

## Module

### 1 Landscape of Top Eigenvector Problem

Consider the following optimization problem for computing the top eigenvector of a positive semidefinite matrix  $M \in \mathbb{R}^{d \times d}$ :

$$\min_{x \in \mathbb{R}^d} f(x) = \frac{1}{4} \|xx^\top - M\|_F^2.$$

Let the eigen-decomposition of  $M$  be  $M = \sum_{i=1}^d \lambda_i v_i v_i^\top$  where  $\{\lambda_i\}_{i=1}^d$  are eigenvalues and  $\{v_i\}_{i=1}^d$  are the corresponding eigenvectors. Assume  $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_d \geq 0$ . Prove that all saddle points and local maxima are strict, i.e., except the global minima, the Hessian matrices of all other first-order stationary points have a negative eigenvalue.

First we calculate the gradient of  $f$ . We will use that to identify stationary points. We rewrite  $f$  in a way that makes allows the partial derivative to be computed.

$$f(x) = \frac{1}{4} \sum_{i=1}^d \sum_{j=1}^d (x_i x_j - M_{ij})^2$$

So, using the chain rule (disclosure: classmate, Roger Wong, helped me figure out this derivative)

$$\begin{aligned} \frac{\partial f}{\partial x_i} &= \frac{1}{4} \sum_{j \neq i, j=1}^d 2x_j (x_i x_j - M_{ij}) + \frac{1}{4} \sum_{j \neq i, j=1}^d 2x_j (x_i x_j - M_{ji}) + \frac{1}{4} (2)(2x_i) (x_i^2 - M_{ii}) \\ &= \sum_{j=1}^d x_j (x_i x_j - M_{ij}) \end{aligned}$$

Finding the partial derivative of each  $x_i$  leads directly to the the gradient:

$$\nabla f(x) = \begin{bmatrix} \sum_{j=1}^d x_j (x_1 x_j - M_{1j}) \\ \sum_{j=1}^d x_j (x_2 x_j - M_{2j}) \\ \vdots \\ \sum_{j=1}^d x_j (x_d x_j - M_{dj}) \end{bmatrix} = \|x\|_2^2 x - Mx$$

The stationary points exist where  $\nabla f(x) = 0$ , which implies

$$\implies \|x\|_2^2 x = Mx$$

Which is the definition of an eigenvector, where  $x$  is an eigenvector with corresponding eigenvalue  $\|x\|_2^2$ . So, stationary points of  $f$  occur when  $x$  is a unit eigenvector of  $M$ , hence we divide by the norm of  $x$ , yielding  $x = \sqrt{\lambda} v$ . Using identities on the matrix calculus wikipedia page, the Hessian of  $f$  is

$$\nabla^2 f(x) = 2xx^T + \|x\|_2^2 I - M$$

where  $I$  is the identity matrix. Plugging the stationary point in

$$\begin{aligned} \nabla^2 f(x) &= 2(\sqrt{\lambda} v)(\sqrt{\lambda} v)^T + (\sqrt{\lambda} v)^T (\sqrt{\lambda} v) I - M \\ &= 2\lambda v v^T + \lambda v^T v I - M \\ &= \lambda(2v v^T + v^T v I) - M \end{aligned}$$

Since  $\lambda$  will always be less than the largest eigenvalue in  $M$ ,  $\lambda_{\min}\{\nabla^2 f(x)\} < 0$

**Problem 2.1** Show  $L(w_t) \rightarrow 0$  as  $t \rightarrow \infty$

$L(w)$  can be rewritten as

$$L(w) = \frac{1}{2n} \|X^T w - y\|_2^2$$

We derive the dynamics of the  $L(w)$  using the general formula given in class

We can conclude that  $\lambda_{\min}(H(t)) > 0$

**Problem 2.2** Show that  $w$  is always in the span of  $(x_1, \dots, x_n)$

We need to show that  $w$  is a linear combination of the column vectors of  $X$ , i.e.

$$w = a_1 x_1 + \dots + a_n x_n$$

Observe that each row of  $H(t)$  (defined in problem 2.1) represents a linear combination of  $x_i$  up to the  $n$ th dimension (where  $n \leq d$ ).

Let  $z = (X^T w - y)$ . It is given that  $\frac{dw_t}{dt} = -\nabla L(w_t)$ , which implies

$$\begin{aligned} w_{t+1} &= w_t + z^T H(0) z \\ &= \sum_{i,j=1}^n [H(0)]_{ij} z_i z_j \end{aligned}$$

So, each update of  $w$  (start with the 0 vector, which is indeed in the span of  $X$ ) adds a linear combination of  $X$  to the previous value of  $w$ . Since the sum of two linear combinations of  $X$  is also a linear combination of  $X$ ,  $w$  is always in the span of  $X$ .

**Problem 2.3**

Assume, given the constraints of the problem, that  $w_t$  minimizes  $L(W)$  but not  $\|w\|_2^2$  as  $t \rightarrow \infty$  (we know  $L(W)$  is minimized from the result of problem 2.1). Since  $w$  is in the span of  $X$ , this can't be true:  $w$  must also shrink as  $L(W)$  shrinks, given  $y_i = x_i^T w$ .

**Problem 3.1**

We are given

$$k(x, x') = x^T x' \cdot \mathbb{E}_w \left[ \sigma'(w_1) \sigma' \left( w_1 x^T x' + w_2 \sqrt{1 - (x^T x')^2} \right) \right]$$

Letting  $x^T x = \cos \theta$  gives

$$k(x, x') = \cos \theta \cdot \mathbb{E}_w [\sigma'(w_1) \sigma'(w_1 \cos \theta + w_2 \sin \theta)]$$

Now, let  $w_1^* = w_1$  and  $w_2^* = w_1 \cos \theta + w_2 \sin \theta$ . Solving for  $w_1$  yields  $w_1 = \frac{w_2^* - w_2 \sin \theta}{\cos \theta}$ , which we plug into  $k$  as follows:

$$\begin{aligned} k(x, x') &= \cos \theta \cdot \mathbb{E}_w [\sigma'(w_1) \sigma'(w_1 \cos \theta + w_2 \sin \theta)] \\ &= \cos \theta \cdot \mathbb{E}_w \left[ \sigma'(w_1^*) \sigma' \left( \frac{w_2^* - w_2 \sin \theta}{\cos \theta} \cos \theta + w_2 \sin \theta \right) \right] \\ &= \cos \theta \cdot \mathbb{E}_w [\sigma'(w_1^*) \sigma'(w_2^*)] \end{aligned}$$

Since  $\|x\|, \|x'\| = 1$ , both  $w^T x^{(\cdot)}$  and  $w_i$  are distributed  $N(0, I)$  (and are therefore rotationally invariant), so:

$$\begin{aligned} k(x, x') &= \cos \theta \cdot \mathbb{E}_w [\sigma'(w_1^*) \sigma'(w_2^*)] \\ &= x^T x \cdot \mathbb{E}_w [\sigma'(w_1^*) \sigma'(w_2^*)] = x^T x \cdot \mathbb{E}_w [\sigma'(w^T x) \sigma'(w^T x')] \end{aligned}$$

### Problem 3.2

Start with

$$\begin{aligned} k(x, x') &= \cos \theta \cdot \mathbb{E}_w [\sigma'(w_1) \sigma'(w_1 \cos \theta + w_2 \sin \theta)] \\ &= \cos \theta \cdot \int_{-\infty}^{\infty} \sigma'(w_1) \sigma'(w_1 \cos \theta + w_2 \sin \theta) P(w) dw \\ &= \frac{\cos \theta}{2\pi} \cdot \int_0^{\infty} w_1 (w_1 \cos \theta + w_2 \sin \theta) (e^{-\frac{1}{2}(w_1^2 + w_2^2)}) dw_1 dw_2 \end{aligned}$$

Now, letting  $u = w_1$  and  $v = w_1 \cos \theta + w_2 \sin \theta$ ...

(Bound by  $\pi/2$  since this is the upper range of the domain when  $\|x\| = 1$ )

$$\begin{aligned} &= \frac{\cos \theta}{2\pi} \cdot \int_0^{\pi/2} u v e^{-\frac{1}{2}(u^2 + (\frac{v-u \cos \theta}{\sin \theta})^2)} du dv \\ &= \frac{\cos \theta}{2\pi} \cdot \int_0^{\pi/2} u v e^{-1(u^2 + v^2 - 2uv \cos \theta)/2 \sin^2 \theta} du dv \end{aligned}$$

Change to polar coordinates where  $u = r \cos \phi$ ,  $v = r \sin \phi$

$$= \frac{\cos \theta}{2\pi} \cdot \int_0^{\pi/2} r^2 \cos \phi \sin \phi \times e^{-1(u^2 + v^2 - 2uv \cos \theta)/2 \sin^2 \theta} dr d\phi$$

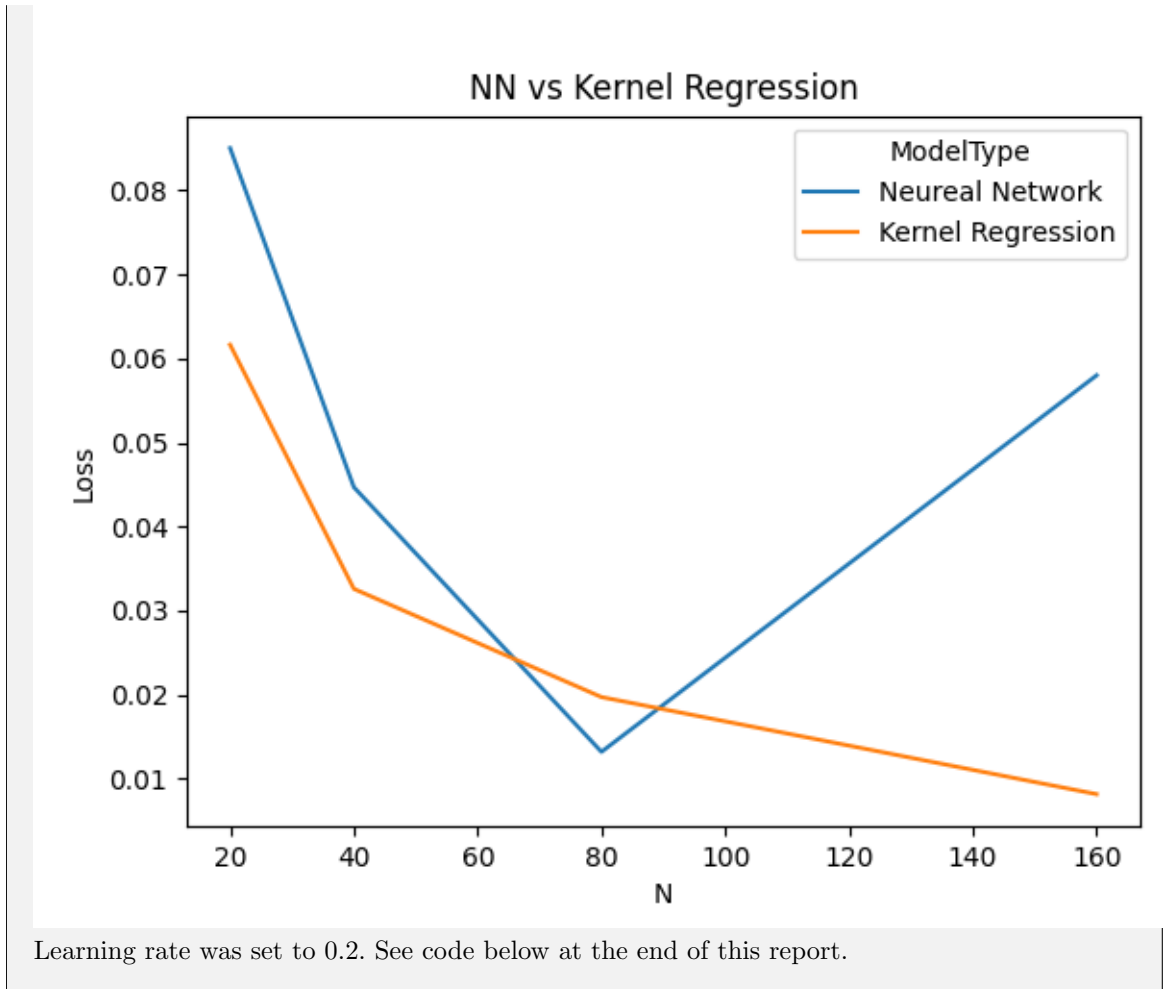
I couldn't figure out how to solve this integral, but I'm sure it evaluates to  $\pi - \theta$ , so we'd have

$$\begin{aligned} k(x, x') &= \frac{\cos \theta}{2\pi} \cdot \int_0^{\pi/2} r^2 \cos \phi \sin \phi \times e^{-1(u^2 + v^2 - 2uv \cos \theta)/2 \sin^2 \theta} dr d\phi \\ &= \frac{\cos \theta}{2\pi} \cdot (\pi - \theta) \\ &= \frac{x^T x' (\pi - \cos^{-1}(x^T x'))}{2\pi}. \end{aligned}$$

The last step follows from the fact that we initially set  $x^T x' = \cos \theta$

### 3.3

The neural network generalized less well to the test data, especially as sample size increased. It's likely that the NN starts to overfit (high variance) the training data as sample size increases since we have much fewer parameters than data.



#### Problem 4.1: Initialization for Leaky ReLU

Expressing  $z^h$  recursively, we have  $z^h = w^h x^h$  and  $x^h = \sigma(z^{h-1})$ . We also know that  $E(z_i^h) = 0$  the weights are given to be initialized normally. We want to find a  $var(z^h)$  such that

$$var(z^h) = d_h var(w^h x^h) = d_{h-1} var(w^{h-1} x^{h-1}) = \dots = d_1 var(w^1 x^1)$$

Which implies

$$var(z^h) = d_h var(w_{ij}^h) E[(x_i^h)^2]$$

Now we rewrite  $E[(x_i^h)^2]$  in terms of variance

$$\begin{aligned}
E[(x_i^h)^2] &= E[(\sigma(z_j^{h-1}))^2] \\
&= E[(\max(0, z_j^{h-1}) + \alpha \min(0, z_j^{h-1}))^2] \\
&= E[\max(0, z_j^{h-1})^2 + \max(0, z_j^{h-1}) \times \alpha \min(0, z_j^{h-1}) + \alpha^2 \min(0, z_j^{h-1})^2] \\
&= E[\max(0, z_j^{h-1})^2] + E[\alpha^2 \min(0, z_j^{h-1})^2] \\
&= \int_{-\infty}^{\infty} \max(0, z_j^{h-1})^2 P(z_j^{h-1}) dz_j^{h-1} + \alpha^2 \int_{-\infty}^{\infty} \min(0, z_j^{h-1})^2 P(z_j^{h-1}) dz_j^{h-1} \\
&= \int_0^{\infty} (z_j^{h-1})^2 P(z_j^{h-1}) dz_j^{h-1} + \alpha^2 \int_{-\infty}^0 (z_j^{h-1})^2 P(z_j^{h-1}) dz_j^{h-1} \\
&= \frac{1}{2} \int_{-\infty}^{\infty} (z_j^{h-1})^2 P(z_j^{h-1}) dz_j^{h-1} + \alpha^2 \frac{1}{2} \int_{-\infty}^{\infty} (z_j^{h-1})^2 P(z_j^{h-1}) dz_j^{h-1} \\
&= \frac{1}{2} \text{var}(z_j^{h-1}) + \frac{\alpha^2}{2} \text{var}(z_j^{h-1}) \\
&= \frac{1}{2} \text{var}(z_j^{h-1}) (1 + \alpha^2)
\end{aligned}$$

Therefore

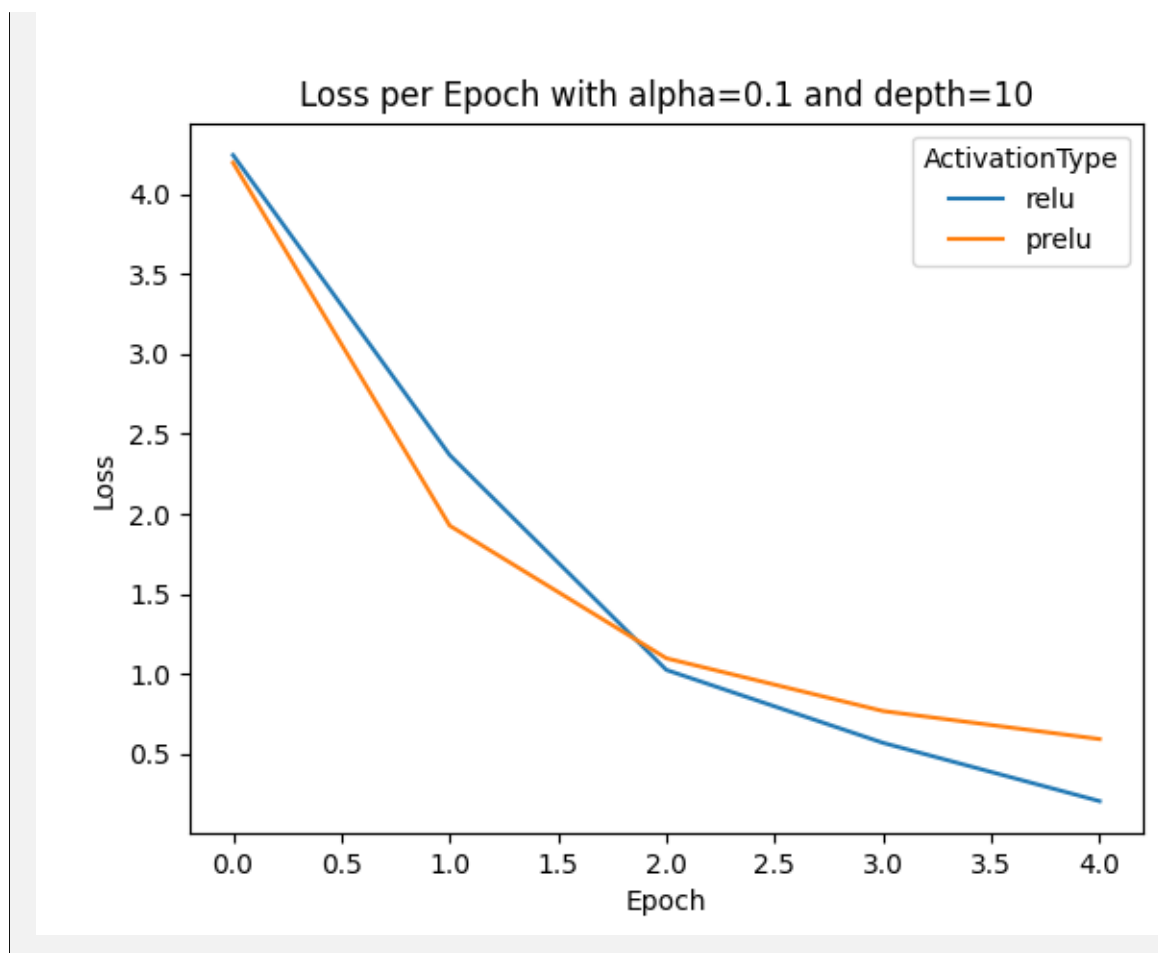
$$\text{var}(z^h) = d_h \text{var}(w_{ij}^h) \frac{1}{2} \text{var}(z_j^{h-1}) (1 + \alpha^2)$$

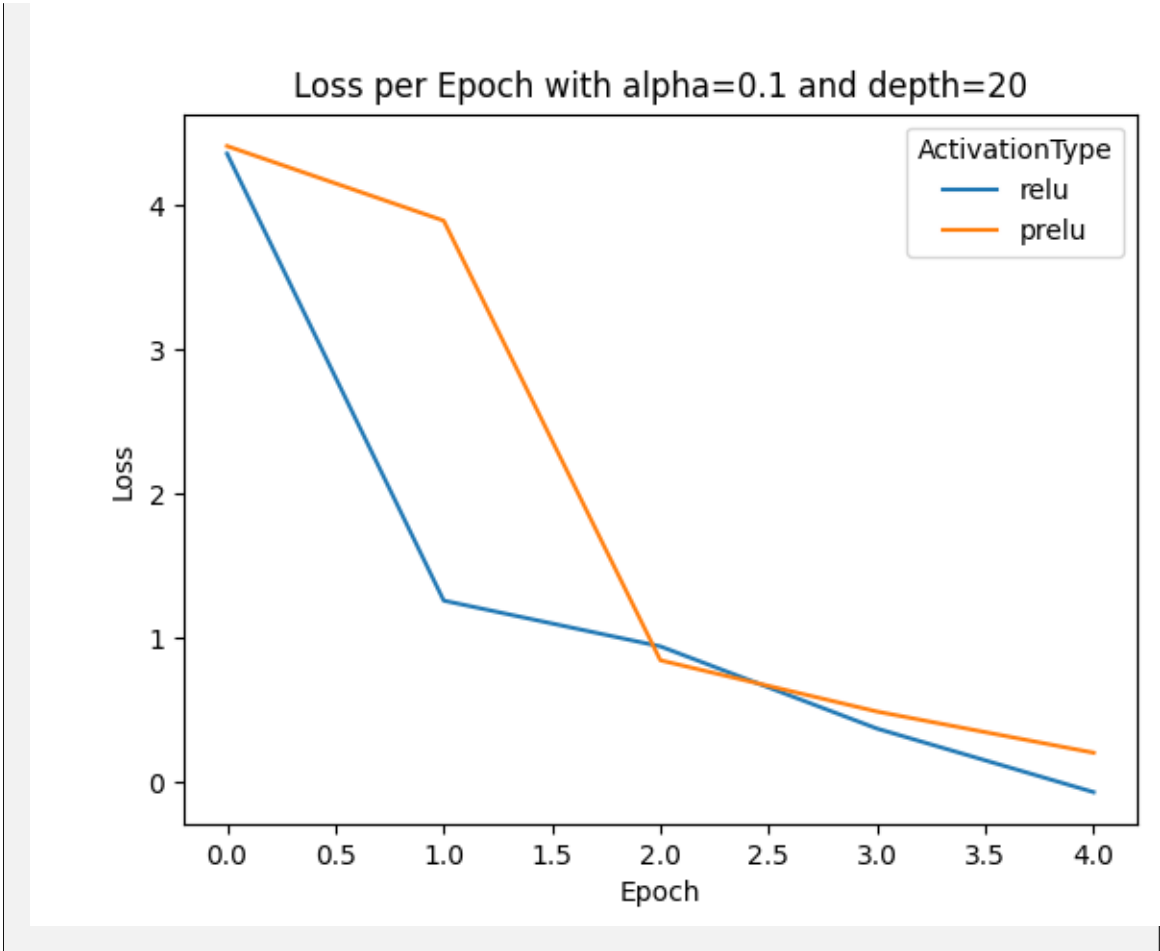
And now solving for  $\text{var}(w_{ij}^h)$ , where all  $z$  has the same variance at all layers

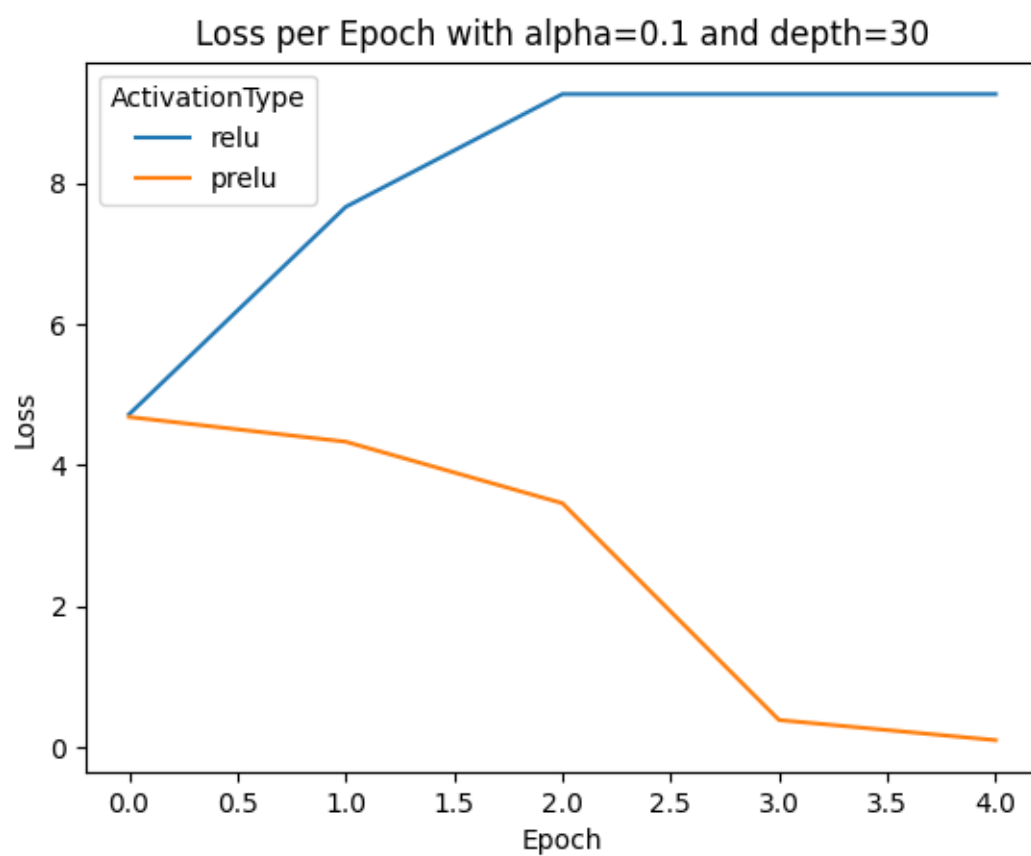
$$\text{var}(w_{ij}^h) = \beta_h = \frac{2}{d_h(1 + \alpha^2)}$$

#### Problem 4.2

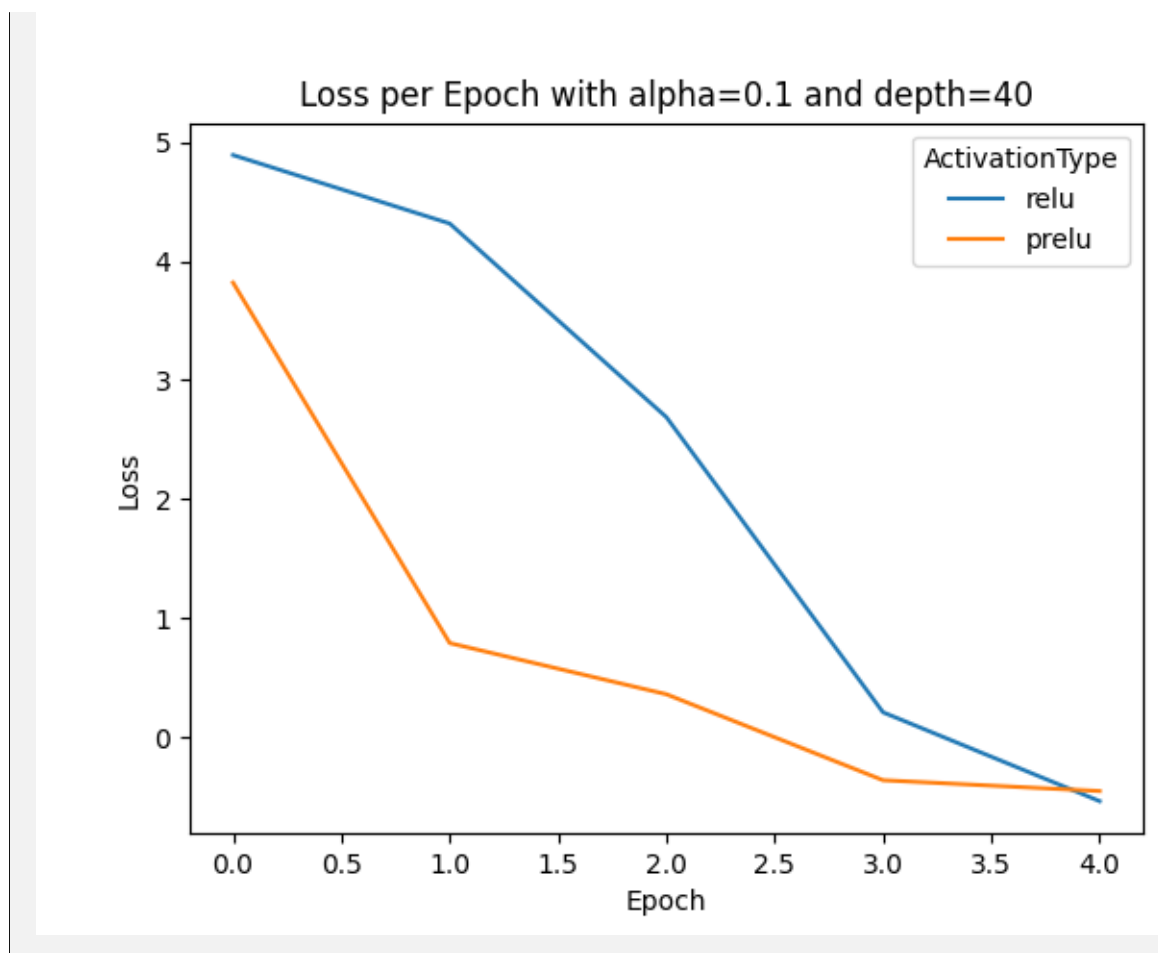
Learning rate for all computations was 0.1. All other hyper-parameters are assigned as specified in the problem statement.

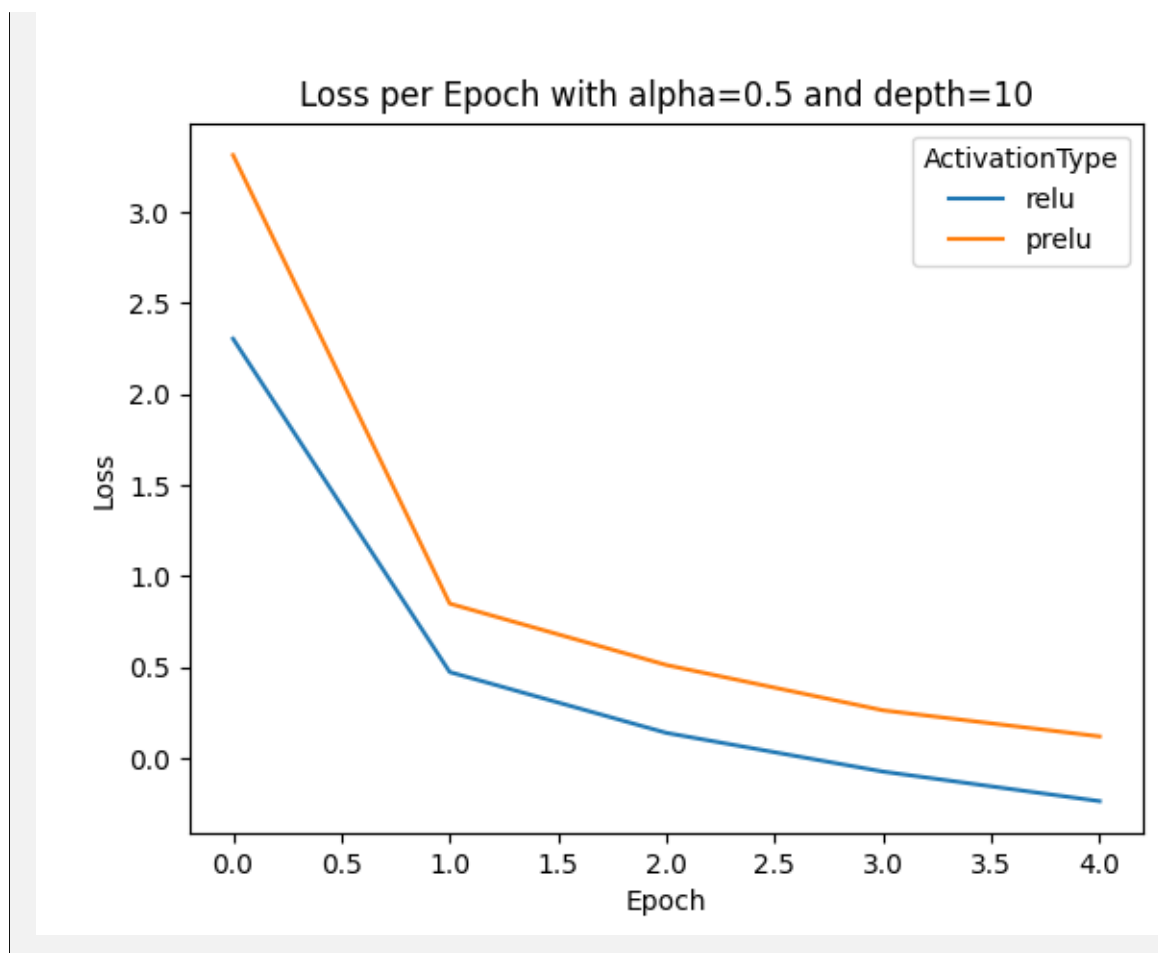


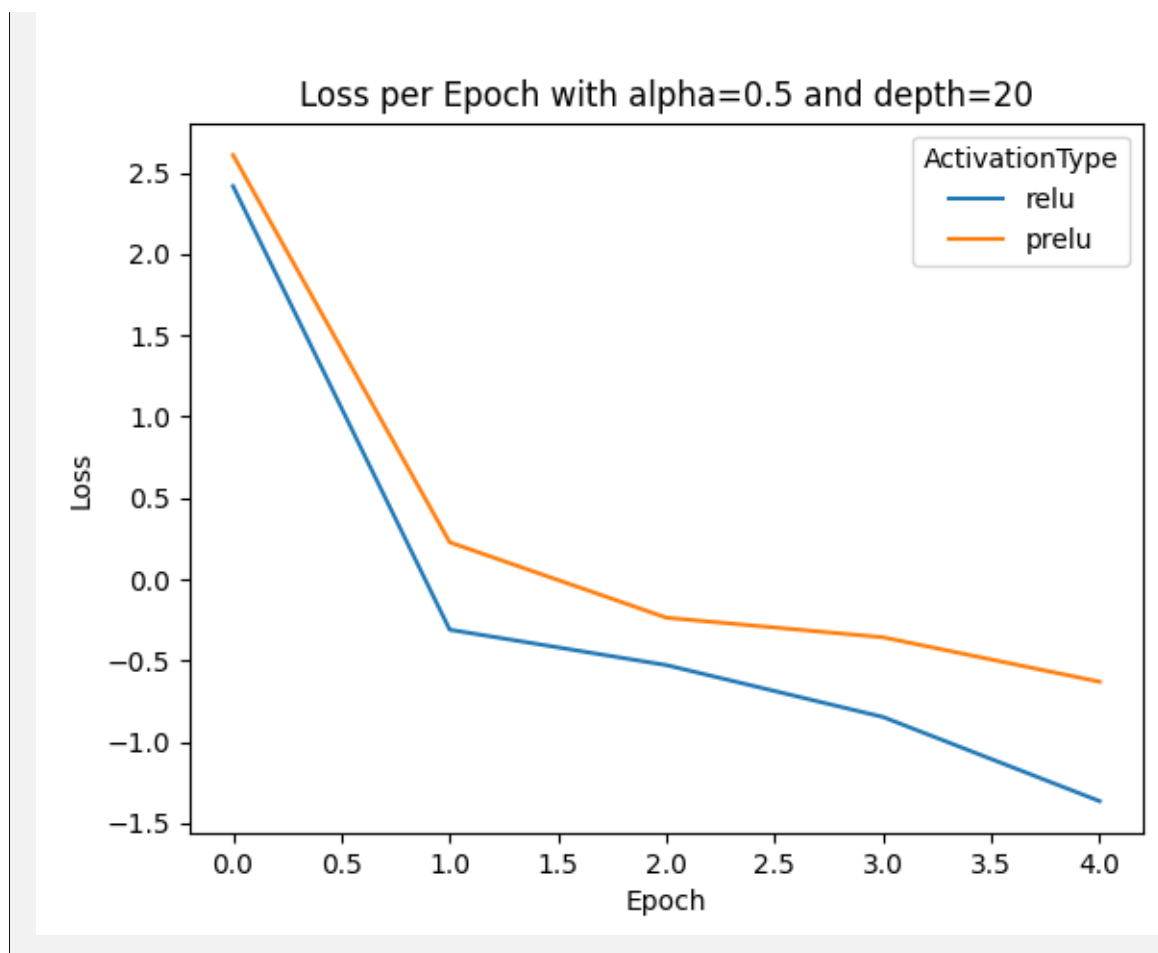


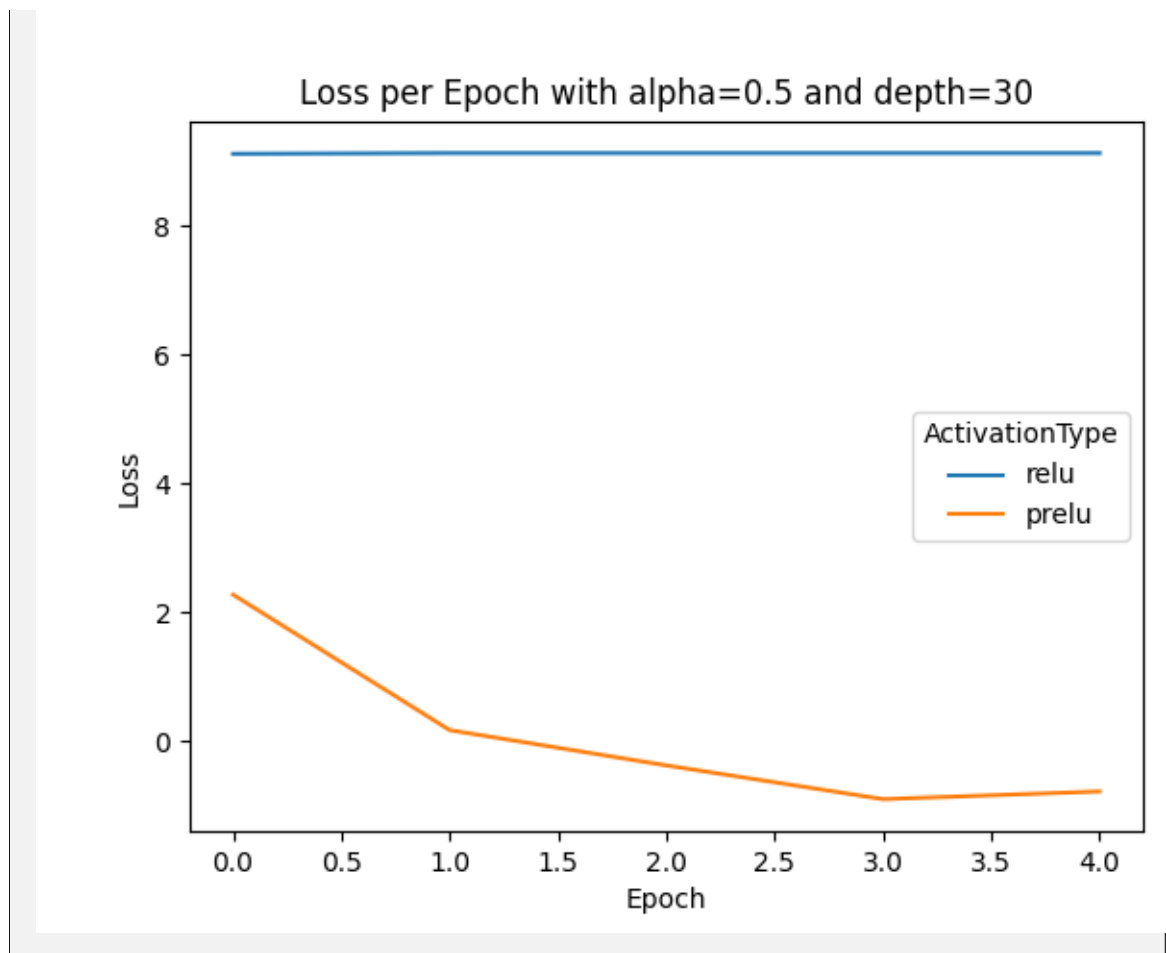


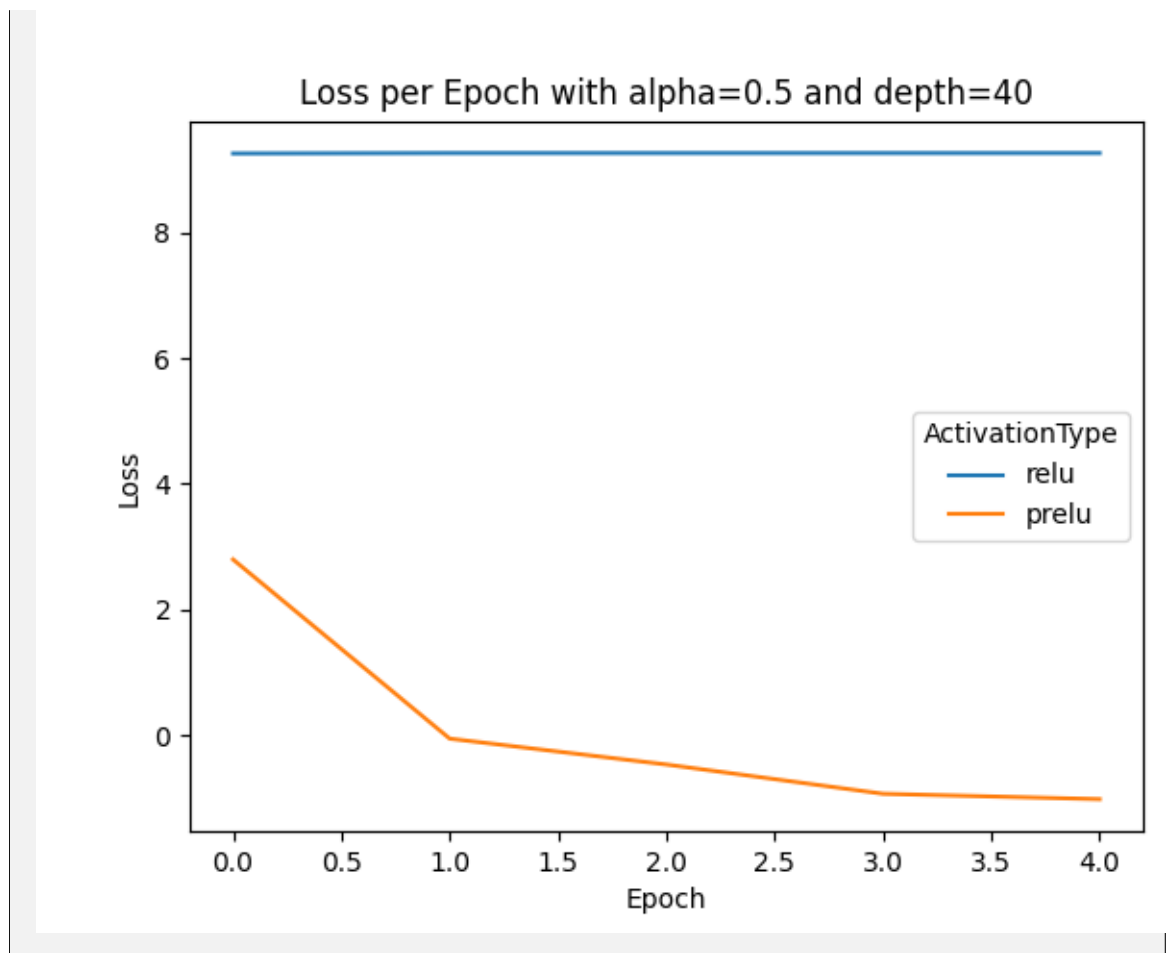


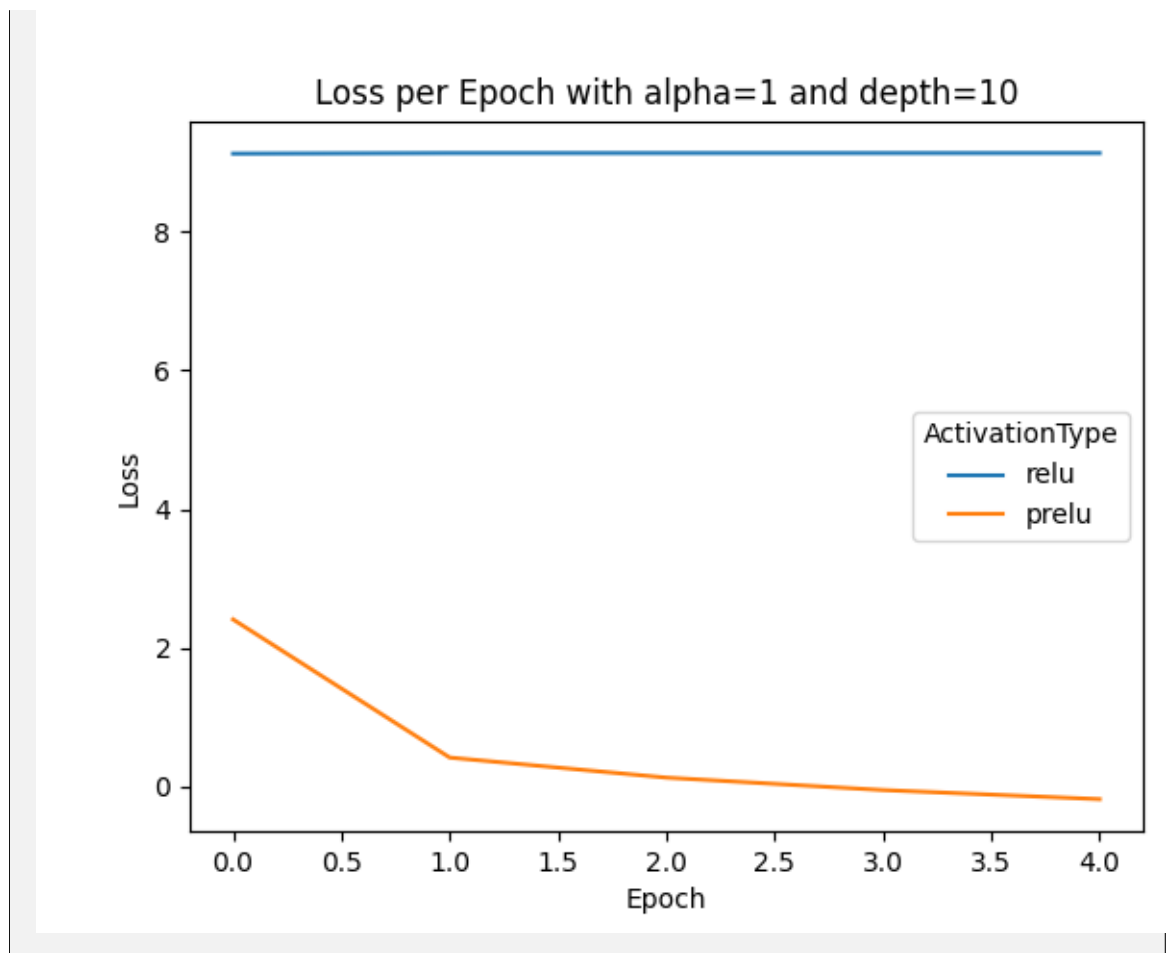


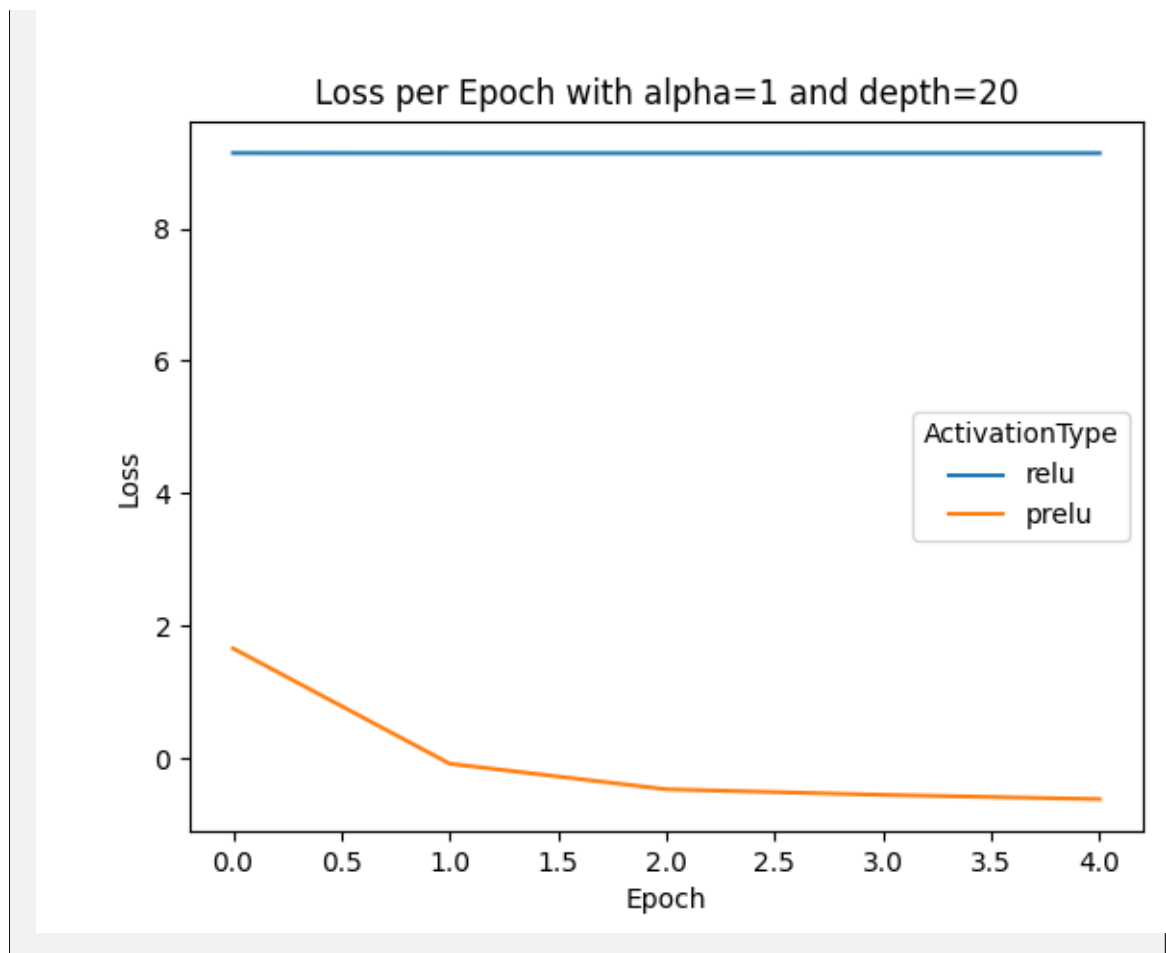


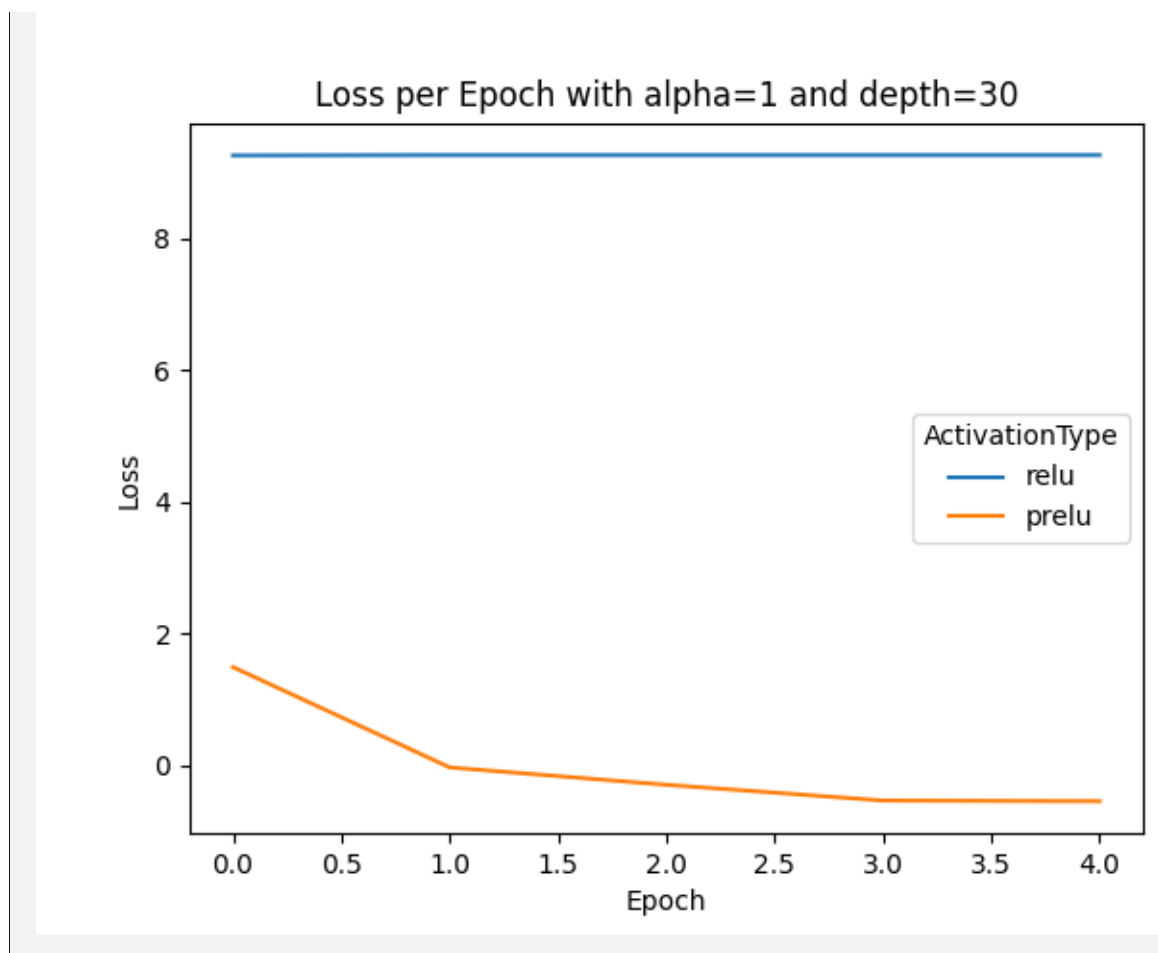




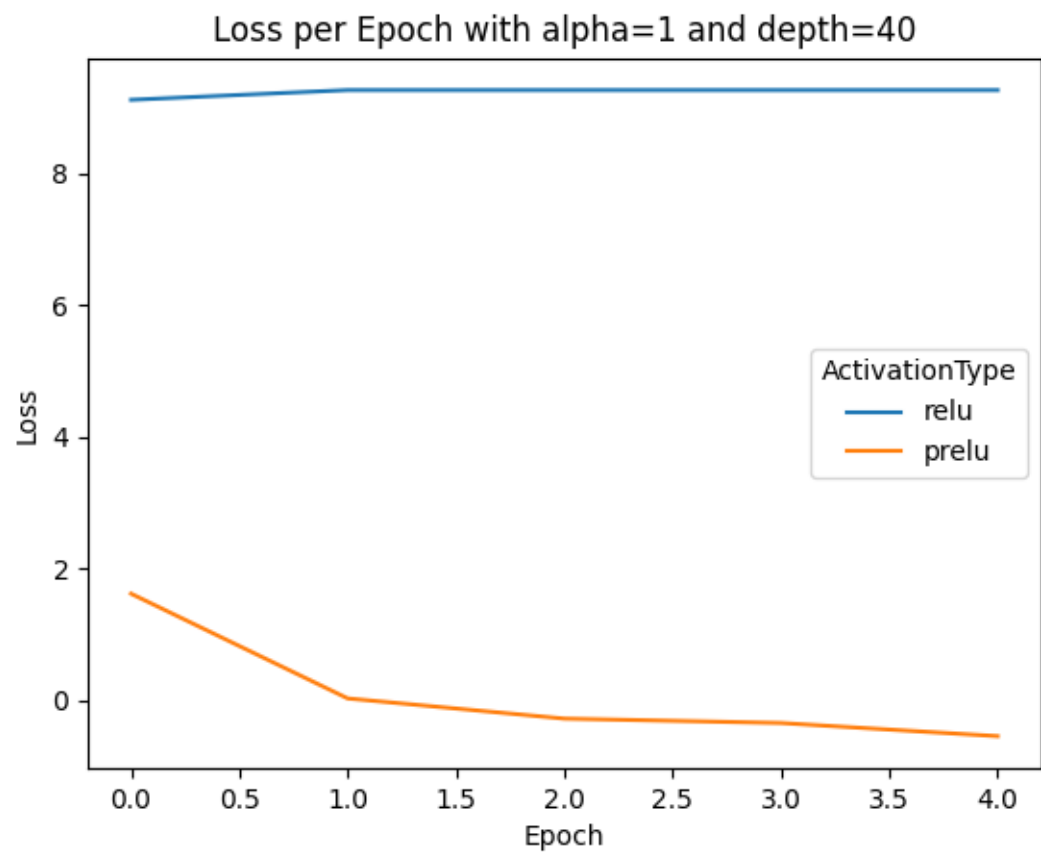


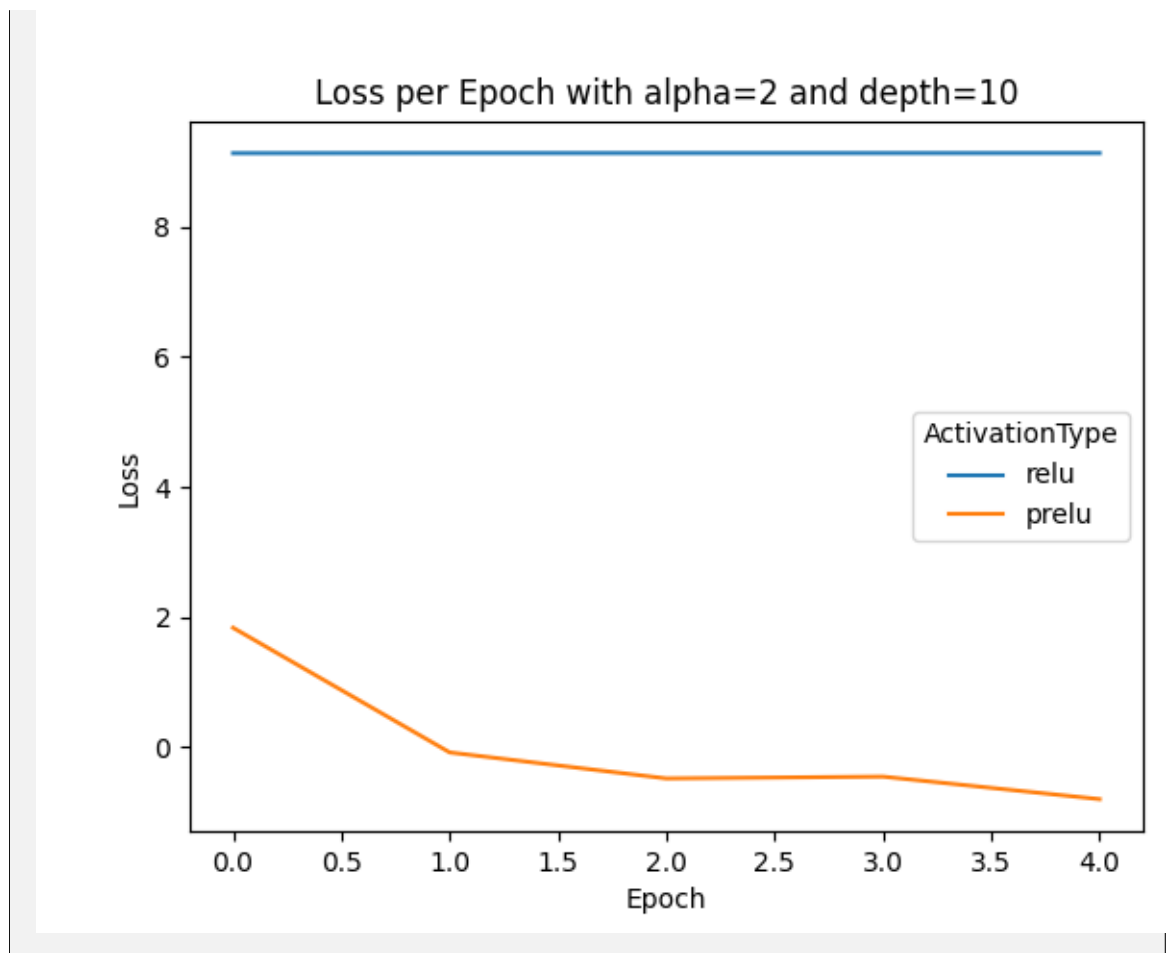


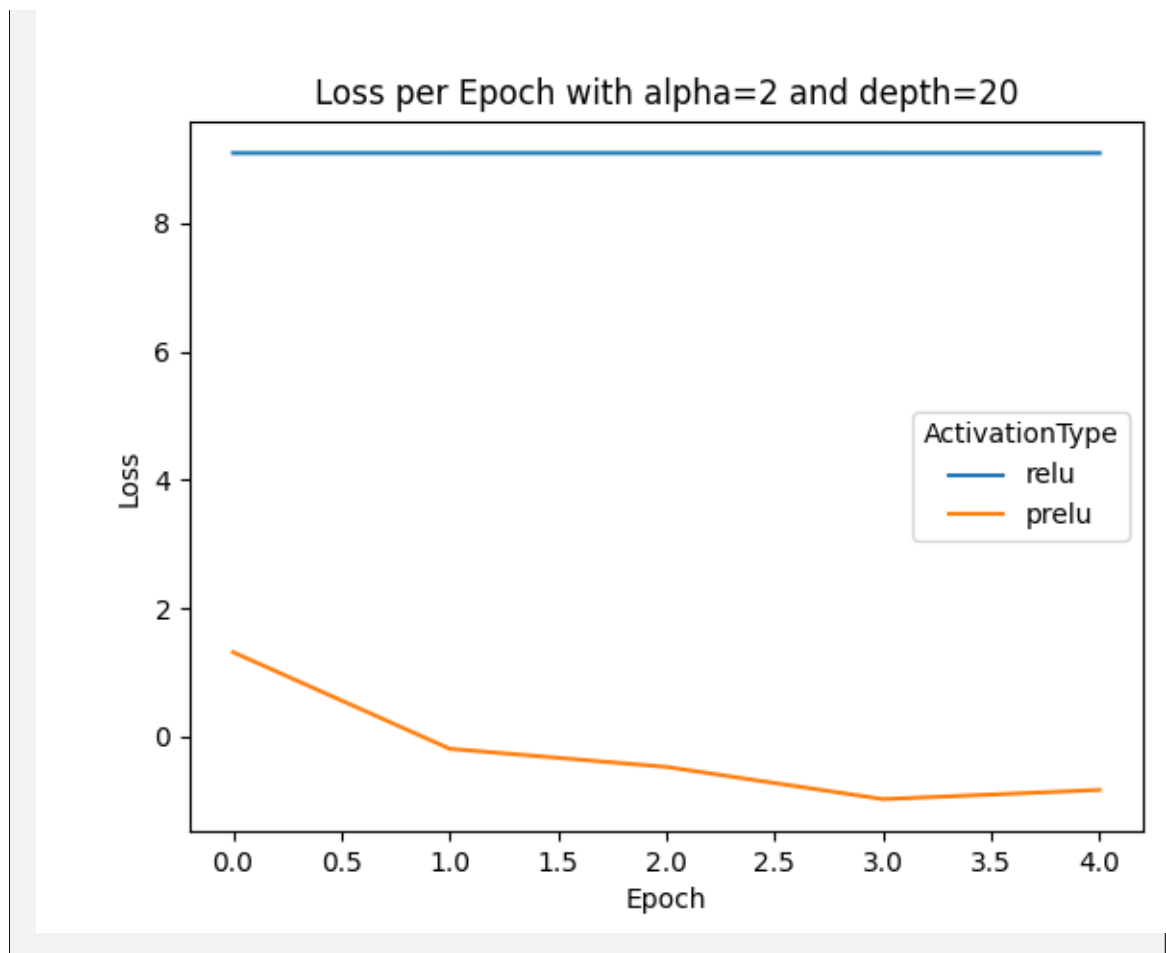


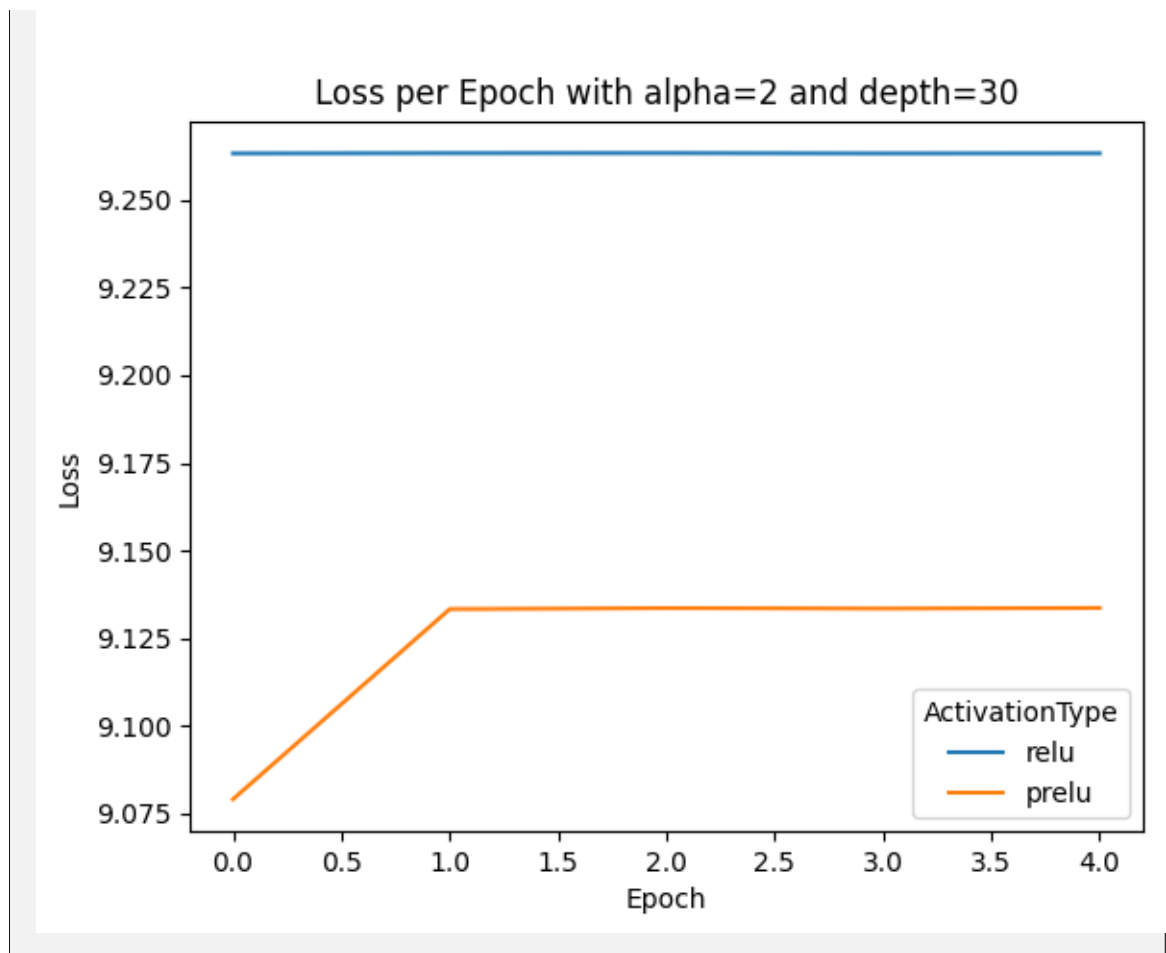


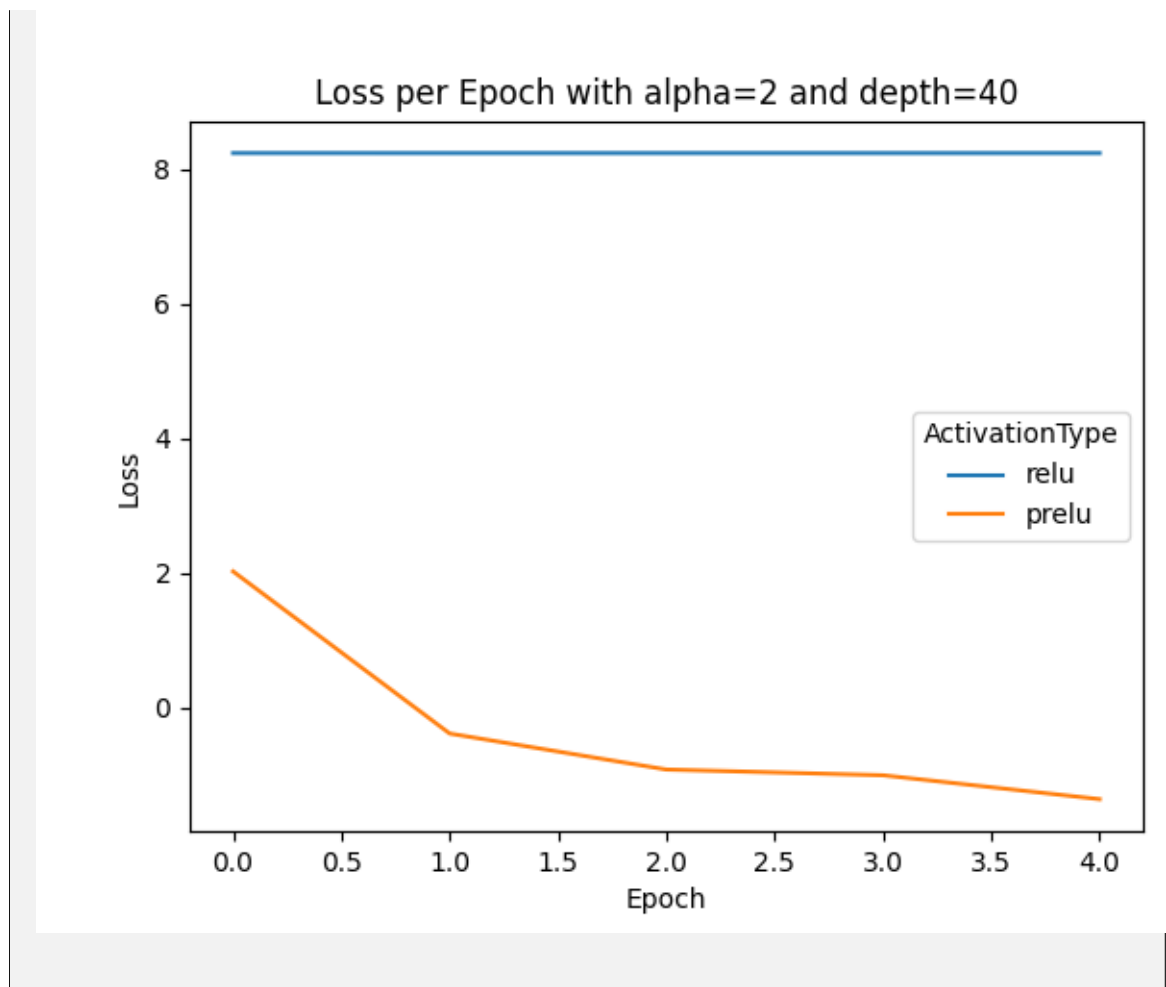












```
1 import torch
2 import torch.nn as nn
3 import torch.nn.functional as F
4 import torch.optim as optim
5
6 from sklearn.kernel_ridge import KernelRidge
7
8 import numpy as np
9 import pandas as pd
10 import seaborn as sns
11
12 DEBUG_MODE = True
13 def pp(s):
14     if(DEBUG_MODE):
15         print(s)
16
17 class Net(nn.Module):
18
19     def __init__(self, depth, width, initVariance):
20         super(Net, self).__init__()
21
22         self.preLayers = nn.ModuleList()
23         for _ in range(depth):
24             newLayer = nn.Linear(width, width)
25             nn.init.normal_(newLayer.weight, 0, np.sqrt(initVariance))
26             self.preLayers.append(newLayer)
27
28         self.outputLayer = nn.Linear(width, 1)
29
30     def forward(self, x):
31         pp(f"x dims: {x.shape}")
32         for l in self.preLayers:
33             x = F.relu(l(x))
34
35         y = F.relu(self.outputLayer(x))
36         return y
37
38
39     def fit(self, xs, ys, learningRate, nEpics=5): # TODO: change back to 10
40
41         optimizer = optim.SGD(self.parameters(), lr=learningRate)
42         lossFn = nn.MSELoss()
43
44         lossPerEpoch = []
45
46         for _ in range(nEpics):
47             self.train()
48
49             optimizer.zero_grad()
50             y_hat = self(xs)
```

```

51         pp(f"y_hats : {y_hat}")
52         pp(f"ys : {ys}")
53         loss_output = lossFn(y_hat, ys)
54         loss_output.backward()
55         optimizer.step()
56         lossPerEpoch.append(loss_output.item()/ys.shape[0])
57
58     return lossPerEpoch
59
60 def genData(n, m, d):
61     def relu(num):
62         return 0 if num < 0 else num
63     def genNSphere(r, d):
64         v = np.random.normal(0, r, d)
65         d = np.sum(v**2) ** (0.5)
66         return v/d
67
68     xss = [genNSphere(1, d) for _ in range(n)]
69     ys = []
70     for xs in xss:
71         ys.append(sum(map(relu, xs))/m)
72
73     return (np.array(xss), np.array(ys))
74
75 def calcError(preds, targets):
76     pp(f"predictions: {preds}")
77     pp(f"targets: {targets}")
78     return ((preds - targets)**2).mean()
79
80 def arcKernel(x1: np.array, x2: np.array):
81     x1Tx2 = np.dot(x1, x2)
82     x1Tx2 = 1.0 if x1Tx2 > 1.0 else x1Tx2
83     x1Tx2 = -1.0 if x1Tx2 < -1.0 else x1Tx2
84     return x1Tx2*(np.pi - np.arccos(x1Tx2))/(2*np.pi)
85
86 def plotResults(df):
87     sns.color_palette("Set2")
88
89     #df['Loss'] = np.log(df['Loss'].astype(float))
90
91     title = f"NN vs Kernel Regression"
92     plot = sns.lineplot(
93         data=df, x="N", y="Loss", hue="ModelType", ci=None
94     ).set_title(title)
95     plot.figure.savefig(f"{title}.png")
96     plot.figure.clf()
97
98 def addHistoryRow(df, n, loss, modelType):
99     print(df.head())
100     new_row = pd.DataFrame(columns=df.columns)

```

```
101     new_row.loc[0] = [n, loss, modelType]
102     df = pd.concat([df, new_row], ignore_index=True)
103     return df
104
105 ##### BEGIN APPLICATION #####
106
107 ns = [20, 40, 80, 160]
108 d = 10
109 m = 5
110 lr = 0.1
111
112 historyDf = pd.DataFrame(columns=[
113     "N", "Loss", "ModelType"
114 ])
115
116 for n in ns:
117     trainXs, trainYs = genData(n, m, d)
118     testXs, testYs = genData(100, m, d)
119
120     #pp(trainXs)
121     #pp(trainYs)
122     net = Net(depth=m, width=d, initVariance=1/m)
123     lossPerEpoch = net.fit(torch.Tensor(trainXs), torch.Tensor(trainYs), lr)
124     pp(f"Loss per eopch: {lossPerEpoch}")
125     nnError = calcError(net(torch.Tensor(testXs)).detach().numpy().flatten(), testYs)
126
127     historyDf = addHistoryRow(historyDf, n, nnError, "Neureal Network")
128
129     krr = KernelRidge(kernel=arcKernel)
130     print(trainXs)
131     krr.fit(trainXs, trainYs)
132     krrError = calcError(krr.predict(testXs), testYs)
133     historyDf = addHistoryRow(historyDf, n, krrError, "Kernel Regression")
134
135
136 plotResults(historyDf)
```



```
1 import torch
2 import torch.nn as nn
3 import torch.nn.functional as F
4 import torch.optim as optim
5 from torch.utils.data import DataLoader, Subset
6
7 import torchvision
8 from torchvision.datasets import MNIST
9 from torchvision import transforms
10
11 import numpy as np
12 import pandas as pd
13 import seaborn as sns
14
15 DEBUG_MODE = True
16 def pp(s):
17     if(DEBUG_MODE):
18         print(s)
19
20 class Net(nn.Module):
21
22     def __init__(self, depth, alpha, width, initVariance):
23         super(Net, self).__init__()
24         self.alpha = alpha
25
26         #self.conv1 = nn.Conv2d(1, 6, 5)
27         #self.conv2 = nn.Conv2d(6, 16, 5)
28
29         self.preLayers = nn.ModuleList()
30         for _ in range(depth):
31             newLayer = nn.Linear(width, width)
32             #pp(f"initVariance: {initVariance}")
33             nn.init.normal_(newLayer.weight, 0, np.sqrt(initVariance))
34             self.preLayers.append(newLayer)
35
36         self.outputLayer = nn.Linear(width, 1)
37         self.outSig = nn.Sigmoid()
38
39     def forward(self, x):
40
41         x = torch.flatten(x, 2, 3)
42
43         for l in self.preLayers:
44             x = F.leaky_relu(l(x), self.alpha)
45
46         x = F.leaky_relu(self.outputLayer(x), self.alpha)
47
48         return torch.squeeze(self.outSig(x))
49
50
```

```

51     def fit(self, batches, learningRate, epochs_n=5): # TODO: change back to 10
52         loss_per_epoch = []
53
54         optimizer = optim.SGD(self.parameters(), lr=learningRate)
55         lossFn = nn.BCELoss()
56
57         for i in range(epochs_n):
58             batch_loss = 0
59
60             self.train()
61             for image, label in batches:
62                 optimizer.zero_grad()
63                 y_hat = self(image)
64                 #pp(f"y_hat: {y_hat}" )
65                 #pp(f"label: {label}" )
66                 loss = lossFn(y_hat, label.float())
67                 loss.backward()
68                 optimizer.step()
69                 #pp(f"loss: {loss}")
70                 batch_loss += loss.item()
71
72             loss_per_epoch.append(batch_loss)
73
74         return loss_per_epoch
75
76 # setup data
77 trainDataRaw = MNIST(
78     root='data',
79     train=True,
80     transform=transforms.Compose([
81         transforms.Resize(16),
82         transforms.ToTensor(),
83     ]),
84     download=True
85 )
86
87
88 def addToDf(df: pd.DataFrame, history, actType):
89     for i, loss in enumerate(history):
90         new_row = pd.DataFrame(columns=df.columns)
91         new_row.loc[0] = [i, loss, actType]
92         df = pd.concat([df, new_row], ignore_index=True)
93
94     return df
95
96 def plotResults(df, d, a, lr):
97     sns.color_palette("Set2")
98
99     df['Loss'] = np.log(df['Loss'].astype(float))
100

```

```
101     title = f"Loss per Epoch with alpha={a} and depth={d}"
102     plot = sns.lineplot(
103         data=df, x="Epoch", y="Loss", hue="ActivationType", ci=None
104     ).set_title(title)
105     plot.figure.savefig(f"{title}_{d}_{a}.png")
106     plot.figure.clf()
107
108     ##### DO THE STUFF #####
109     batchSize = 64
110     width = 256
111     depths = [10, 20, 30, 40]
112     alphas = [2, 1, 0.5, 0.1]
113
114     keepIdxs = (trainDataRaw.targets==0) | (trainDataRaw.targets==1)
115     trainDataRaw.targets = trainDataRaw.targets[keepIdxs]
116     trainDataRaw.data = trainDataRaw.data[keepIdxs]
117
118     trainBatches = DataLoader(trainDataRaw, batch_size=batchSize, shuffle=True)
119
120     initFuncs = {
121         "relu": (lambda alpha: 2/width),
122         "prelu": (lambda alpha: 2/(width*(1 + alpha**2))),
123     }
124
125     history = []
126     learningRate = 0.01
127
128     for depth in depths:
129         for alpha in alphas:
130
131             historyDf = pd.DataFrame(columns=[
132                 "Epoch", "Loss", "ActivationType"
133             ])
134
135             for activationType, initFunc in initFuncs.items():
136                 net = Net(depth, alpha, width, initFunc(alpha))
137                 losses = net.fit(trainBatches, learningRate, epochs_n=5)
138                 pp(f"Losses: {losses}")
139                 historyDf = addToDf(historyDf, losses, activationType) # TODO
140
141             print(historyDf.head())
142             plotResults(historyDf, d=depth, a=alpha, lr=learningRate)
```