09.3 - Deep Learning - Extending Deep Neural Network

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1 Programming for Data Science and Artificial Intelligence

1.1 9.3 Deep Learning - Extending Deep Neural Network

1.1.1 Readings

- [WEIDMAN] Ch4
- [CHARU] Ch2-3

```
[1]: #import from last time work so we can extend further from neuralnet.first_version import *

#To make this simple, I have stored all our stuff #that we have develop so far in the folder #<code>/neuralnet/first_version.py</code>
```

In the last two classes, we focus on understanding deep neural net and I hope it's going fantastic. Anyhow, what we have been discovering so far is the most basic form of it and most of the time, it is insufficient for most real-world problems.

Today, we shall explore some well-understood techniques that make neural network training more likely to succeed.

Before doing that, let's review the intuition behind neural network:

In a high-level view, we can say that Neural Network is trying to most optimal parameters which is commonly defined as W that **minimizes the loss**, which can be described using the figure like this:

Now, if we use non-linear activation function like sigmoid, **each W will have a non-linear relationship with the loss**. If we plot one W against loss, while keeping everything constant, we get this oversimplistic graph:

At the beginning, we will probably randomize a W value, and we iterate to update our W by finding the gradients. How large should we move along the slope then? We use learning rate. Small learning rate means small step of update which can be slow but risk ending up in a local minimia, while large learning mean large step of update what will be faster but risk hopping over" the global minimum

Now we can imagine there are many areas we can perhaps improve on:

1. The **loss function**. We used MSE as our loss function. We chose this because it is convex (i.e., imagining a shape of U), meaning that when the loss is huge, the gradient is steeper

(imagine the curve is very steep on the top of U but become less toward the bottom of U), allowing the model to quickly improve. The good question we can ask here is **whether we** can find a loss function that is steeper and also is differentiable so gradient can be easily find, in order to accelerate the learning.

- 2. The activation function. We used sigmoid as our activation function, but the gradient of sigmoid, at best, can have derivative of 0.25 which is quite small. The good question we can ask here is whether we can find a activation function that can provide larger range of derivative and thus can accelerate the learning.
- 3. The **update rule**. Now we only simply multiply the learning rate with the current gradient. However, our batch X and y keeps changing. It may be nice if we can update the params based on histories of gradients, not only on the current gradient.
- 4. The **learning rate**. Currently, we put a static learning rate, but it does not make so much sense. In fact, it can be safely assumed that our randomized weight is greatly far from the optimal weight and thus learning rate should be large. However, as iterations run, learning rate should be slowly reduce so we do not keep hopping over and over again, not finding the minimum.
- 5. The **weight initialization** We currently simply randomize our Ws but the good question is whether we can improve this process a bit.
- 6. Last, the **overfitting**. You may already realize that we so far is hesistant to add more layers. Why? Because more layers though may be more accurate but could potentially overfit. Thus, we need to add some mechanisms to counter the act of adding more layers, in order to prevent overfitting.

Phew....they may look a lot but that's the point of the beauty of deep neural net. Let's start with the loss function.

1.1.2 Extension #1. Softmax Cross Entropy Function

So recall the question whether we can find a loss function that is steeper.

Indeed, if we consider a **classification problem**, **softmax cross entropy** as a loss function has a steeper gradients, exploiting the fact that we know the predicted results are probabilities that sum up to 1

The **Softmax Cross Entropy** function has two components: (1) softmax function, and (2) cross entropy function.

Let's first focus on the softmax function:

The Softmax Function For example, let's have a classification problem with N classes, let's say 3 classes. Then for sample 1, the predicted values can be written as:

Vector of probabilities for sample 1 = [5, 3, 2]

5, 3, 2 represent the regressed probabilities of each class. For example, 5 represent the probability of sample 1 to belong to class 1, 3 for class 2, and 2 for class 3.

To make it more clear, it is desirable to convert [5, 3, 2] to something like [0.5, 0.3, 0.2] so they sum up to 1 and are really probabilities.

Indeed, this can be easily done by simply normalizing them like this:

Normalize
$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$
 $= \begin{bmatrix} \frac{x_1}{x_1 + x_2 + x_3} \\ \frac{x_2}{x_1 + x_2 + x_3} \\ \frac{x_3}{x_1 + x_2 + x_3} \end{bmatrix}$

However, there turns out a way that both produces **steeper** gradients, and at the same time, **has elegant mathematical properties**. This is called **softmax function** like this:

Softmax(
$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$
) = $\begin{bmatrix} \frac{e^{x_1}}{e^{x_1} + e^{x_2} + e^{x_3}} \\ \frac{e^{x_1} + e^{x_2} + e^{x_3}}{e^{x_3}} \\ \frac{e^{x_1} + e^{x_2} + e^{x_3}}{e^{x_3}} \end{bmatrix}$

The good properties include: 1. The softmax function makes the bigger value much bigger, forcing the neural network to be "less neutral". This is doable since we are most interested in the class with biggest probability anyway. If we apply softmax([5, 3, 2]), we get [0.84, 0.11, 0.04] which is different with the more neutral method of normalization which get [0.5, 0.3, 0.2]

2. The softmax function has a steeper gradients, comparing to simple normalization, since derivative of e^x is e^x !

Cross Entropy Loss Recall that loss function in classification problems take a vector of predicted probabilities

$$\begin{bmatrix} p_1 \\ \cdot \\ \cdot \\ p_n \end{bmatrix}$$

For N=3, we can have like this [0.84, 0.11, 0.04]

The loss function will then calculate the loss based on the differences between this vector of predicted probabilities and a vector of actual values that look like this:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix}$$

If sample 1 belongs to class 1, then this vector will look like this: [1, 0, 0]

The cross entropy loss function, for each index i in these vectors, is

$$CE(p_i, y_i) = -y_i * log(p_i) - (1 - y_i) * log(1 - p_i)$$

Why this loss function make sense? Here is the breakdown situation when $y_i = 0$ and $y_i = 1$

$$CE(p, y_i) = \begin{cases} -log(1 - p_i) & \text{if } y_i = 0\\ -log(p_i) & \text{if } y_i = 1 \end{cases}$$

If our $y_i = 0$,

• When our p_i is near 0 which means we are correct, the loss become

$$-log(1) = 0$$

• otherwise, if our p_i is near 1 which means we are incorrect, the loss becomes

$$-log(0) = \infty$$

If our $y_i = 1$

• When our p_i is near 0 which means we are incorrect, the loss become

$$-log(0) = \infty$$

• otherwise, if our p_i is near 1 which means we are correct, the loss becomes

$$-log(1) = 0$$

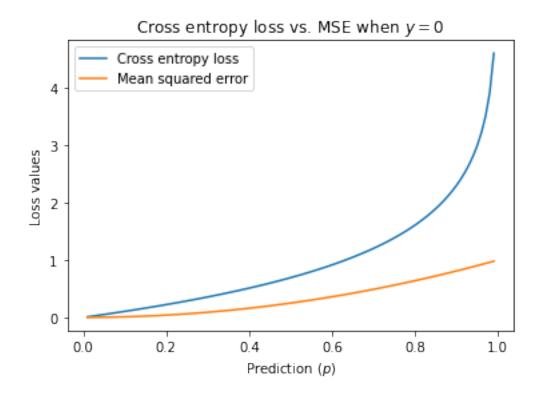
If we were to plot the situation when $y_i = 0$, here is the plot:

```
import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(0.01, 0.99, 99) #range of p
y1 = -1.0 * np.log(1 - x) #the cross entropy
y2 = (x - 0) ** 2 #the MSE
plt.plot(x, y1);
plt.plot(x, y2);
plt.legend(['Cross entropy loss', 'Mean squared error'])

plt.title("Cross entropy loss vs. MSE when $y = 0$")
plt.xlabel("Prediction ($p$)")
plt.ylabel("Loss values")
```

[2]: Text(0, 0.5, 'Loss values')

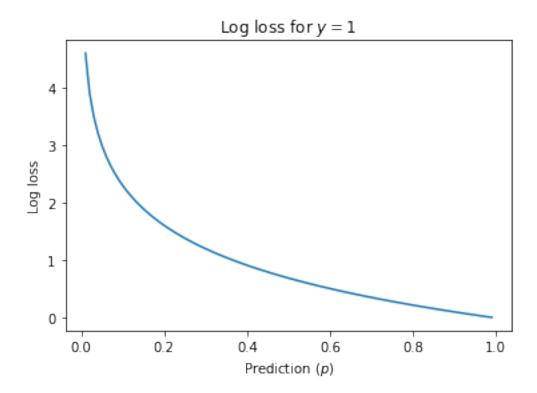


You can clearly see that **cross entrophy** has a steeper gradient when the prediction is very far from the actual values

Similarly, we can plot when $y_i = 1$

```
[3]: x = np.linspace(0.01, 0.99, 99)
y = -1.0 * np.log((x))

plt.plot(x, y);
plt.title("Log loss for $y = 1$")
plt.xlabel("Prediction ($p$)")
plt.ylabel("Log loss");
```



The real magic happens when we combine this loss with the softmax function like this:

$$SCE_1 = -y_1 * log(\frac{e^{x_1}}{e^{x_1} + e^{x_2} + e^{x_3}}) - (1 - y_1) * log(1 - \frac{e^{x_1}}{e^{x_1} + e^{x_2} + e^{x_3}})$$

This **softmax cross entropy** function first converts $x_1...x_n$ into probabilities, and then insert these probabilities into the cross entrophy function.

It turns out that the gradient can also be very easily calculated as follows:

$$\frac{\partial SCE_1}{\partial x_1} = \frac{e^{x_1}}{e^{x_1} + e^{x_2} + e^{x_3}} - y_1$$

That means that the total gradient is as follows:

$$\operatorname{softmax}(\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}) - \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

Enough talk. Let's code this up.

[4]: from numpy import ndarray class SoftmaxCrossEntropy(Loss):

```
def __init__(self, eps: float=1e-9):
       super().__init__()
       self.eps = eps
   def _output(self) -> float:
       # applying the softmax function to each row (observation)
       softmax_preds = self.softmax(self.prediction, axis=1)
       # clipping the softmax output to prevent numeric instability
       #numpy.clip(a, a min, a max, out=None, **kwarqs)
       #To prevent extremely large loss values that could lead to numericu
\rightarrow instability,
       #we'll clip the output of the softmax function to be no less than 10-7_{\sqcup}
→and no greater than 10~7
       self.softmax_preds = np.clip(softmax_preds, self.eps, 1 - self.eps)
       # actual loss computation
       softmax_cross_entropy_loss = (
           -1.0 * self.target * np.log(self.softmax_preds) - \
               (1.0 - self.target) * np.log(1 - self.softmax_preds)
       )
       #return average loss
       return np.sum(softmax_cross_entropy_loss) / self.prediction.shape[0]
   def input grad(self) -> ndarray:
       #return average grad
       return (self.softmax_preds - self.target) / self.prediction.shape[0]
   def softmax(self, x, axis=None):
       #keepdims so that this number can be broadcasted and divided
       return np.exp(x) / np.sum(np.exp(x), axis=axis, keepdims=True)
```

1.1.3 Extension #2. Activation Function

We use sigmoid in previous classes because we say that sigmoid was: - non-linear and monotonic (one to one mapping) - actually help overfitting by forcing all values to be between 0 and 1

Nevertheless, sigmoid produces relatively flat gradients with maximum slopoe of only 0.25, i.e., any gradient that gets passed to the sigmoid function is at best, be divided by 4 when sent backward. Worse still, when the input to the sigmoid is less than -2 or greater than 2, the gradient is almost zero. See this graph for example:

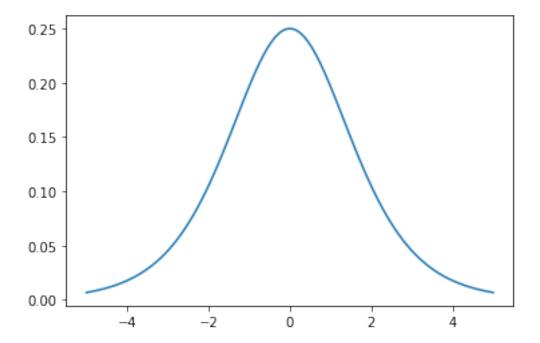
```
[5]: import matplotlib.pyplot as plt
def sigmoid(x):
```

```
return 1.0/(1.0 + np.exp(-1.0 * x))

def sigmoid_derivative(x):
    return sigmoid(x) * (1.0 - sigmoid(x))

x = np.linspace(-5, 5, 100)
plt.plot(x, sigmoid_derivative(x))
```

[5]: [<matplotlib.lines.Line2D at 0x119292490>]



What this means is that any parameters influencing these inputs will receive small gradients, and our network could elarn slowly as a result. Worse yet, if we have multiple sigmoid functions in successive layers, it will further diminish the gradients.

So the question is, is there any other activation function that has bigger derivative. Let's explore other activation function including **ReLu**, **Tanh**, and **Relu Leaky**.

ReLu (Rectified Linear Unit) ReLu is simply defined to be 0 if x is less than 0, and x otherwise. It's derivative is simply if x is more than 0, then the derivative is 1, otherwise is 0.

This is a valid activation function because it is monotonic and non-linear. It produces much greater gradients. However, the downside is that it draws a somewhat strange distinction between values less than or greater than 0. That can be fixed with **Leaky ReLu** which is simply using some alpha to make sure values smaller than zero does not completely gone. Another one is **ReLu6** which is simply having the positive cap at 6 (it will not exceed 6), adding even more non-linearity into the network.

Nevertheless, if we are dealing with simple problems such as MNIST, then adding more sophiscated activation functions are NOT encouraged, since it adds more complexity and make the network harder to learn.

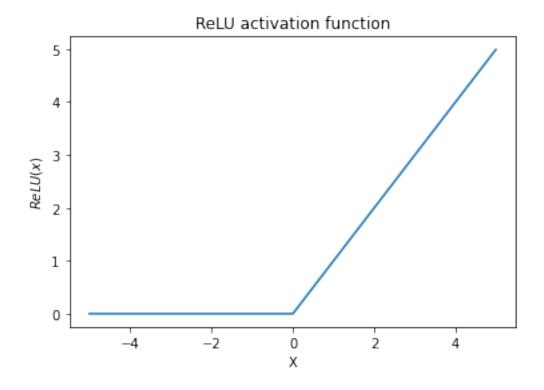
Luckily, there is a simple activation function that also produces strong gradients but is also simple: Tanh function

```
[6]: def relu(x):
    return np.array([el if el > 0 else 0 for el in x])

def relu_derivative(x):
    x[x<=0] = 0
    x[x>0] = 1
    return x

x = np.arange(-5, 5, 0.01)
plt.plot(x, relu(x))
# plt.plot(x, relu_derivative(x))
plt.title("ReLU activation function")
plt.xlabel("X")
plt.ylabel("$ReLU(x)$")
```

[6]: Text(0, 0.5, '\$ReLU(x)\$')



Tanh The Tanh function is shaped similarly to the sigmoid function but maps inputs to values between -1 and 1. It produces strong gradient with maximum of 1. It also has a simple derivative of

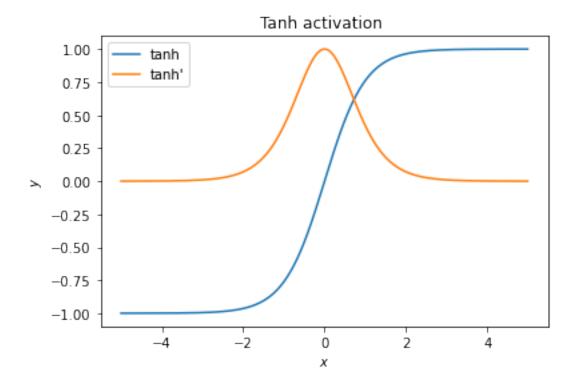
$$1 - tanh(x)^2$$

Given that tanh has strong gradient of 1, it is commonly a natural replacement of sigmoid since tanh is better than sigmoid in the gradient, but share the same downside of sigmoid, i.e., having gradient of 0 after x is around the left/right side of the curve.

Tanh is also considered a balance between sigmoid and ReLu. Sigmoid is very conservative, while Relu is very progressive - always producing gradient of 1 when x is greater than 0. In common problem, Tahn is sufficient to improve the performance over sigmoid. In more sophiscated problems with many non-linearity, we may use ReLu.

```
[7]: x = np.arange(-5, 5, 0.01)
  plt.plot(x, np.tanh(x), label="tanh")
  plt.plot(x, 1 - (np.tanh(x) **2), label="tanh")
  plt.title("Tanh activation ")
  plt.xlabel("$x$")
  plt.ylabel("$y$")
  plt.legend()
```

[7]: <matplotlib.legend.Legend at 0x119345c50>



Finally, we can write the Tanh function as a class like this:

```
[8]: class Tanh(Operation):
    def __init__(self):
        super().__init__()

    def _output(self) -> ndarray:
        return np.tanh(self.input_)

    def _input_grad(self, output_grad: ndarray) -> ndarray:
        return output_grad * (1 - self.output * self.output)
```

1.1.4 Experiments

Before we dive into other possible extensions. Let's try out our techniques using MNIST dataset, which consists of black and white images of handwritten digits that are 28 x 28 pixels, with the value of each pixel range from 0 to 255.

Here we gonna have 60,000 images on training and 10,000 images for testing

```
[9]: from sklearn.datasets import fetch_openml

mnist = fetch_openml('mnist_784', version=1, cache=True)
mnist.target = mnist.target.astype(int)

X_train = mnist['data'][:60000]
y_train = mnist['target'][:60000]

X_test = mnist['data'][60000:]
y_test = mnist['target'][60000:]
```

Data Preprocessing

1. Always help to standardize our data The reason we do this is because in the process of training our network, we're going to be multiplying (weights) and adding to (biases) these initial inputs in order to cause activations that we then backpropagate with the gradients to train the model. We'd like in this process for each feature to have a similar range so that our gradients don't go out of control (and that we only need one global learning rate multiplier).

```
[10]: from sklearn.preprocessing import StandardScaler
    scaler = StandardScaler()
    X_train = scaler.fit_transform(X_train)
    X_test = scaler.transform(X_test)
```

2. We need to convert our y which current is a single digit showing the class (e.g., 9), we need to convert to a vector of probabilities like this [0, 0, 0, 0, 0, 0, 0, 0, 1] which indicates that this sample is of class 9. This process is also commonly known as *one hot encoding* We can use sklearn.preprocessing to make our life easier:

```
[11]: from sklearn import preprocessing
  onehot = preprocessing.OneHotEncoder()

#sklearn expects a 2D array thus we have to reshape to (-1, 1)
  y_train_encode = onehot.fit_transform(y_train.reshape(-1, 1)).toarray()
  y_test_encode = onehot.fit_transform(y_test.reshape(-1, 1)).toarray()
  print(y_train_encode.shape, y_test_encode.shape)
```

(60000, 10) (10000, 10)

```
[12]: #define a simple accuracy function

from sklearn.metrics import accuracy_score

def calc_accuracy(model, X_test, y_test):
    #getting the accuracy score with testing data
    preds = model.forward(X_test)
    preds = np.argmax(preds, axis=1)
    print("Accuracy: ", accuracy_score(y_test, preds))
```

1. Sigmoid activation function

We gonna first use Tanh activation on the first Dense layer. Then on the second layer (i.e., last layer), since the output has 10 numbers with number in range of [0, 1], thus the last layer has 10 neurons with Sigmoid activation to squeeze the result into that range of [0, 1]

A key question is how many neurons should be our hidden layer which is the Tanh layer. This is a entire field of its own and there are really tough to determine the right number. However, the one consensus is that number of neurons should be between the number of neurons in the input layer (e.g., 784) and the number of neurons in the output layer (e.g., 10)

Anyhow, this leave us still doubtful what number to choose between 10 and 784. Another useful technique is to take the **number of sample** / (alpha * number of neurons in both input and output layers). This can often prevent overfitting. For example, let alpha be 1 (typically around 2 - 10), it can be calculated as:

$$60,000/(1*784+10) = 75.6$$

Thus we can use around 76 neurons. Another technique is to use the mean. Since we are talking about images, we can take the **geometric mean of 784 and 10** which can be calculated as:

$$\sqrt{784 * 10} = 88.54$$

Thus we can use around 89 neurons.

Anyhow, talking about this probably require all of us to read tons of research papers! Here is some discussion you can read (https://stats.stackexchange.com/questions/181/how-to-choose-the-

number-of-hidden-layers-and-nodes-in-a-feedforward-neural-netw). The general idea is that the more neurons you have, it usually helps in model more complex relationships, but it also come with a downside that it takes much more time to learn.

Also note that all what we discuss only apply to feed-forward neural network...

Let's stick with 89 neurons for now.

```
Validation loss after 10 epochs is 0.300 Validation loss after 20 epochs is 0.245 Validation loss after 30 epochs is 0.225 Validation loss after 40 epochs is 0.216 Validation loss after 50 epochs is 0.210 Accuracy: 0.8758
```

2. Softmax Cross Entropy Loss

Let's prove our claim that softmax cross entropy can help our model learn faster.

Similarly, we gonna use Tanh activation on the beginning. Since we are now feeding our results to the SoftmaxCrossEntropy which has a softmax function to make things into probabilities, we simply use a Linear activation function in the last layer.

```
epochs = 50,
    eval_every = 10,
    seed=20200720,
    batch_size=60)

calc_accuracy(model, X_test, y_test)
```

```
Validation loss after 10 epochs is 0.683
Validation loss after 20 epochs is 0.645
Validation loss after 30 epochs is 0.636
Validation loss after 40 epochs is 0.635
Validation loss after 50 epochs is 0.633
Accuracy: 0.8924
```

Yay, we see a 2% increase. Although this is minimal, they stack up with other improvements!

1.1.5 Extension #3: Momentum

So far, we've been using only one update rule for our weights at each time step. Simply take the derivative of the loss with respect to the weights and move the weights in the resulting correct direction.

Here we gonna introduce a new way based on using the history of gradients called momentum

Basing our parameter updates on momentum means that the parameter update at each time step will be a weighted average of the parameter updates at past time steps, with the weights decayed exponentially. There will thus be a second parameter we have to choose, the momentum parameter, which will determine the degree of this decay; the higher it is, the more the weight update at each time step will be based on the parameter's accumulated momentum as opposed to its current velocity

Mathematically, if our momentum parameter is μ , and the gradient at each time step is ∇_t , our weight update is

update =
$$\nabla_t + \mu * \nabla_{t-1} + \mu^2 * \nabla_{t-2} + \dots$$

If our momentum parameter was 0.9, for example, we would multiply the gradient from one time step ago by 0.9, the one from two time steps ago by $0.9^2 = 0.81$, the one from three time steps ago by $0.9^3 = 0.729$, and so on, and then finally add all of these to the gradient from the current time step to get the overall weight update for the current time step.

Why momentum? The problem of the old way is that it is possible that it stucks at the local minima, just like the picture below.

To avoid this situation, we use a momentum term in the objective function, which is a value between 0 and 1 that increases the size of the steps taken towards the minimum by trying to jump from a local minima. If the momentum term is large then the learning rate should be kept smaller. A large value of momentum also means that the convergence will happen fast. But if both the momentum and learning rate are kept at large values, then you might skip the minimum with a huge step. A

small value of momentum cannot reliably avoid local minima, and can also slow down the training of the system.

Momentum also helps in smoothing out the variations, if the gradient keeps changing direction, just like in this graph

A right value of momentum can be either learned by hit and trial or through cross-validation.

To implement this, a simple way is just to keep track of what you have added so far, and simply add the current gradient on top of it, like this:

```
1. \nabla_1
2. \nabla_2 + \mu * \nabla_1
3. \nabla_3 + \mu * (\nabla_2 + \mu * \nabla_1)
```

We can call the right side after the first time, called velocity which is the history of momentum * gradients. In every iteration, we simply multiply the velocity by momentum again, and add up the current grad.

```
[15]: class SGDMomentum(Optimizer):
          def __init__(self,
                       lr: float = 0.01,
                       momentum: float = 0.9):
              super().__init__(lr)
              self.momentum = momentum
              self.first = True
          def step(self):
              if self.first:
                  self.velocities = [np.zeros_like(param)
                                     for param in self.net.params()]
                  self.first = False
              for (param, param_grad, velocity) in zip(self.net.params(),
                                                        self.net.param_grads(),
                                                        self.velocities):
                  self._update_rule(param=param,
                                     grad=param_grad,
                                     velocity=velocity)
          def _update_rule(self, **kwargs):
                  # Update velocity
                  kwargs['velocity'] *= self.momentum
                  kwargs['velocity'] += self.lr * kwargs['grad']
                  # Use this to update parameters
                  kwargs['param'] -= kwargs['velocity']
```

Let's try this replacing SGD with SGDMomentum

Validation loss after 10 epochs is 0.549 Loss increased after epoch 20, final loss was 0.549, using the model from epoch 10 Accuracy: 0.9154

Yay, it improves another 2\%! These improvements slowly stack up.

1.1.6 Extension #4: Learning rate decay

In previous classes, we fix the learning rate. However, learning rate decay is the idea that while we want to take big steps toward the beginning of training, we want to smoothly declines so it does not skip over the minimum.

There are different types. The simplest is **linear decay**. At time step t with N iterations (epochs), if the learning rate we want to start with is α_{start} , and our final learning rate is α_{end} , then our learning rate at each time step is:

$$\alpha_t = \alpha_{start} - (\alpha_{start} - \alpha_{end}) * \frac{t}{N}$$

Another simple method is **exponential decay** where the formula is:

$$\alpha_t = \alpha_{start} * \left(\left(\frac{\alpha_{end}}{\alpha_{start}} \right)^{\frac{1}{N}} \right)^t$$

Implementing this requires us to update our Optimizer function as the following:

```
self.final_lr = final_lr #<---added
       self.decay_type = decay_type #<---added</pre>
   def _setup_decay(self): #<---added</pre>
       if not self.decay_type:
           return
       elif self.decay_type == 'exponential':
           self.decay_per_epoch = np.power(self.final_lr / self.lr,
                                       1.0 / (self.max_epochs - 1))
       elif self.decay_type == 'linear':
           self.decay_per_epoch = (self.lr - self.final_lr) / (self.max_epochs_
→- 1)
   def _decay_lr(self): #<---added</pre>
       if not self.decay_type:
           return
       if self.decay_type == 'exponential':
           self.lr *= self.decay_per_epoch
       elif self.decay_type == 'linear':
           self.lr -= self.decay_per_epoch
   def step(self, epoch: int = 0): #<---added epoch info</pre>
       for (param, param_grad) in zip(self.net.params(),
                                       self.net.param_grads()):
           self._update_rule(param=param,
                              grad=param_grad)
   def _update_rule(self, **kwargs):
       raise NotImplementedError()
```

Our SGDMomentum class is also updated:

```
def step(self):
    if self.first:
        self.velocities = [np.zeros_like(param)
                           for param in self.net.params()]
        self.first = False
    for (param, param_grad, velocity) in zip(self.net.params(),
                                              self.net.param_grads(),
                                              self.velocities):
        self._update_rule(param=param,
                          grad=param_grad,
                          velocity=velocity)
def _update_rule(self, **kwargs):
        # Update velocity
        kwargs['velocity'] *= self.momentum
        kwargs['velocity'] += self.lr * kwargs['grad']
        # Use this to update parameters
        kwargs['param'] -= kwargs['velocity']
```

We also need to update our Trainer to call this decay function like this:

```
[19]: from copy import deepcopy
      from typing import Tuple
      class Trainer(object):
          #NeuralNetwork and Optimizer as attributes
          def __init__(self,
                       net: NeuralNetwork,
                       optim: Optimizer):
              #Requires a neural network and an optimizer in order for
              #training to occur.
              self.net = net
              self.optim = optim
              self.best_loss = 1e9 #use for comparing the least amount of loss
              #Assign the neural network as an instance variable to
              #the optimizer when the code runs
              setattr(self.optim, 'net', self.net)
          # helper function for shuffling
          def permute_data(self, X, y):
              perm = np.random.permutation(X.shape[0])
              return X[perm], y[perm]
```

```
# helper function for generating batches
  def generate_batches(self,
                        X: ndarray,
                        y: ndarray,
                        size: int = 32) -> Tuple[ndarray]:
       #X and y should have same number of rows
       assert X.shape[0] == y.shape[0]
       N = X.shape[0]
       for i in range(0, N, size):
           X_batch, y_batch = X[i:i+size], y[i:i+size]
           #return a generator that can be loop
           yield X_batch, y_batch
  def fit(self, X_train: ndarray, y_train: ndarray,
           X_test: ndarray, y_test: ndarray,
           epochs: int=100,
           eval_every: int=10,
           batch_size: int=32,
           seed: int = 20200720,
           restart: bool = True):
       setattr(self.optim, 'max_epochs', epochs) #<---added</pre>
       self.optim._setup_decay() #<---added</pre>
       np.random.seed(seed)
       #for resetting
       if restart:
           for layer in self.net.layers:
               layer.first = True
           self.best_loss = 1e9
       #Fits the neural network on the training data for a certain
       #number of epochs.
       for e in range(epochs):
           if (e+1) % eval_every == 0:
               # for early stopping
               # deepcopy is a hardcopy function that make sure it construct a_{\sqcup}
→new object (copy() is a shallow copy)
```

```
last_model = deepcopy(self.net)
           X_train, y_train = self.permute_data(X_train, y_train)
           batch_generator = self.generate_batches(X_train, y_train,
                                                     batch_size)
           for (X_batch, y_batch) in batch_generator:
               self.net.train_batch(X_batch, y_batch)
               self.optim.step()
           #Every "eval_every" epochs, it evaluated the neural network
           #on the testing data.
           if (e+1) % eval_every == 0:
               test_preds = self.net.forward(X_test)
               loss = self.net.loss.forward(test_preds, y_test)
               if loss < self.best_loss:</pre>
                   print(f"Validation loss after {e+1} epochs is {loss:.3f}")
                   self.best_loss = loss
               #if the validation loss is not lower, it stop and perform early \Box
\hookrightarrowstopping
               else:
                   print(f"""Loss increased after epoch {e+1}, final loss was⊔
→{self.best_loss:.3f}, using the model from epoch {e+1-eval_every}""")
                   self.net = last_model
                    # ensure self.optim is still updating self.net
                   setattr(self.optim, 'net', self.net)
                   break
           #call this at the end of each epoch
           if self.optim.final_lr: #<----added</pre>
               self.optim._decay_lr()
                                        #<----added
```

Validation loss after 10 epochs is 0.505 Loss increased after epoch 20, final loss was 0.505, using the model from epoch 10 Accuracy: 0.9339

Yay, another 1.5% increase!!! Hopefully we can reach 0.95...

1.1.7 Extension #5: Weight Initialization

As we mentioned in the section on activation functions, several activation functions, such as sigmoid and Tanh, have their steepest gradients when their inputs are 0, with the functions quickly flattening out as the inputs move away from 0. This can potentially limit the effectiveness of these functions, because if many of the inputs have values far from 0, the weights attached to those inputs will receive very small gradients on the backward pass.

This turns out to be a major problem in the neural networks we are now dealing with. Consider the hidden layer in the MNIST network we've been looking at. This layer will receive 784 inputs and then multiply them by a weight matrix, ending up with some number n of neurons (and then optionally add a bias to each neuron).

This figure shows the distribution of these n values in the hidden layer of our neural network (with 784 inputs) before and after feeding them through the Tanh activation function.

After being fed through the activation function, most of the activations are either -1 or 1!

The reason is because we initialized each weight to have variance 1 (Recall that we use random.rand(num_feature, num_neurons) which basically create a uniform distribution of [0, 1) with variance 1. Also for bias, we use random.rand(1, num_neurons)):

$$Var(w_{i,j}) = 1$$

Thus, if we have 785 features (784 + 1 for b), each having one variance, this gives us a standard deviation of:

$$\sqrt{785} = 28.02$$

This is pretty huge. So what should be the right distribution of weights? Well, it certainly should depend on the number of neurons in the in and out layer. The weight matrix should have a roughly normal distribution across all neurons. But now we have in- and out- layer, which should we use as basis? Let's think each of them first.

For in-layer, the standard deviation of each weight on the forward pass should be

 $\frac{1}{n_{in}}$

At the same time, for the next layer,

 $\frac{1}{n_{out}}$

As a compromise between these, what is most often called **Glorot initialization (also known as Xavier)**, the idea is to initialize each weight with a small Gaussian value with mean = 0.0 and variance based on the fan-in and fan-out of the weight like this:

$$\frac{2}{n_{in} + n_{out}}$$

where n_{in} is the number of input neurons, and n_{out} is the number of output neurons.

By doing this, we make sure the distribution of the weights in the beginning is uniformed across all neurons in the beginning.

To do this is simple, we add a weight_init argument to each layer, and we add the following to our _setup_layer function

```
[21]: class Dense(Layer):
          def __init__(self, neurons: int,
                       activation: Operation = Sigmoid(),
                       weight_init: str = "glorot"): #<---added</pre>
              #define the desired non-linear function as activation
              super().__init__(neurons)
              self.activation = activation
              self.weight_init = weight_init #<---added
          def _setup_layer(self, input_: ndarray):
              #in case you want reproducible results
              if self.seed:
                  np.random.seed(self.seed)
              #---->added section
              num_in = input_.shape[1]
              if self.weight_init == "glorot":
                  scale = 2/(num_in + self.neurons)
              else:
                  scale = 1.0
              #---->revised section
              self.params = []
```

We can then try our models with this function:

```
[22]: model = NeuralNetwork(
          layers=[Dense(neurons=89,
                        activation=Tanh(),
                        weight init="glorot"),
                  Dense(neurons=10,
                        activation=Linear(),
                        weight_init="glorot")],
                  loss = SoftmaxCrossEntropy(),
      seed=20200720)
      trainer = Trainer(model, SGDMomentum(lr=0.2, momentum=0.9,
                                          final_lr=0.05, decay_type='exponential'))
      trainer.fit(X_train, y_train_encode, X_test, y_test_encode,
                  epochs = 50,
                  eval_every = 10,
                  seed=20200720,
                  batch_size=60)
      calc_accuracy(model, X_test, y_test)
```

```
Validation loss after 10 epochs is 0.396
Loss increased after epoch 20, final loss was 0.396, using the model from epoch 10
Accuracy: 0.9487
```

Yay, another 1% increase!

1.1.8 Extension #6: Dropout

Recall the discussion in the beginning of the class that adding more layers are prone to overfitting, and thus we are quite hesitant to add more layers than we need. Indeed, with one hidden layer, we are doing good job so far.

The good question to ask is what if we want to add more layers in the future, for example, for more complex data?

The answer is yes, with **Dropout**. **Dropout** is a mechanism to make our neural network less likely to overfit

Dropout is actually a simple idea of randomly choosing some proportion p of the neurons in a layer and setting them equal to 0 during each forward pass of training. By randomly setting some neurons to null in each iteration, the other neurons become more generalized in learning.

Though dropout can help our network avoid overfitting during training, we still want to give our network its *best shot* of making correct predictions when it comes time to predict. So, the Dropout operation will have **two modes**: a **training** mode in which dropout is applied, and an **inference** mode, in which it is not.

To make sure the distribution of the values during inference time is close to that during training time, we should multiply values by P_{keep} . For example, say we have a vector of x=1,2,3,4,5. Let's set p=0.8 which means 20% of data will be turn to 0. In training, $x_{train}=1,0,3,4,5$; do not confuse why I turn off 2 and not others, I just turn 20% off randomly. In inference, we turn off dropout, but to make sure the distribution remains similar, we multiply the values by 0.8, which becomes $x_{inference}=0.8,1.6,2.4,3.2,4.0$

We can implement **Dropout** as an Operation, that we can attach onto the end of each layer like this:

```
[23]: class Dropout(Operation):
          def __init__(self,
                       keep_prob: float = 0.8):
              super().__init__()
              self.keep_prob = keep_prob
          def _output(self, inference: bool) -> ndarray:
              if inference:
                  return self.input_ * self.keep_prob #multiply input by probability
                  #binomial will give us list of O and 1s with 1s of probability_
       \rightarrow equal to keep_prob
                  self.mask = np.random.binomial(1, self.keep_prob,
                                                  size=self.input .shape)
                  return self.input_ * self.mask
          def _input_grad(self, output_grad: ndarray) -> ndarray:
              #since gradient of 0 is nothing, thus the input_grad is simply whatever_
       →output_grad multiply with self.mask
              return output_grad * self.mask
```

You may have noticed that we included an inference flag in the _output method that affects whether dropout is applied or not. For this flag to be called properly, we actually have to add it in several other places throughout training

1. The **NeuralNetwork** > **Layer** > **Operation** forward methods will take in inference as an argument (False by default) and pass the flag into each Operation, so that every Operation will behave differently in training mode than in inference mode.

```
[24]: class NeuralNetwork(object):
          def __init__(self,
                        layers: List[Layer],
                        loss: Loss,
                        seed: int = 1):
              self.layers = layers
              self.loss = loss
              self.seed = seed
              if seed:
                   for layer in self.layers:
                       setattr(layer, "seed", self.seed)
          def forward(self, X_batch: ndarray,
                       inference=False) -> ndarray: #<---added inference as param</pre>
              X_out = X_batch
              for layer in self.layers:
                   X_out = layer.forward(X_out, inference) #<---added inference as_
       \hookrightarrow param
              return X_out
          def backward(self, loss_grad: ndarray):
              grad = loss_grad
              for layer in reversed(self.layers):
                  grad = layer.backward(grad)
                   #you may wonder why I did not return anything
                   #it's because in Layer.backward, it is appending this value to
       → param_grads to each layer
                   #this return "grad" is simply something it returns
          def train_batch(self,
                           X_batch: ndarray,
                           y_batch: ndarray,
                           inference: bool = False) -> float: #<----added inference_
       \hookrightarrow as param
              prediction = self.forward(X_batch, inference) #<---added inference as_
       \hookrightarrow param
              batch_loss = self.loss.forward(prediction, y_batch)
              loss_grad = self.loss.backward()
```

```
self.backward(loss_grad)
   return batch_loss
def params(self):
    #get the parameters for the network
    #use for updating w and b
    for layer in self.layers:
        #equivalent for-loop yield
        #yield is different from return is that
        #it will return a sequence of values
        yield from layer.params
def param_grads(self):
    #get the gradient of the loss with respect to the parameters
    #for the network
    #use for updating w and b
   for layer in self.layers:
        yield from layer.param_grads
```

```
[25]: class Layer(object):
          def __init__(self,
                       neurons: int) -> None:
              self.neurons = neurons
              self.first = True
              self.params: List[ndarray] = []
              self.param_grads: List[ndarray] = []
              self.operations: List[Operation] = []
          def _setup_layer(self, input_: ndarray) -> None:
              pass
          def forward(self, input_: ndarray,
                      inference=False) -> ndarray: #<----added</pre>
              if self.first:
                  self._setup_layer(input_)
                  self.first = False
              self.input_ = input_
              for operation in self.operations:
                  input_ = operation.forward(input_, inference) #<----added_
       \rightarrow inference as param
```

```
self.output = input_
    return self.output
def backward(self, output_grad: ndarray) -> ndarray:
    assert self.output.shape == output_grad.shape
    for operation in self.operations[::-1]:
        output_grad = operation.backward(output_grad)
    input_grad = output_grad
    assert self.input_.shape == input_grad.shape
    self._param_grads()
    return input_grad
def _param_grads(self) -> None:
    self.param_grads = []
    for operation in self.operations:
        if issubclass(operation.__class__, ParamOperation):
            self.param_grads.append(operation.param_grad)
def _params(self) -> None:
    self.params = []
    for operation in self.operations:
        if issubclass(operation.__class__, ParamOperation):
            self.params.append(operation.param)
```

```
def backward(self, output_grad: ndarray) -> ndarray:
        #make sure output and output grad has same shape
        assert self.output.shape == output_grad.shape
        self.input_grad = self._input_grad(output_grad)
        #input grad must have same shape as input
        assert self.input_.shape == self.input_grad.shape
        return self.input_grad
    def _output(self, inference: bool) -> ndarray: #<----inference</pre>
        raise NotImplementedError()
    def _input_grad(self, output_grad: ndarray) -> ndarray:
        raise NotImplementedError()
class Linear(Operation):
    def __init__(self) -> None:
        super().__init__()
    def _output(self, inference: bool) -> ndarray: #<---inference</pre>
        return self.input_
    def _input_grad(self, output_grad: ndarray) -> ndarray:
        return output grad
class Sigmoid(Operation):
    def __init__(self) -> None:
        super().__init__()
    def _output(self, inference: bool) -> ndarray: #<---inference</pre>
        return 1.0/(1.0+np.exp(-1.0 * self.input_))
    def _input_grad(self, output_grad: ndarray) -> ndarray:
        sigmoid_backward = self.output * (1.0 - self.output)
        input_grad = sigmoid_backward * output_grad
        return input_grad
class Tanh(Operation):
    def __init__(self) -> None:
        super().__init__()
```

```
def _output(self, inference: bool) -> ndarray: #<---inference</pre>
       return np.tanh(self.input_)
   def _input_grad(self, output_grad: ndarray) -> ndarray:
       return output_grad * (1 - self.output * self.output)
class ParamOperation(Operation):
   def __init__(self, param: ndarray):
        super().__init__() #inherit from parent if any
        self.param = param #this will be used in _output
   def backward(self, output_grad: ndarray) -> ndarray:
        #make sure output and output_grad has same shape
        assert self.output.shape == output_grad.shape
        #perform gradients for both input and param
        self.input_grad = self._input_grad(output_grad)
        self.param_grad = self._param_grad(output_grad)
       assert self.input_.shape == self.input_grad.shape
       assert self.param.shape == self.param_grad.shape
       return self.input_grad
   def _param_grad(self, output_grad: ndarray) -> ndarray:
       raise NotImplementedError()
class WeightMultiply(ParamOperation):
   def __init__(self, W: ndarray):
        #initialize Operation with self.param = W
        super().__init__(W)
   def _output(self, inference: bool) -> ndarray: #<----inference</pre>
        return self.input_ @ self.param
   def _input_grad(self, output_grad: ndarray) -> ndarray:
        return output_grad @ self.param.T #same as last class
   def _param_grad(self, output_grad: ndarray) -> ndarray:
       return self.input_.T @ output_grad #same as last class
class BiasAdd(ParamOperation):
   def __init__(self, B: ndarray):
        #initialize Operation with self.param = B.
        assert B.shape[0] == 1 #make sure it's only B
```

```
super().__init__(B)
    def _output(self, inference: bool) -> ndarray: #<----inference</pre>
        return self.input_ + self.param
    def _input_grad(self, output_grad: ndarray) -> ndarray:
        return np.ones_like(self.input_) * output_grad
    def _param_grad(self, output_grad: ndarray) -> ndarray:
        param_grad = np.ones_like(self.param) * output_grad
        return np.sum(param grad, axis=0).reshape(1, param grad.shape[1])
#we have to define Dropout again, so it refers to the new Operation class
class Dropout(Operation):
    def __init__(self,
                 keep_prob: float = 0.8):
        super().__init__()
        self.keep_prob = keep_prob
    def _output(self, inference: bool) -> ndarray:
        if inference:
            return self.input * self.keep_prob #multiply input by probability
        else:
            #binomial will give us list of 0 and 1s with 1s of probability_
\rightarrow equal to keep prob
            self.mask = np.random.binomial(1, self.keep_prob,
                                            size=self.input_.shape)
            return self.input_ * self.mask
    def _input_grad(self, output_grad: ndarray) -> ndarray:
        #since gradient of 0 is nothing, thus the input_grad is simply whatever_
 →output_grad multiply with self.mask
        return output_grad * self.mask
```

2. Recall that in the Trainer, we evaluate the trained model on the testing set every eval_every epochs. Now, every time we do that, we'll evaluate with the inference flag equal to True:

```
#training to occur.
    self.net = net
    self.optim = optim
    self.best_loss = 1e9 #use for comparing the least amount of loss
    #Assign the neural network as an instance variable to
    #the optimizer when the code runs
    setattr(self.optim, 'net', self.net)
# helper function for shuffling
def permute_data(self, X, y):
    perm = np.random.permutation(X.shape[0])
    return X[perm], y[perm]
# helper function for generating batches
def generate_batches(self,
                     X: ndarray,
                     y: ndarray,
                     size: int = 32) -> Tuple[ndarray]:
    #X and y should have same number of rows
    assert X.shape[0] == y.shape[0]
    N = X.shape[0]
    for i in range(0, N, size):
        X_batch, y_batch = X[i:i+size], y[i:i+size]
        #return a generator that can be loop
        yield X_batch, y_batch
def fit(self, X_train: ndarray, y_train: ndarray,
        X_test: ndarray, y_test: ndarray,
        epochs: int=100,
        eval_every: int=10,
        batch_size: int=32,
        seed: int = 20200720,
        restart: bool = True):
    setattr(self.optim, 'max_epochs', epochs)
    self.optim._setup_decay()
    np.random.seed(seed)
    #for resetting
    if restart:
```

```
for layer in self.net.layers:
               layer.first = True
           self.best_loss = 1e9
       #Fits the neural network on the training data for a certain
       #number of epochs.
       for e in range(epochs):
           if (e+1) % eval_every == 0:
               # for early stopping
               # deepcopy is a hardcopy function that make sure it construct a_
→new object (copy() is a shallow copy)
               last_model = deepcopy(self.net)
           X_train, y_train = self.permute_data(X_train, y_train)
           batch_generator = self.generate_batches(X_train, y_train,
                                                    batch_size)
           for (X_batch, y_batch) in batch_generator:
               self.net.train_batch(X_batch, y_batch)
               self.optim.step()
           #Every "eval_every" epochs, it evaluated the neural network
           #on the testing data.
           if (e+1) % eval_every == 0:
               test_preds = self.net.forward(X_test, inference=True)_
→#<---inference #<---make sure validation does not use dropout
               loss = self.net.loss.forward(test_preds, y_test)
               if loss < self.best_loss:</pre>
                   print(f"Validation loss after {e+1} epochs is {loss:.3f}")
                   self.best_loss = loss
               #if the validation loss is not lower, it stop and perform early_{\sqcup}
\rightarrowstopping
               else:
                   print(f"""Loss increased after epoch {e+1}, final loss was u
→{self.best_loss:.3f}, using the model from epoch {e+1-eval_every}""")
                   self.net = last model
                   # ensure self.optim is still updating self.net
                   setattr(self.optim, 'net', self.net)
                   break
```

```
#call this at the end of each epoch
if self.optim.final_lr:
    self.optim._decay_lr()
```

Finally, we add a dropout keyword to the Dense class and we append the dropout operation

```
[28]: class Dense(Layer):
          def __init__(self, neurons: int,
                       activation: Operation = Sigmoid(),
                       dropout: float = 1.0, #<---add default dropout as 1.0 which
       \rightarrowmeans all values are kept
                       weight_init: str = "glorot"):
              #define the desired non-linear function as activation
              super().__init__(neurons)
              self.activation = activation
              self.weight_init = weight_init
              self.dropout = dropout #<---added</pre>
          def _setup_layer(self, input_: ndarray):
              #in case you want reproducible results
              if self.seed:
                  np.random.seed(self.seed)
              num_in = input_.shape[1]
              if self.weight init == "glorot":
                  scale = 2/(num_in + self.neurons)
              else:
                  scale = 1.0
              self.params = []
              # weights
              self.params.append(np.random.normal(loc=0,
                                                   scale=scale,
                                                   size=(num_in, self.neurons)))
              # bias
              self.params.append(np.random.normal(loc=0,
                                                   scale=scale,
                                                   size=(1, self.neurons)))
              self.operations = [WeightMultiply(self.params[0]),
                                 BiasAdd(self.params[1]),
                                  self.activation]
```

```
#-----added this section
if self.dropout < 1.0:
    self.operations.append(Dropout(self.dropout))
#------</pre>
```

Let's try out the previous one but with dropout!

```
[29]: model = NeuralNetwork(
          layers=[Dense(neurons=89,
                        activation=Tanh(),
                        weight_init="glorot",
                        dropout=0.8),
                  Dense(neurons=10,
                        activation=Linear(),
                        weight_init="glorot")],
                  loss = SoftmaxCrossEntropy(),
      seed=20200720)
      trainer = Trainer(model, SGDMomentum(lr=0.2, momentum=0.9,
                                           final_lr=0.05, decay_type='exponential'))
      trainer.fit(X_train, y_train_encode, X_test, y_test_encode,
                  epochs = 50,
                  eval_every = 10,
                  seed=20200720,
                  batch_size=60)
      calc_accuracy(model, X_test, y_test)
```

```
Validation loss after 10 epochs is 0.314
Validation loss after 20 epochs is 0.294
Validation loss after 30 epochs is 0.281
Loss increased after epoch 40, final loss was 0.281, using the model from epoch 30
Accuracy: 0.9448
```

Hmm...very similar accuracy. The power of Dropout is best worked with deep models! Let's try add one more hidden layer, and use with and without dropout! For the first layer, let's have twice as many (178) and the second hidden layer has half as many (46). This will make sure our distribution still looks good.

Without Dropout

```
Validation loss after 10 epochs is 0.345
Validation loss after 20 epochs is 0.338
Loss increased after epoch 30, final loss was 0.338, using the model from epoch 20
Accuracy: 0.9555
```

Wow, even without dropout, it still performs quite well...This is not always the case but when you are lucky, with more layers, even without Dropout, you can get better accuracy

With Dropout

```
[31]: model = NeuralNetwork(
          layers=[Dense(neurons=178,
                        activation=Tanh(),
                        weight_init="glorot",
                        dropout=0.8),
                  Dense(neurons=46,
                        activation=Tanh(),
                        weight_init="glorot",
                        dropout=0.8),
                  Dense(neurons=10,
                        activation=Linear(),
                        weight_init="glorot")],
                  loss = SoftmaxCrossEntropy(),
      seed=20200720)
      trainer = Trainer(model, SGDMomentum(lr=0.2, momentum=0.9,
                                           final_lr=0.05, decay_type='exponential'))
      trainer.fit(X_train, y_train_encode, X_test, y_test_encode,
                  epochs = 50,
                  eval_every = 10,
```

```
seed=20200720,
batch_size=60)

calc_accuracy(model, X_test, y_test)
```

```
Validation loss after 10 epochs is 0.305
Validation loss after 20 epochs is 0.281
Validation loss after 30 epochs is 0.254
Validation loss after 40 epochs is 0.254
Validation loss after 50 epochs is 0.251
Accuracy: 0.9522
```

Well....unluckily, Dropout does not show that much of a performance. However, it should be noted that Boston dataset is quite small and thus Dropout has less effect. Dropout is especially good when training in a really deep network with huge datasets.

Indeed, dropout was an essentially component of the ImageNet-winning model from 2012 that kicked off the modern deep learning era!

https://arxiv.org/pdf/1207.0580.pdf

[]: