLU
          dy1_dh1 = np.where(y1 > 0, 1, 0)
13
          dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
14
        elif self.activation_method == 1:
15
          # Leaky ReLU
          dy1_dh1 = np.where(y1 > 0, 1, self.leaky_relu_c)
17
          dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
        elif self.activation_method == 2:
19
          # SWISH
          dy1_dh1 = sigmoid(y1) * (1+y1*(1-sigmoid(y1)))
21
          dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
23
        else:
          # SELU
25
          dy1_dh1 = self.selu_lambda * np.where(y1 > 0, 1, self.selu_alpha * np.exp(y1))
26
          dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
28
        grads['w1'] = x.T.dot(dY1_dLoss)
        grads['b1'] = np.sum(dY1_dLoss, axis=0)
30
```

1.3 Training: Stochastic Gradient Descent (SGD)

We add a regularization to the loss \mathcal{L} by adding the regularization term $\lambda \mathcal{R} = \frac{\lambda}{2}\theta$, where $\theta = \frac{1}{2}w^2$, in our case $w^2 = \|\mathbf{W}^{(2)}\|_2^2 + \|\mathbf{W}^{(1)}\|_2^2$. We compute the norm-2 with the formula $\sum_i \sum_j w_{i,j}^2$.

We need to compute the new gradient of weights:

$$\frac{\partial \mathcal{L} + \lambda \mathcal{R}}{\partial \theta} = \frac{\partial \mathcal{L}}{\partial \theta} + \frac{\partial \lambda \mathcal{R}}{\partial \theta}$$

$$\frac{\partial \mathcal{R}}{\partial \theta} = \lambda \frac{\partial \mathcal{R}}{\partial \theta} = \frac{\lambda}{2} \frac{\partial \theta^2}{\partial \theta} = \lambda \theta.$$

So we update the parameters of the model with the following formula (notice the $-\eta\lambda\theta$ which have been added from the usual formula):

$$\theta = \theta - \eta \nabla_{\theta} J(\theta; x^{(i)}, y^{(i)}) - \eta \lambda \theta$$
$$= \theta - \eta (\nabla_{\theta} J(\theta; x^{(i)}, y^{(i)}) + \lambda \theta)$$

From the backward propagation equations 1 we have :

$$\begin{split} \mathbf{W}^{(2)} \leftarrow \mathbf{W}^{(2)} - \eta \left(\frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{h}^{(1)} + \lambda \mathbf{W}^{(2)} \right) \\ \mathbf{b}^{(2)} \leftarrow \mathbf{b}^{(2)} - \eta \left(\frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \cdot \mathbf{1} \right) \\ \mathbf{W}^{(1)} \leftarrow \mathbf{W}^{(1)} - \eta \left(\frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{W}^{(2)} \sigma'(\mathbf{y}^{(1)}) \mathbf{x} + \lambda \mathbf{W}^{(1)} \right) \\ \mathbf{b}^{(1)} \leftarrow \mathbf{b}^{(1)} - \eta \left(\frac{1}{n} (\hat{\mathbf{y}}^{(2)} - \mathbf{t}) \mathbf{W}^{(2)} \sigma'(\mathbf{y}^{(1)}) \cdot \mathbf{1} \right) \end{split}$$

```
def loss(self, x, y=None, regular=0.0, enable_margin=False):
    # PLACE YOUR CODE HERE (REGULARIZATION)
    # TODO: Implement weight regularization
    loss += 0.5 * regular * (np.sum(w1 * w1) + np.sum(w2 * w2))
    #add regularization effect to the gradient terms
9
    grads['w2'] += regular * w2
10
    grads['w1'] += regular * w1
11
12
    # END OF YOUR CODE
     14
```

```
def train(self, x, y, x_v, y_v,
           eta=1e-3, lamdba=0.95,
2
           regular=1e-5, num_iters=50,
           batch_size=100, verbose=False):
       # PLACE YOUR CODE HERE
       # TODO: Create a random minibatch of training data and labels, storing
       # them in x_batch and y_batch respectively.
10
       rand_indexes = np.random.choice(num_train, batch_size, replace=True)
11
       x_batch = x[rand_indexes]
       y_batch = y[rand_indexes]
13
14
       # END OF YOUR CODE
15
       17
       # Compute loss and gradients using the current minibatch
       loss, grads = self.loss(x_batch, y=y_batch, regular=regular)
19
       loss_history.append(loss)
20
21
       # PLACE YOUR CODE HERE
23
       # TODO: Update the parameters of the network stored in self.params by
25
       # using the gradients in the grads dictionary. For that, use stochastic #
26
       # gradient descent.
       self.params['w1'] += -eta * grads["w1"]
28
       self.params['w2'] += -eta * grads["w2"]
       self.params['b1'] += -eta * grads["b1"]
30
       self.params['b2'] += -eta * grads["b2"]
32
       # END OF YOUR CODE
33
       34
```

```
Selected using ReLU

The #iteration 0 / 1000: loss -2.301592

The #iteration 100 / 1000: loss -1.983305

The #iteration 200 / 1000: loss -1.673172

The #iteration 300 / 1000: loss -1.604143

The #iteration 400 / 1000: loss -1.563334

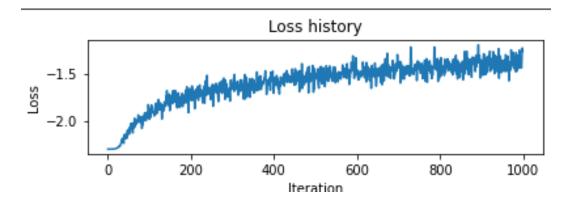
The #iteration 500 / 1000: loss -1.552667

The #iteration 600 / 1000: loss -1.450022

The #iteration 700 / 1000: loss -1.402927

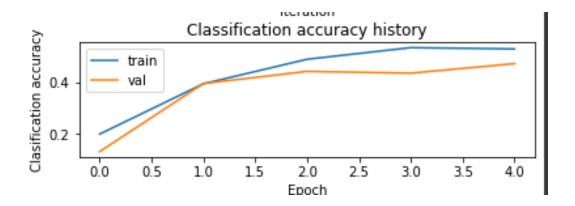
The #iteration 800 / 1000: loss -1.480540

The #iteration 900 / 1000: loss -1.486115
```



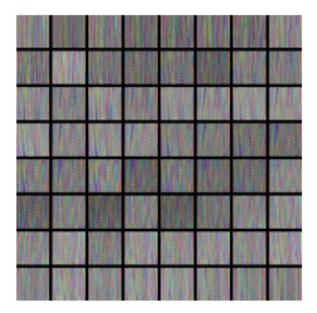
1.4 Prediction

```
def predict(self, x):
1
    2
    # PLACE YOUR CODE HERE
    # TODO: Implement the predict function
    out, _ = self.forward_pass(x, self.params['w1'],
                   self.params['b1'],
                   self.params['w2'],
                   self.params['b2'])
10
    y_pr = np.argmax(out, axis=1)
11
12
    # END OF YOUR CODE
    14
```



1.5 Visualization

Here is the weights visualization, we can see that there is no human recognizable pattern in the image.



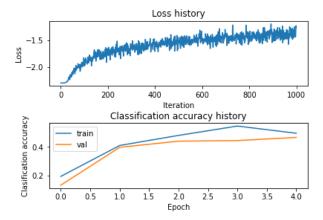
```
def predict(self, x):
1
    2
    # PLACE YOUR CODE HERE
3
    # TODO: Implement the predict function
                                             #
    out, _ = self.forward_pass(x, self.params['w1'],
                   self.params['b1'],
                   self.params['w2'],
                   self.params['b2'])
9
10
    y_pr = np.argmax(out, axis=1)
11
12
    # END OF YOUR CODE
13
    14
```

1.6 Advanced - Activation functions

We can compute the derivatives of the other activation functions as follow : The derivative of LeakyReLU is:

$$\frac{d}{dx} \text{LeakyReLU}(x) = \begin{cases} 1 & \text{if } x > 0 \ \alpha \\ \text{otherwise} \end{cases}$$

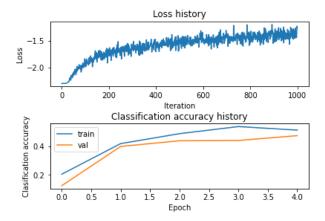
This is the result of using this activation function



The derivative of Swish is:

$$\frac{d}{dx}Swish(x) = Swish(x) + \sigma(x)(1 - Swish(x))$$

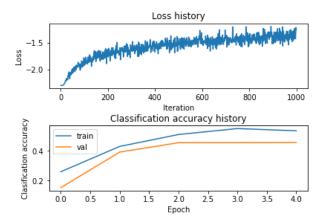
This is the result of using this activation function



The derivative of SELU is:

$$\frac{d}{dx} SELU(x) = \lambda \begin{cases} 1 & \text{if } x > 0 \ \alpha e^x \\ \text{otherwise} \end{cases}$$
 (7)

This is the result of using this activation function



```
def forward_pass(self, x, w1, b1, w2, b2):
      2
      # PLACE YOUR CODE HERE
      # TODO: Design the fully-connected neural network and compute its forward
      #
            pass output,
6
            Input - Linear layer - LeakyReLU - Linear layer.
            You have use predefined variables above
      y1 = x.dot(w1) + b1
10
11
      if self.activation_method == 0:
12
       # ReLU
13
       h1 = np.where(y1 > 0, y1, 0)
14
      elif self.activation_method == 1:
15
       # Leaky ReLU
       h1 = np.where(y1 > 0, y1, self.leaky_relu_c*y1)
17
      elif self.activation_method == 2:
       # SWISH
19
       h1 = y1 * sigmoid(y1)
20
      else:
21
         h1 = self.selu_lambda * np.where(y1 > 0, y1, self.selu_alpha * (np.exp(y1) - 1))
23
      y2 = h1.dot(w2) + b2
25
26
      # END OF YOUR CODE
27
      28
```

```
def backward_pass(self, dY2_dLoss, x, w1, y1, h1, w2):
       2
       # PLACE YOUR CODE HERE
       # TODO: Compute the backward pass, computing the derivatives of the weights #
       # and biases. Store the results in the grads dictionary. For example,
6
       # the gradient on W1 should be stored in grads['w1'] and be a matrix of same#
       # size
       #without regularization
10
11
       dY2_dw2 = h1.T
       dY2_dh1 = dY2_dLoss.dot(w2.T)
13
14
       grads['w2'] = dY2_dw2.dot(dY2_dLoss)
15
       grads['b2'] = dY2_dLoss.sum(axis=0) #we do the sum to match the dimensions
17
       if self.activation_method == 0:
        # ReLU
19
        dy1_dh1 = np.where(y1 > 0, 1, 0)
        dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
21
       elif self.activation_method == 1:
        # Leaky ReLU
23
        dy1_dh1 = np.where(y1 > 0, 1, self.leaky_relu_c)
24
        dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
25
       elif self.activation_method == 2:
26
        # SWISH
        dy1_dh1 = sigmoid(y1) * (1+y1*(1-sigmoid(y1)))
28
        dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
30
       else:
31
        # SELU
32
        dy1_dh1 = self.selu_lambda * np.where(y1 > 0, 1, self.selu_alpha * np.exp(y1))
33
        dY1_dLoss = dY2_dLoss.dot(w2.T) * dy1_dh1
34
       grads['w1'] = x.T.dot(dY1_dLoss)
36
       grads['b1'] = np.sum(dY1_dLoss, axis=0)
38
       # END OF YOUR CODE
       40
```

We notice that the LeakyReLU have the best accuracy score even though there is a very small difference between these different activation functions.