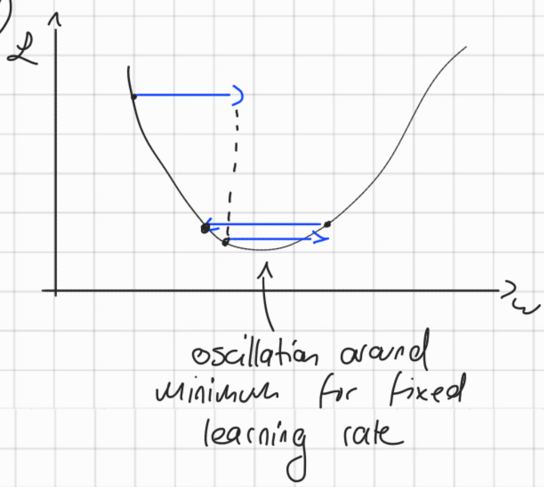
Exercise 1: Optimization and Training Tricks

1)

- Batch Gradient Descent (BGD): The Loss gradient is computed on the whole Training set before an update is made. While this is ideal for convex problems because the gradient is noiseless, pointing to the true minimum, the computational cost of just doing one update per epoch is very high. Thus BGD is rather slow and not apt for very large data sets. Additionally, BGD might get stuck in a local minimum due to the absence of noise.
- Stochastic Gradient Descent (SGD): The loss gradient is computed and the update to the model's parameters is computed for each instance. This reduces computational cost making it ideal for large datasets. The thus computed gradient is very noise, which helps to escape local minima, but can also cause oscillation around a minima.
- Minibatch SGD: The Loss gradient is computed and the update is performed on a (small) subset of the training set. This is a compromise between BGD and SGD. Consequently it benefits from the advantages of both, ie. reduced noise and computational cost, while mitigating the disadvantages, ie. no noise or too much noise and high computational cost. Minibatch is still able to escape local minima, due to the noise introduced by subsampling the training set.

		BGD	SGD	Minibatch SGD
Computational cost		high	low	medium
Speed of convergence	#epochs	few	many	moderately many
	time	slow (esp. for large Datasets)	fast	often fastest (=> allows vectorized operations)

2) a)



Getting closer to a Loss minimum while maintaining the same large learning rate makes it likely to "jump" over that minimum and eventually oscillate around it.

Thus it is common practice to reduce the learning rate going further into training to be able to go deeper into a minimum, while still approaching these minima fast by the initially large learning rate and jumping over sub-optimal local minima.

b)

Exponential decay: $\tau(t) = \tau_0 \exp(-\lambda t)$

with decay rate λ and training step t.

Reduces the learning rate exponentially which yields the above mentioned advantage.

3)

a)

The training set is used to train model.

The validation set is used to judge the model performance and optimise its hyperparameters accordingly

The test set is not involved in training or hyperparameter optimisation, but merely serves to measure the models generalisation capability.

b) This would implicitly involve the test set in the training process, which contradicts the principle of generalisation to unseen data and thus undermines the purpose of the test set.

c) In grid search the hypermeter space is scanned over and for each point the model is trained and test using the validation set. That way the best hyperparameters are determined.

4)

a)

i) RMSProp: The gradient is normalised using the root mean square of the previous gradients:

$$\Delta\theta_{t-1}^{RMS} = \sqrt{\frac{1}{t-1}\sum_{\tau=1}^{t-1}\Delta\theta_{\tau}^{2}} \qquad (10)$$

where this RMS is updated using a decay $\beta < 1$:

$$\Delta\theta_t^{RMS} = \beta\,\Delta\theta_{t-1}^{RMS} + (1-\beta)\,\Delta\theta_t$$

Leading to a training step of the form:

$$\theta_t = \theta_{t-1} + \tau\frac{\Delta\theta_t}{\sqrt{\Delta\theta_{t-1}^{2}+\varepsilon}}$$ with $\varepsilon \ll 1$ preventing division by zero.

This leads to a reduced learning relatively fast because the gradients commonly decrease faster than the accumulated RMS if $\beta \gg 0$.

However, this method is able to adapt too large or too small learning rates through the RMS.

ii) Momentum: The gradient is combined with the gained "momentum" of past gradients via:

$$p_t = \gamma \, p_{t-1} + (1-\gamma)\Delta\Theta_t$$

with momentum p_i and momentum decay γ.
That way even if the current gradient would be zero, there would still be some momentum left, "pushing" the model out of e.g. a local minimum.

b) Adam: $$\omega_t = \omega_{t-1} - \alpha \frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \varepsilon}$$

$$m_t = \beta_1 m_{t-1} + (1-\beta)g_t \, , \quad v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

$m_{t-1} = 0{,}5$, $v_{t-1} = 0{,}2$, $g_t = 2$, $\beta_1 = 0.9$, $\beta_2 = 0{,}99$, $\alpha = 0.01$, $\varepsilon = 10^{-8}$

i) $m_t = 0{,}65$, $v_t = 0{,}238$

ii) $\Delta w = -0{,}0133$

iii)
- $v_t' \gg v_t$: the history factors in much more than the current gradient with $\beta_2 = 0{,}99$
- $|\Delta w_t'| \ll |\Delta w_t|$: the effective learning rate decreases accounting for the previous very large gradients
- Adam seeks to keep the learning rate on an appropriate level since the history of second moments counters the development of too large/small training steps.

Machine Learning Essentials SS25 - Exercise Sheet 5

Instructions

- `TODO` 's indicate where you need to complete the implementations.
- You may use external resources, but **write your own solutions**.
- Provide concise, but comprehensible comments to explain what your code does.
- Code that's unnecessarily extensive and/or not well commented will not be scored.

Exercise 1

Exercise 2

In [1]:
```
import matplotlib.pyplot as plt
import numpy as np
# TODO: Import the stuff you need from torch and torchvision
import torch
from torchvision import transforms
from torchvision.datasets import FashionMNIST
from torch.utils.data import random_split, DataLoader
from torch import nn, optim

""""
If you stay in ML-related fields, you will likely be working on a server
always remember to set the number of CPU (or even GPU) threads you're usi
might sometimes use all available threads by default, which will lead to
also want to use some of the threads.
"""
# Example of limiting CPU threads:
# import os
# os.environ["OMP_NUM_THREADS"] = "15"
# os.environ["MKL_NUM_THREADS"] = "15"
# torch.set_num_threads(15) # If you only want to use PyTorch threads
```

Out[1]:
```
'"\nIf you stay in ML-related fields, you will likely be working on a se
rver or cluster. If you do so,\nalways remember to set the number of CPU
(or even GPU) threads you\'re using, as Jupyter notebooks or Python scri
pts \nmight sometimes use all available threads by default, which will l
ead to unhappy colleagues or classmates that\nalso want to use some of t
he threads.\n'
```

In [2]:
```
num_workers = 8
```

2.1

In [3]:
```
# TODO: Define transformations
# Given statistics of training set:
mu_train = 0.286
```

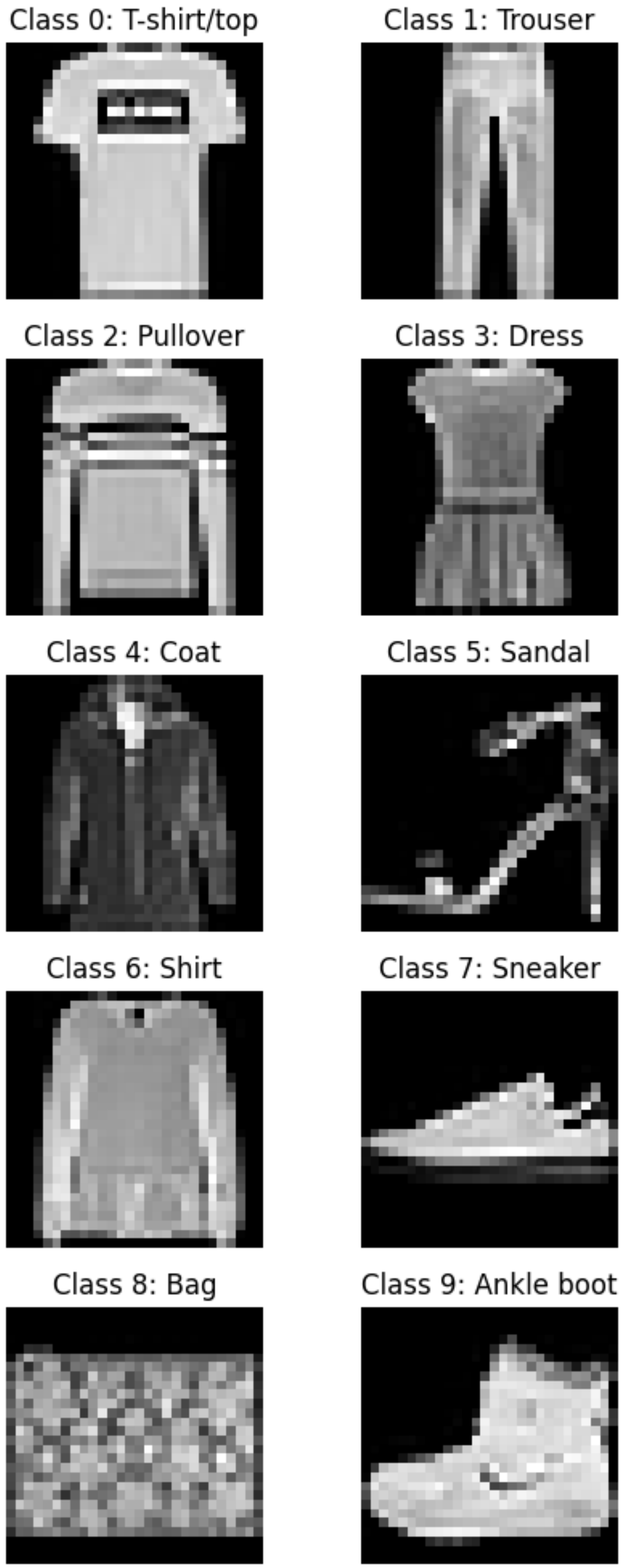
```python
std_train = 0.353
transform = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((mu_train,), (std_train,))
])

# TODO: Load FashionMNIST train/testsets
train_dataset_full = FashionMNIST(
    root='./data',
    train=True,
    download=True,
    transform=transform
)
test_dataset = FashionMNIST(
    root='./data',
    train=False,
    download=True,
    transform=transform
)

print(f"Full training dataset size: {len(train_dataset_full)}")
print(f"Test dataset size: {len(test_dataset)}")
```

```
Full training dataset size: 60000
Test dataset size: 10000
```

In [4]:

```python
# TODO: Create 5x2 subplot grid w/ example image for each class
fig, axes = plt.subplots(5, 2, figsize=(5, 10))
for i in range(10):
    img = np.where(train_dataset_full.targets == i)[0][0]
    img_tensor = train_dataset_full[img][0]
    img_array = img_tensor.numpy().squeeze()
    ax = axes[i // 2, i % 2]
    ax.imshow(img_array, cmap='gray')
    ax.set_title(f'Class {i}: {train_dataset_full.classes[i]}')
    ax.axis('off')

plt.tight_layout()
plt.show()
```


Class 0: T-shirt/top
Class 1: Trouser
Class 2: Pullover
Class 3: Dress
Class 4: Coat
Class 5: Sandal
Class 6: Shirt
Class 7: Sneaker
Class 8: Bag
Class 9: Ankle boot

In [5]:
```
# TODO: Create a validation set from the training set
validation_size = 10000
train_size = len(train_dataset_full) - validation_size
train_dataset, validation_dataset = random_split(
    train_dataset_full, [train_size, validation_size]
)
```

2.2

In [6]:
```
# TODO: Define your model architecture: A class called MLP that inherits
class MLP(nn.Module):
    def __init__(self, input_size=28*28, k=10, hidden_size=128, output_si
        super(MLP, self).__init__()
        layers = []
        layers.append(nn.Linear(input_size, hidden_size))
        layers.append(nn.ReLU())
        for _ in range(k):
            layers.append(nn.Linear(hidden_size, hidden_size))
            layers.append(nn.ReLU())
        layers.append(nn.Linear(hidden_size, output_size))
        self.model = nn.Sequential(*layers)
    def forward(self, x):
        x = x.view(x.size(0), -1)
        return nn.functional.softmax(self.model(x), dim=1)


# TODO: Define appropriate loss
criterion = nn.CrossEntropyLoss()
```

2.3

In [7]:
```
BATCH_SIZE_DEFAULT = 2048 # TODO: Set your default batch size. The capita

#TODO: Define DataLoaders for training, validation, and test sets
train_loader = DataLoader(
    train_dataset,
    batch_size=BATCH_SIZE_DEFAULT,
    shuffle=True,
    num_workers=num_workers
)
validation_loader = DataLoader(
    validation_dataset,
    batch_size=BATCH_SIZE_DEFAULT,
    shuffle=False,
    num_workers=num_workers
)
test_loader = DataLoader(
    test_dataset,
    batch_size=BATCH_SIZE_DEFAULT,
    shuffle=False,
    num_workers=num_workers
)
```

In [14]:
```
def calculate_accuracy(outputs, labels):
    """
    Calculate accuracy given model outputs and true labels.
    """
```

```
    _, predicted = torch.max(outputs.data, 1) # Prediction = class with h
    total = labels.size(0)
    correct = (predicted == labels).sum().item() #.item() converts a sing
    return correct / total

def train_model(model, criterion, optimizer, train_loader, val_loader, nu
    # Device configuration: if available use GPU (needs CUDA installed an
    device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
    model.to(device)
    print(f"Training on device: {device}")

    # TODO: Define training loop that for each epoch iterates over all mi
    # Record and return the training&validation loss and accuracy for eac
    train_losses = []
    val_losses = []
    train_accuracies = []
    val_accuracies = []

    for epoch in range(num_epochs):

        # mini batches
        model.train()
        running_loss = 0.0
        running_accuracy = 0.0

        for _ , (images, labels) in enumerate(train_loader):

            images, labels = images.to(device), labels.to(device)

            optimizer.zero_grad()
            outputs = model(images)
            loss = criterion(outputs, labels)
            loss.backward()
            optimizer.step()

            running_loss += loss.item()

            running_accuracy += calculate_accuracy(outputs, labels)

        train_loss = running_loss / len(train_loader)
        train_losses.append(train_loss)

        train_accuracy = running_accuracy / len(train_loader)
        train_accuracies.append(train_accuracy)

        model.eval()

        with torch.no_grad():
            running_val_acc = 0.0
            running_val_loss = 0.0
            for _, (images, labels) in enumerate(val_loader):
                images, labels = images.to(device), labels.to(device)
                outputs = model(images)

                running_val_acc += calculate_accuracy(outputs, labels)
                loss = criterion(outputs, labels)
                running_val_loss += loss.item()

            val_accuracy = running_val_acc / len(val_loader)
            val_accuracies.append(val_accuracy)
```

```
            val_loss = running_val_loss / len(val_loader)
            val_losses.append(val_loss)

        print(f'Epoch [{epoch+1}/{num_epochs}], '
              f'Train Loss: {train_loss:.4f}, Train Accuracy: {train_accu
              f'Val Accuracy: {val_accuracy:.4f}')

    return train_losses, val_losses, train_accuracies, val_accuracies
```

2.4

In [16]:
```
# TODO: Define hyperparameter grid for tuning
k = [2, 5, 10]
hidden_size = [32, 64, 128, 256]
batch_size = [256, 512, 1024, BATCH_SIZE_DEFAULT]

# fixed hybperparameters
num_epochs = 100
input_size = 28 * 28
output_size = 10

default_k = 2
default_hidden_size = 64


# TODO: For each hyperparameter setting, instantiate model&optimizer,
# train the model, and store the results for evaluation later
results_k_adam = {}
results_k_sgd = {}
for k_value in k:
    model_adam = MLP(input_size=input_size, k=k_value, hidden_size=defaul
    model_sgd = MLP(input_size=input_size, k=k_value, hidden_size=default_
    optimizer_adam = optim.Adam(model_adam.parameters())
    optimizer_sgd = optim.SGD(model_sgd.parameters(), lr=0.01, momentum=0

    print(f"Training model with k={k_value} using Adam optimizer")
    train_losses_adam, val_losses_adam, train_accuracies_adam, val_accura
        model_adam, criterion, optimizer_adam, train_loader, validation_l
    )
    results_k_adam[k_value] = {
        'train_losses': train_losses_adam,
        'val_losses': val_losses_adam,
        'train_accuracies': train_accuracies_adam,
        'val_accuracies': val_accuracies_adam
    }
    print(f"Training model with k={k_value} using SGD optimizer")
    train_losses_sgd, val_losses_sgd, train_accuracies_sgd, val_accuracie
        model_sgd, criterion, optimizer_sgd, train_loader, validation_loa
    )
    results_k_sgd[k_value] = {
        'train_losses': train_losses_sgd,
        'val_losses': val_losses_sgd,
        'train_accuracies': train_accuracies_sgd,
        'val_accuracies': val_accuracies_sgd
    }
```

```
Epoch [93/100], Train Loss: 1.6367, Train Accuracy: 0.8293, Val Accuracy:
0.8144
Epoch [94/100], Train Loss: 1.6365, Train Accuracy: 0.8291, Val Accuracy:
0.8146
Epoch [95/100], Train Loss: 1.6359, Train Accuracy: 0.8299, Val Accuracy:
0.8154
Epoch [96/100], Train Loss: 1.6353, Train Accuracy: 0.8307, Val Accuracy:
0.8148
Epoch [97/100], Train Loss: 1.6354, Train Accuracy: 0.8303, Val Accuracy:
0.8146
Epoch [98/100], Train Loss: 1.6347, Train Accuracy: 0.8310, Val Accuracy:
0.8158
Epoch [99/100], Train Loss: 1.6352, Train Accuracy: 0.8303, Val Accuracy:
0.8139
Epoch [100/100], Train Loss: 1.6346, Train Accuracy: 0.8311, Val Accuracy:
0.8146
```

In [ ]:
```
results_batch_size_adam = {}
results_batch_size_sgd = {}

for batch_size_value in batch_size:
    train_loader = DataLoader(
        train_dataset,
        batch_size=batch_size_value,
        shuffle=True,
        num_workers=num_workers
    )
    validation_loader = DataLoader(
        validation_dataset,
        batch_size=batch_size_value,
        shuffle=False,
        num_workers=num_workers
    )

    model_adam = MLP(input_size=input_size, k=default_k, hidden_size=defa
    model_sgd = MLP(input_size=input_size, k=default_k, hidden_size=defau
    optimizer_adam = optim.Adam(model_adam.parameters())
    optimizer_sgd = optim.SGD(model_sgd.parameters(), lr=0.01, momentum=0

    print(f"Training model with batch size={batch_size_value} using Adam 
    train_losses_adam, val_losses_adam, train_accuracies_adam, val_accura
        model_adam, criterion, optimizer_adam, train_loader, validation_l
    )
    results_batch_size_adam[batch_size_value] = {
        'train_losses': train_losses_adam,
        'val_losses': val_losses_adam,
        'train_accuracies': train_accuracies_adam,
        'val_accuracies': val_accuracies_adam
    }

    print(f"Training model with batch size={batch_size_value} using SGD o
    train_losses_sgd, val_losses_sgd, train_accuracies_sgd, val_accuracie
        model_sgd, criterion, optimizer_sgd, train_loader, validation_loa
    )
    results_batch_size_sgd[batch_size_value] = {
        'train_losses': train_losses_sgd,
        'val_losses': val_losses_sgd,
        'train_accuracies': train_accuracies_sgd,
        'val_accuracies': val_accuracies_sgd
    }
```

In [26]:
```
# TODO: Plot evolution of validation accuracy for each hyperparameter set

def plot_results(results, title):
    plt.figure(figsize=(12, 8))
    for key, value in results.items():
        plt.plot(value['val_accuracies'], label=f'k={key}' if 'k' in titl
    plt.title(title)
    plt.xlabel('Epochs')
    plt.ylabel('Validation Accuracy')
    plt.legend()
    plt.grid()
    plt.show()
```

In [27]:
```
print(results_hidden_size_adam.values())
```

dict_values([{'train_losses': [2.2086666584014893, 1.9124801301956176, 1.7
935973978042603, 1.72051860332489, 1.694562406539917, 1.682826418876648, 1
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In [28]:
```
plot_results(results_k_adam, 'Validation Accuracy for Different k Values
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plot_results(results_hidden_size_sgd, 'Validation Accuracy for Different
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plot_results(results_batch_size_sgd, 'Validation Accuracy for Different B
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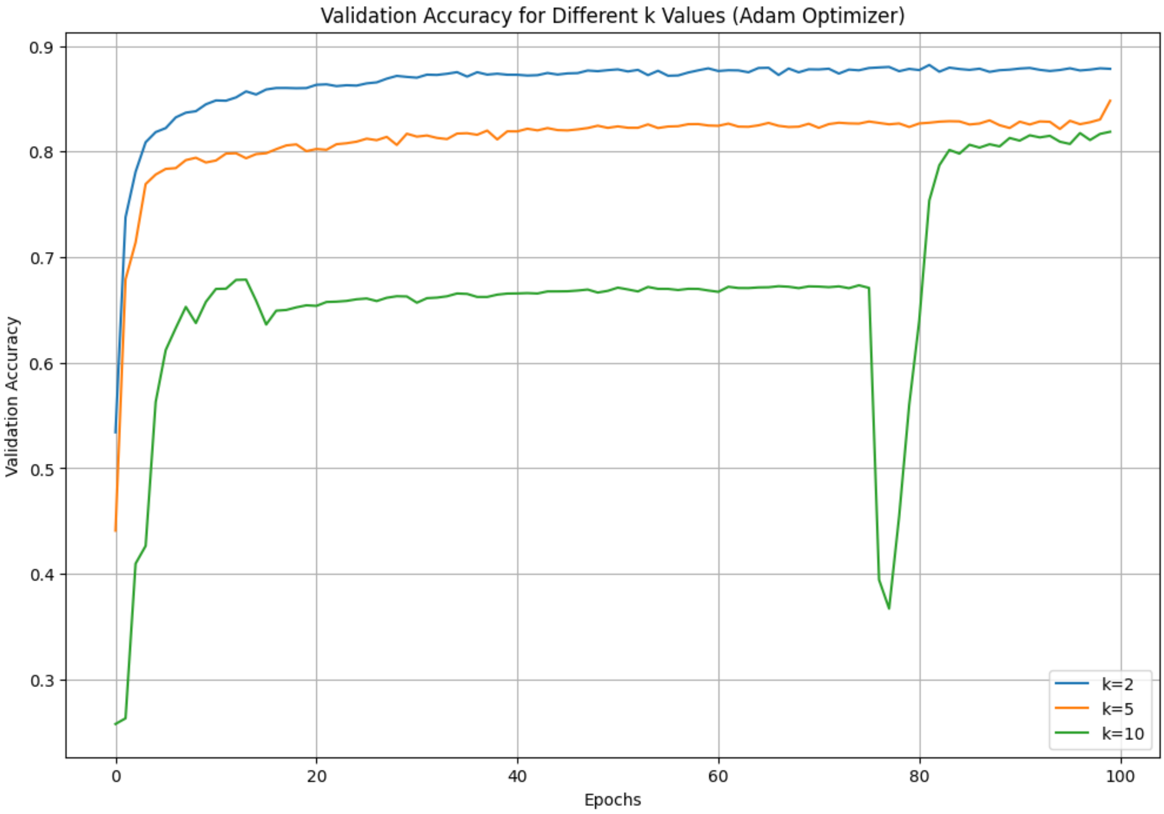
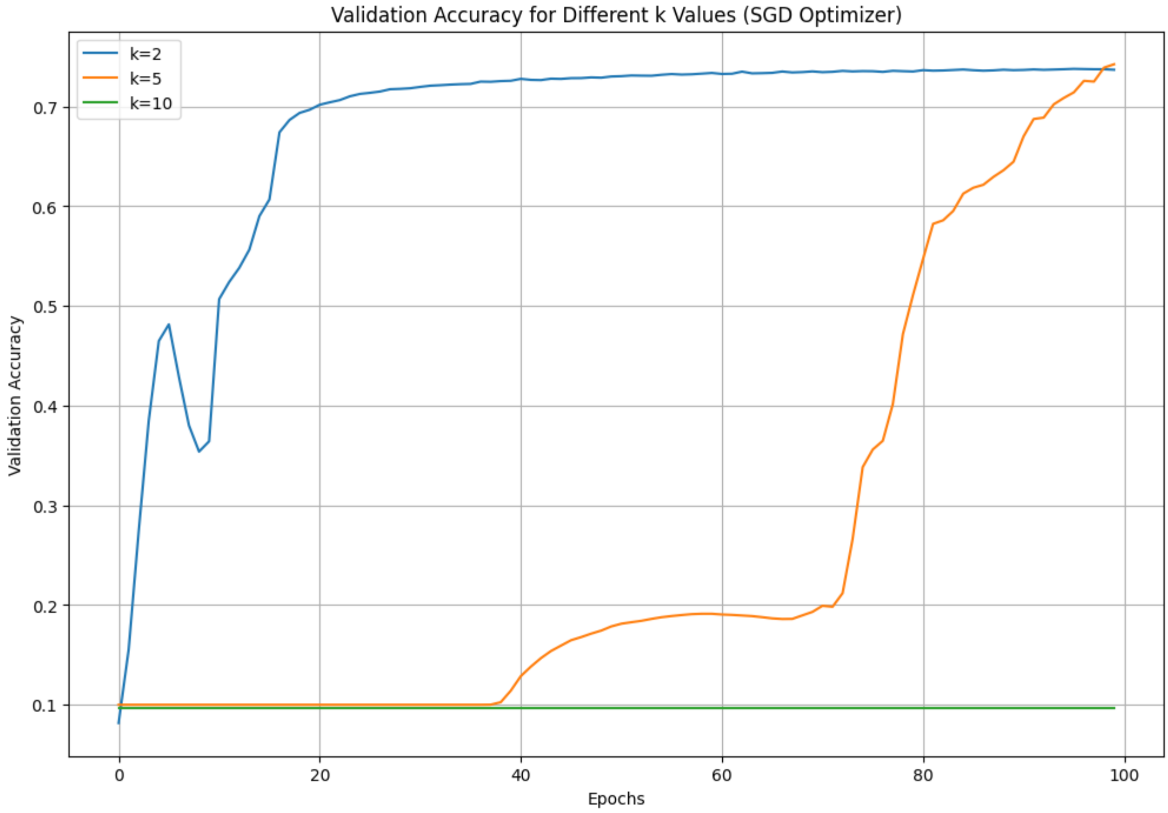
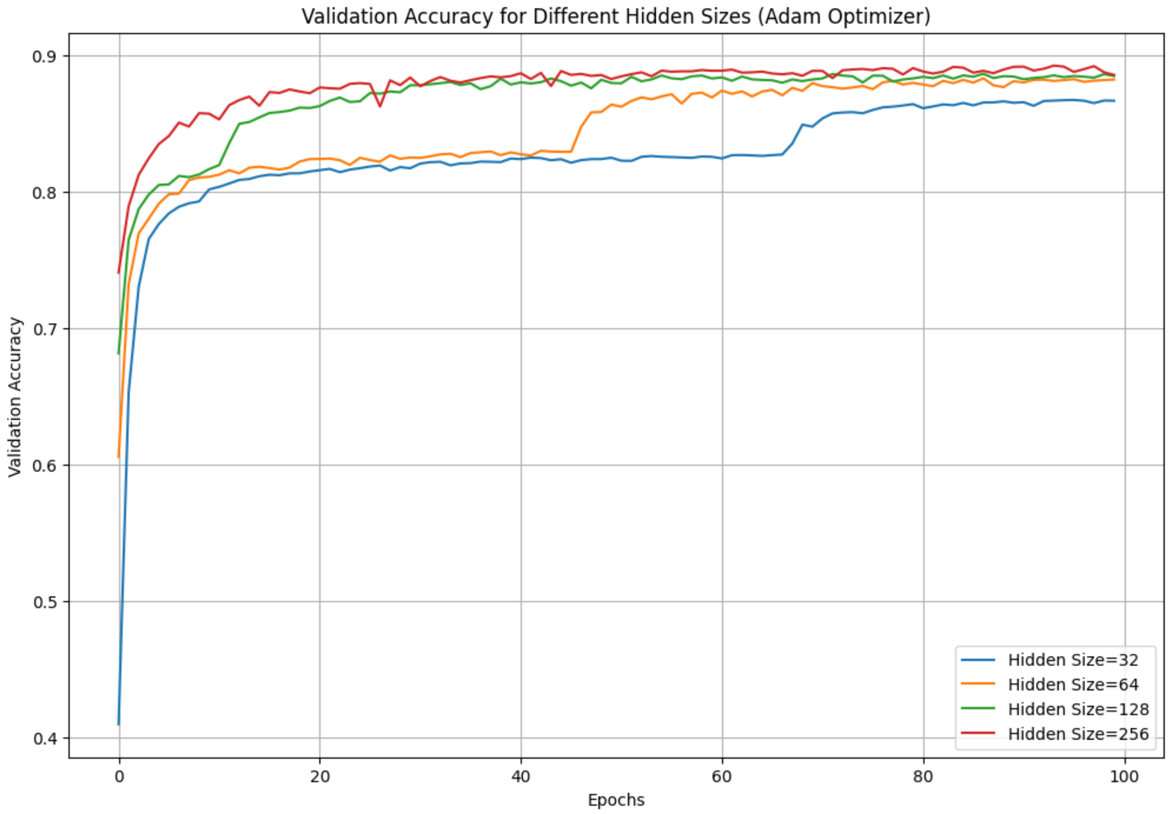
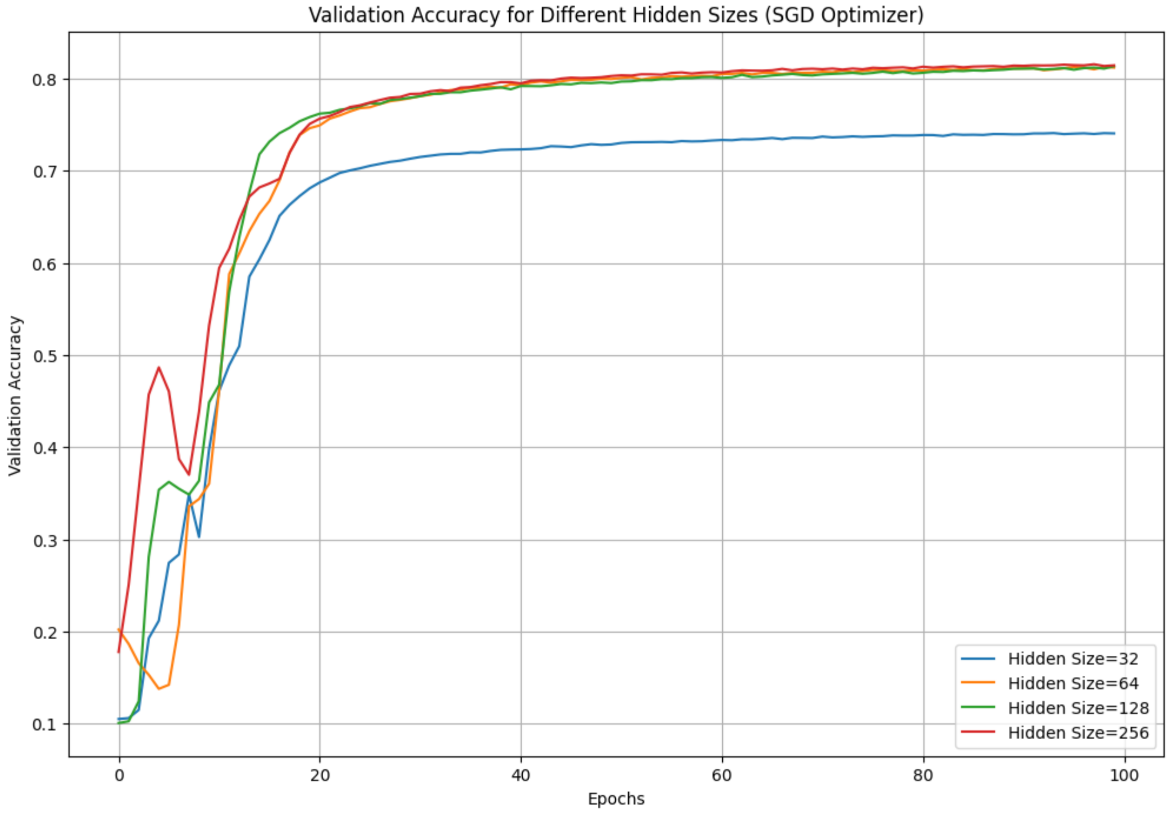
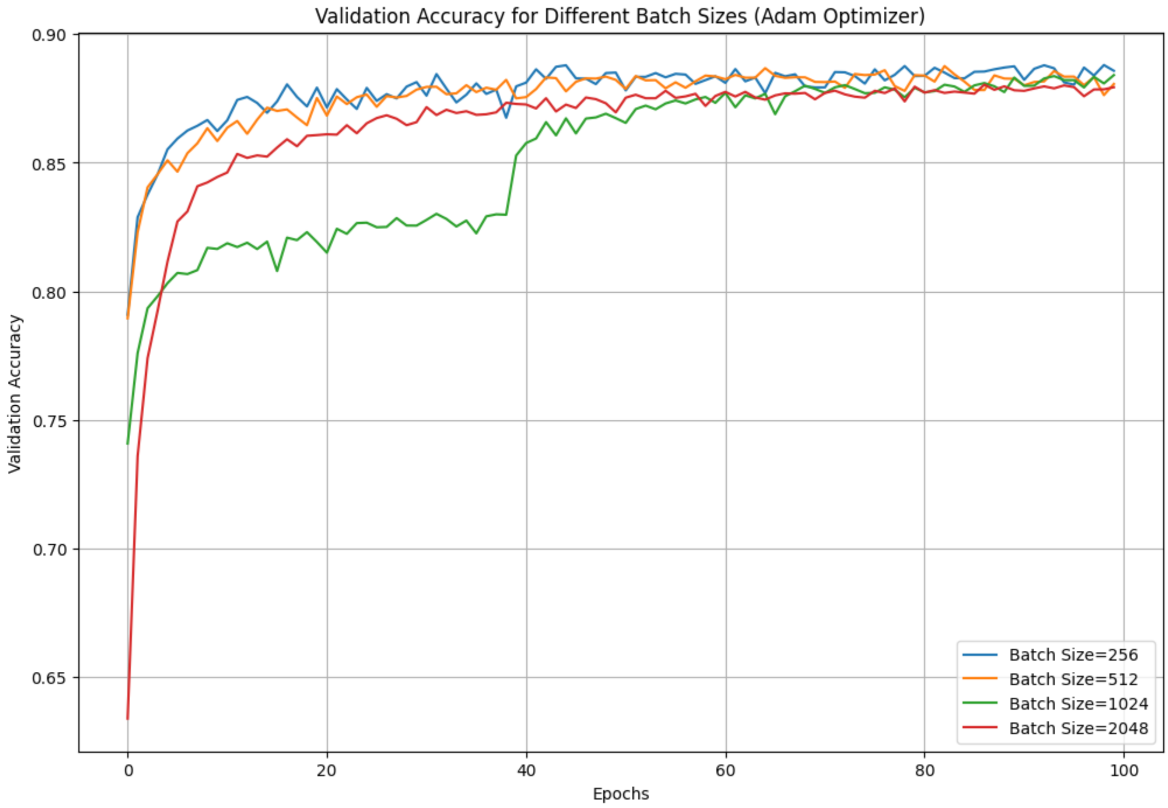
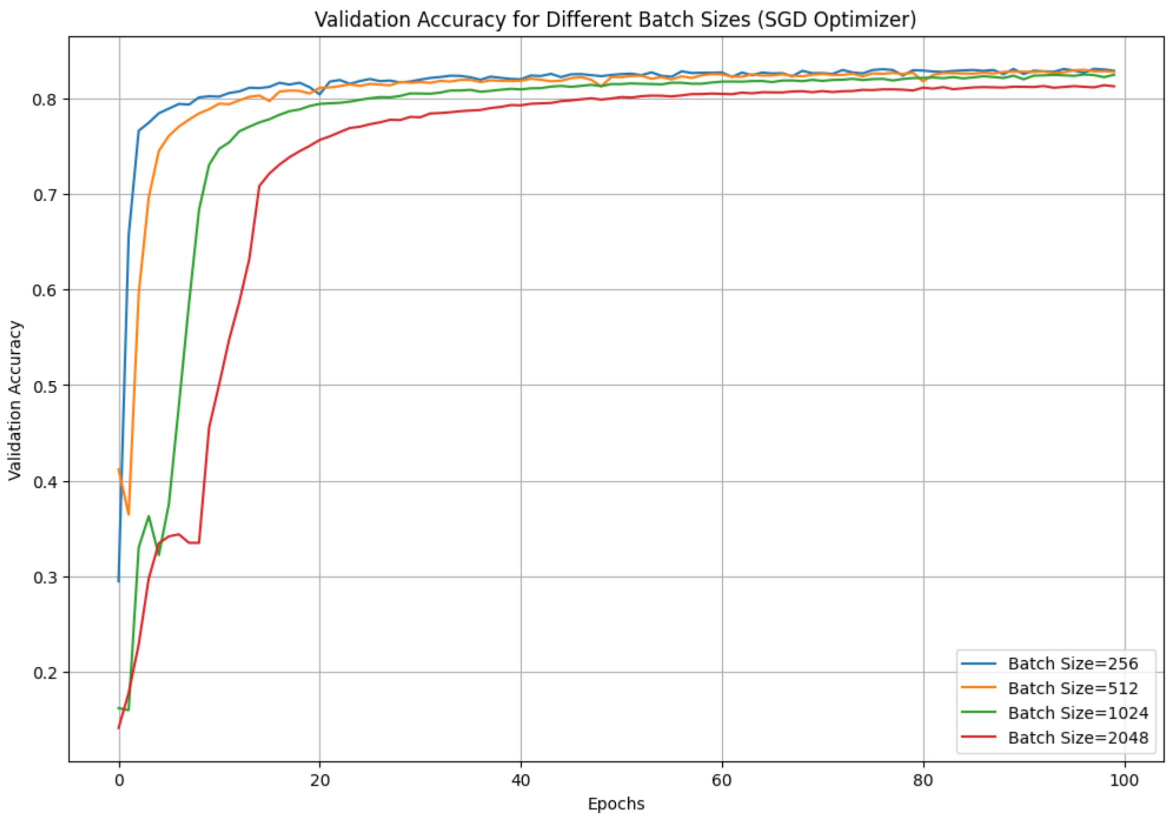



Validation Accuracy for Different k Values (SGD Optimizer)
k=2
k=5
k=10
Validation Accuracy
Epochs
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
20
40
60
80
100


Validation Accuracy for Different Hidden Sizes (Adam Optimizer)
Hidden Size=32
Hidden Size=64
Hidden Size=128
Hidden Size=256
Validation Accuracy
Epochs
0.4
0.5
0.6
0.7
0.8
0.9
0
20
40
60
80
100


Validation Accuracy for Different Hidden Sizes (SGD Optimizer)
Validation Accuracy
Epochs
Hidden Size=32
Hidden Size=64
Hidden Size=128
Hidden Size=256


Validation Accuracy for Different Batch Sizes (Adam Optimizer)
Validation Accuracy
Epochs
Batch Size=256
Batch Size=512
Batch Size=1024
Batch Size=2048



TODO: Justify which batch size and learning rate combination you will go with.

For the Batch Size it seems to not make a large difference for the convergence. Smaller Batch size seems to converge faster but you make much more mini opitmization steps, which results in this behavior, so we choose 1024, because 2048 performed slightly worse, if we choose the batch size too small the training takes longer because the CPU and GPU communication takes longer.

For the hidden size 64 performed equally well compared to the others, but we will choose 128 because, the learning seems to not go beyond the 0.75 accurracy mark, and a larger network maybe helps to achieve better accuracies and learns the underlying distribution better.

For the hidden layers k, we choose 5. It seems sufficient to use 2, but we choose more for the same reason as before.

But we train for more epochs than before

2.4

In [32]:
```
# TODO: Train model w/ best hyperparameters for SGD and compare to defaul
best_k = 5
best_hidden_size = 128
best_batch_size = 1024

train_loader = DataLoader(
    train_dataset,
    batch_size=best_batch_size,
    shuffle=True,
    num_workers=12
```

```
)
validation_loader = DataLoader(
    validation_dataset,
    batch_size=best_batch_size,
    shuffle=False,
    num_workers=12
)


model_best_sgd = MLP(input_size=input_size, k=best_k, hidden_size=best_hi
optimizer_best_sgd = optim.SGD(model_best_sgd.parameters(), lr=0.01, mome

print("Training model with best hyperparameters using SGD optimizer")
train_losses_best_sgd, val_losses_best_sgd, train_accuracies_best_sgd, va
    model_best_sgd, criterion, optimizer_best_sgd, train_loader, validati

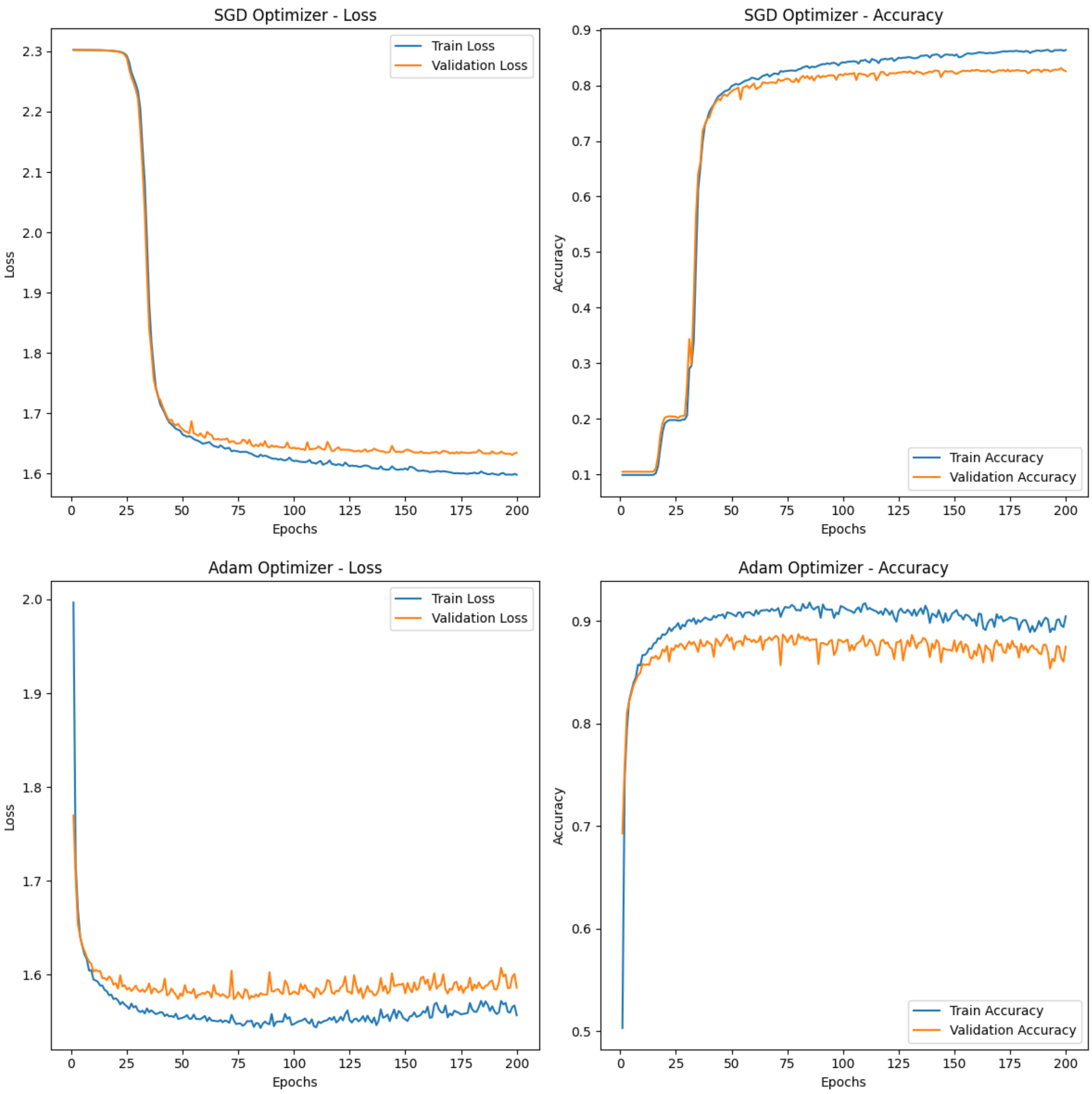
model_best_adam = MLP(input_size=input_size, k=best_k, hidden_size=best_h
optimizer_best_adam = optim.Adam(model_best_adam.parameters())

print("Training model with best hyperparameters using Adam optimizer")
train_losses_best_adam, val_losses_best_adam, train_accuracies_best_adam,
    model_best_adam, criterion, optimizer_best_adam, train_loader, valida
```

```
Epoch [189/200], Train Loss: 1.5663, Train Accuracy: 0.8948, Val Accuracy:
0.8675
Epoch [190/200], Train Loss: 1.5610, Train Accuracy: 0.9001, Val Accuracy:
0.8766
Epoch [191/200], Train Loss: 1.5580, Train Accuracy: 0.9032, Val Accuracy:
0.8769
Epoch [192/200], Train Loss: 1.5597, Train Accuracy: 0.9014, Val Accuracy:
0.8694
Epoch [193/200], Train Loss: 1.5721, Train Accuracy: 0.8889, Val Accuracy:
0.8535
Epoch [194/200], Train Loss: 1.5682, Train Accuracy: 0.8928, Val Accuracy:
0.8631
Epoch [195/200], Train Loss: 1.5699, Train Accuracy: 0.8912, Val Accuracy:
0.8608
Epoch [196/200], Train Loss: 1.5605, Train Accuracy: 0.9007, Val Accuracy:
0.8755
Epoch [197/200], Train Loss: 1.5596, Train Accuracy: 0.9016, Val Accuracy:
0.8749
Epoch [198/200], Train Loss: 1.5655, Train Accuracy: 0.8957, Val Accuracy:
0.8636
Epoch [199/200], Train Loss: 1.5672, Train Accuracy: 0.8940, Val Accuracy:
0.8604
Epoch [200/200], Train Loss: 1.5567, Train Accuracy: 0.9044, Val Accuracy:
0.8749
```

In [33]:

```python
# TODO: Plot "learning curves" of the best SGD model and the Adam model
def plot_learning_curves(train_losses, val_losses, train_accuracies, val_
    epochs = range(1, len(train_losses) + 1)

    plt.figure(figsize=(12, 6))

    plt.subplot(1, 2, 1)
    plt.plot(epochs, train_losses, label='Train Loss')
    plt.plot(epochs, val_losses, label='Validation Loss')
    plt.title(f'{title} - Loss')
    plt.xlabel('Epochs')
    plt.ylabel('Loss')
    plt.legend()

    plt.subplot(1, 2, 2)
    plt.plot(epochs, train_accuracies, label='Train Accuracy')
    plt.plot(epochs, val_accuracies, label='Validation Accuracy')
    plt.title(f'{title} - Accuracy')
    plt.xlabel('Epochs')
    plt.ylabel('Accuracy')
    plt.legend()

    plt.tight_layout()
    plt.show()

plot_learning_curves(train_losses_best_sgd, val_losses_best_sgd, train_ac
plot_learning_curves(train_losses_best_adam, val_losses_best_adam, train_
```



TODO: Based on plots, compare (mini-batch) SGD and Adam, select overall best Model

Select Adam because overall performance is better

In [34]:
```
#TODO: Evaluate the best model on the test set, print the test/train/vali

def evaluate_model(model, test_loader, train_loader, validation_loader):
    device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
    model.to(device)
    model.eval()

    test_accuracy = 0.0
    train_accuracy = 0.0
    validation_accuracy = 0.0
    with torch.no_grad():
        for images, labels in test_loader:
            images, labels = images.to(device), labels.to(device)
            outputs = model(images)

            test_accuracy += calculate_accuracy(outputs, labels)

        for images, labels in train_loader:
            images, labels = images.to(device), labels.to(device)
            outputs = model(images)
```

```
            train_accuracy += calculate_accuracy(outputs, labels)
        for images, labels in validation_loader:
            images, labels = images.to(device), labels.to(device)
            outputs = model(images)
            validation_accuracy += calculate_accuracy(outputs, labels)

    test_accuracy /= len(test_loader)
    train_accuracy /= len(train_loader)
    validation_accuracy /= len(validation_loader)

    return test_accuracy, train_accuracy, validation_accuracy

test_acc_best, train_acc_best, val_acc_best = evaluate_model(
    model_best_adam, test_loader, train_loader, validation_loader
)

print(f"Adam best model test accuracy: {test_acc_best:.4f}")
print(f"Adam best model train accuracy: {train_acc_best:.4f}")
print(f"Adam best model validation accuracy: {val_acc_best:.4f}")
```

```
Adam best model test accuracy: 0.8669
Adam best model train accuracy: 0.9016
Adam best model validation accuracy: 0.8749
```

TODO: Briefly discuss your results.

Adam converged faster than SGD and also had a steeper learning curve. SGD took more epochs to achieve higher accuracies compared to Adam. With more epochs, the results maybe would have been better, but this network is not designed for image classification, odher models would achieve better results.