

CS203 Lab 6

Team

Team Number: 33

Team Members

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Repository Details

- Link to Repository: https://github.com/VivekRaj2708/Lab6_CS203

Procedure

Dataset

1. We get the IRIS Dataset from `sklearn`

```
from sklearn.datasets import load_iris
```

2. Dataset Cleaning and labelling. We clean the dataset, append the labels and then normalise the data.

```
data = load_iris()
X = data['data']
Y = data['target']
labels = []

for x in range(len(Y)):
    if Y[x] == 0:
        labels.append('setosa')
    elif Y[x] == 1:
        labels.append('versicolor')
    else:
        labels.append('virginica')

X_normed = X / X.max(axis=0)
```

3. Now we have to split the dataset into `Train` (70%), `Validation` (20%) and `Test` (10%). We use `sklearn` for that also.

```
X_train, X_testing, y_train, y_testing = train_test_split(X_normed, Y, test_size=0.3,
random_state=20)
X_validation, X_test, y_validation, y_test = train_test_split(X_testing, y_testing,
test_size=0.33, random_state=20)
print(X_train.shape, X_validation.shape, X_test.shape, y_train.shape, y_validation.shape,
y_test.shape)
```

4. We make torch dataset out of our generated Train/Validation and Test Splits

```
X_train_model = tensor(X_train, dtype=torch.float32)
y_train_model = tensor(y_train)

train_dataset = TensorDataset(X_train_model, y_train_model)
train_loader = DataLoader(train_dataset, batch_size=32, shuffle=True)

val_dataset = TensorDataset(tensor(X_validation, dtype=torch.float32), tensor(y_validation))
val_loader = DataLoader(val_dataset, batch_size=32, shuffle=True)

test_dataset = TensorDataset(tensor(X_test, dtype=torch.float32), tensor(y_test))
test_loader = DataLoader(test_dataset, batch_size=32, shuffle=True)
```

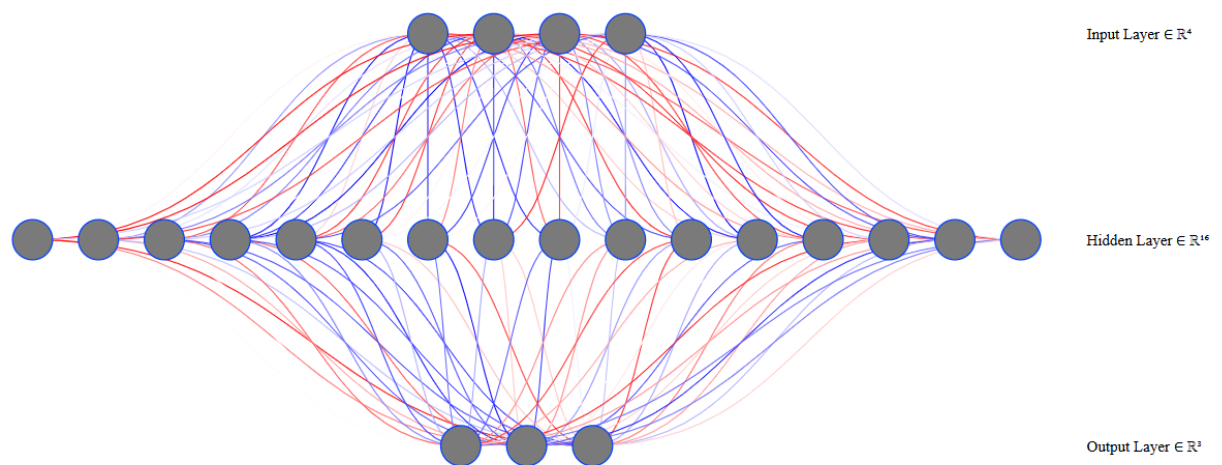
Torch Initialisation

1. Device Selection

```
import torch
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

2. Architecture Declaration

We use the following architecture for training on the IRIS Dataset. We will use pytorch to make the model as well



```
class MLP(nn.Module):
    def __init__(self) -> None:
        super(MLP, self).__init__()
        self.layer1 = nn.Linear(4, 16)
        self.activation = nn.ReLU()
        self.layer2 = nn.Linear(16, 3)
        self.softmax = nn.Softmax()

    def forward(self, x):
        x = self.layer1(x)
        x = self.activation(x)
        x = self.layer2(x)
        x = self.softmax(x)
        return x

model = MLP()
model.to(device)
optimiser = AdamW(model.parameters(), lr=0.001)
criteria = CrossEntropyLoss()
```

Model Training

We train the model on the following parameters:

1. 50 Epochs
2. 10^{-3} Learning Rate
3. AdamW Optimiser
4. CrossEntropyLoss Loss Criteria

```
epochs = 50
model.train()

training_loss = []
valid_loss = []

for epoch in range(epochs):
    running_loss = 0.0
    val_loss = 0.0
    model.train()
    for X_batch, Y_batch in train_loader:
        X_batch, Y_batch = X_batch.to(device), Y_batch.to(device)
        optimiser.zero_grad()
        outputs = model(X_batch)
        loss = criteria(outputs, Y_batch)
        loss.backward()
        optimiser.step()
        running_loss += loss.item()
    avg_loss = running_loss / len(train_loader)
    training_loss.append(avg_loss)

    model.eval()
    with torch.no_grad():
        for inputs, labels in val_loader:
            inputs, labels = inputs.to(device), labels.to(device)
            outputs = model(inputs)
            loss = criteria(outputs, labels)
            val_loss += loss.item()
        avg_val_loss = val_loss / len(val_loader)
        valid_loss.append(avg_val_loss)

    if (epoch+1) % 10 == 0:
        print(f'Epoch {epoch+1}/{epochs}, Test Loss: {avg_loss:.4f}, , Val Loss: {avg_val_loss:.4f}')
```

Model Evaluation

Now we test the model on our test dataset (10%)

```
model.eval()

pred = []
label = []
with torch.no_grad():
    for inputs, labels in test_loader:
        label.append(labels)
        inputs, labels = inputs.to(device), labels.to(device)
        outputs = model(inputs)

        # Update the test accuracy
        _, preds = torch.max(outputs, 1)
        pred.append(preds.cpu().numpy())
```

Model Metrics

We will calculate the F1 score, Prescision, Recall and Accuracy using the `skealrn` module

```
pred = np.array(pred).flatten()
label = np.array(label).flatten()
accuracy = accuracy_score(pred, label)
recall = recall_score(pred, label, average="weighted")
precision = precision_score(pred, label, average="weighted")
f1 = f1_score(pred, label, average="weighted")

print("Acc: ", accuracy, "\nRecall:", recall, "\nPrescision:", precision, "\nF1:", f1)

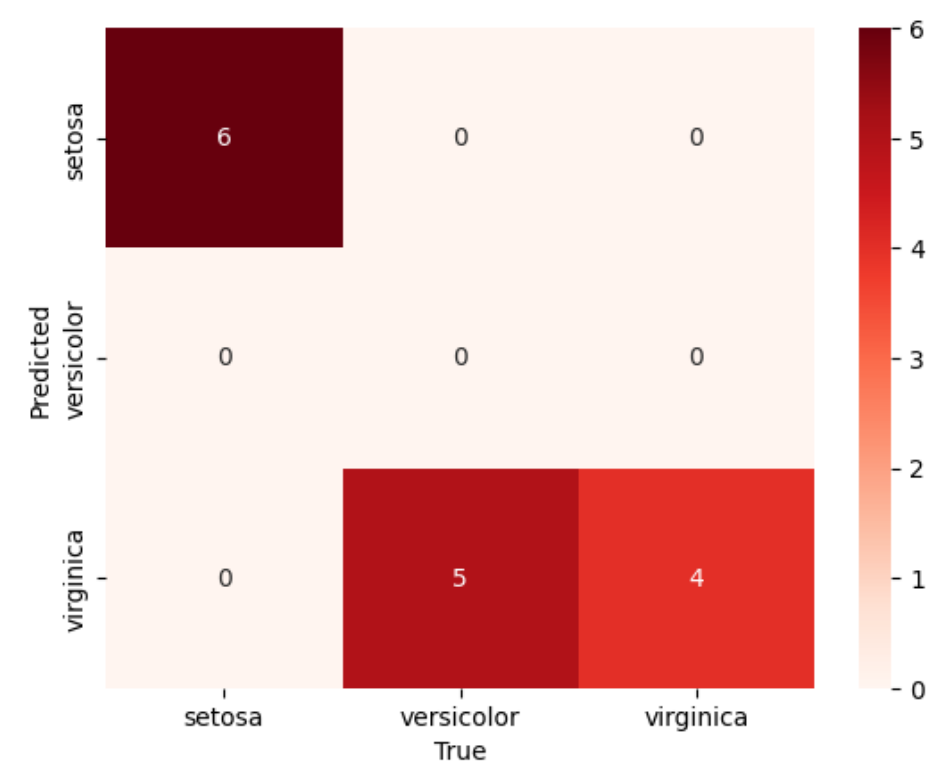
df_cm = pd.DataFrame(confusion_matrix(pred, label),
                     index = data['target_names'],
                     columns = data['target_names'])

sn.heatmap(df_cm, annot=True, cmap="Reds")
plt.xlabel("True")
plt.ylabel("Predicted")
```

Metric Details:

Metric	Value
Accuracy	0.667
Recall	0.667
Precision	1.000
F1 Score	0.769

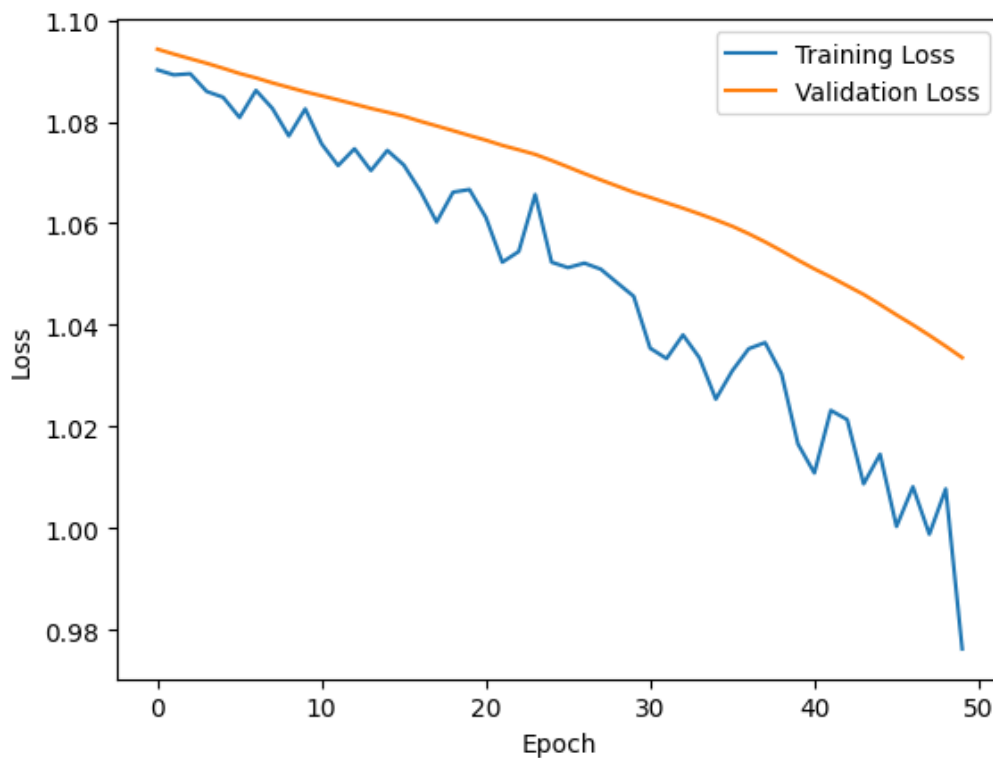
Confusion Matrics



Training Loss vs Vaidation Loss

According to the question we have to plot the training and the validation loss using `Matplotlib`

```
plt.plot(training_loss, label='Training Loss')
plt.plot(valid_loss, label='Validation Loss')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
```



The plot above represents the **Training Loss** and **Validation Loss** over **50 epochs**.

Observations:

- The **Training Loss** (blue line) steadily decreases with fluctuations, indicating that the model is learning.
- The **Validation Loss** (orange line) also decreases but remains consistently higher than the training loss.
- The gap between training and validation loss suggests some level of **overfitting**, where the model generalizes less effectively on unseen data.
- The fluctuations in training loss could be due to **learning rate variations** or **batch randomness**.

WandB Initialisation

Installation

```
pip install wandb
```

Login

```
wandb login
```

We give the API Key generated by <https://wandb.ai/authorize>

Initialisation Parameters

We register the following details to WandB before we proceed to the actual model training

Project Details

- **Project Name:** STT-For-AI-Lab6
- **Run Name:** Run 24022025-4

Model Architecture

- **Type:** Multi-Layer Perceptron (MLP)
- **Layers:**
 - **Input Layer:** 4 neurons
 - **Hidden Layer:** 16 neurons
 - **Output Layer:** 3 neurons

Activation Functions

- **Hidden Layer Activation:** ReLU
- **Output Layer Activation:** Softmax

Hyperparameters

- **Batch Size:** 32
- **Epochs:** 50
- **Learning Rate:** 0.001

Dataset

- **Dataset Used:** IRIS

Code

This is the initialisation function:

```
wandb.init(  
    project="STT-For-AI-Lab6",  
    name="Run 24022025-4",  
    config={  
        "architecture": "MLP",  
        "Layers": {  
            "Input": 4,  
            "Hidden": 16,  
            "Output": 3  
        },  
        "Activation": ["ReLU", "Softmax"],  
        "Hyperparameter": {  
            "batch_size": 32,  
            "epochs": 50,  
            "learning_rate": 0.001  
        },  
        "dataset": "IRIS",  
    }  
)
```

Actual Training in WandB

We training the model again and log the losses and metrics using the `log` method in the `wandb` module

Initialisation Parameters

▼

Config parameters: {} 5 keys

▼

Activation: [] 2 items

0: "ReLU"

1: "Softmax"

architecture: "MLP"

dataset: "IRIS"

▼

Hyperparameter: {} 3 keys

batch_size: 32

epochs: 50

learning_rate: 0.001

▼

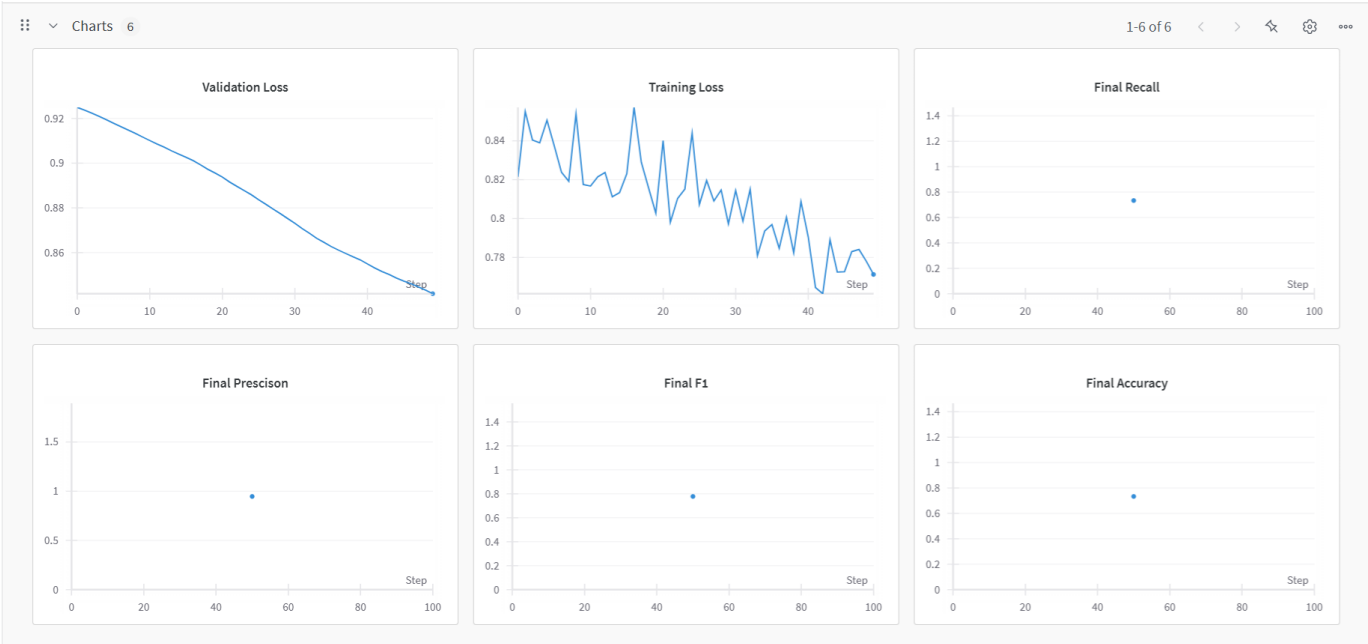
Layers: {} 3 keys

Hidden: 16

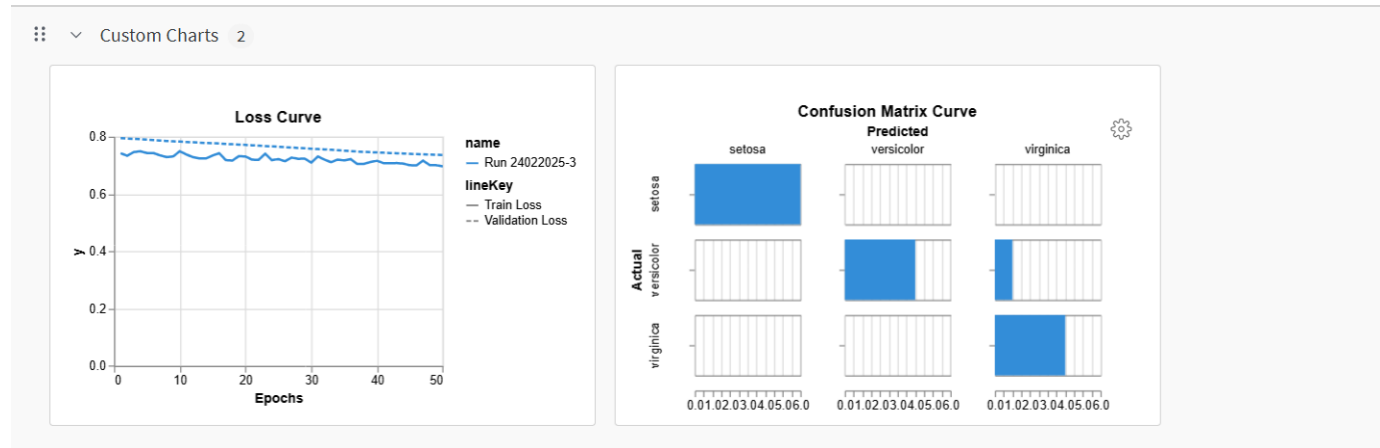
Input: 4

Output: 3

Charts



Loss Curve and Confusion Matrics



Autogluen Initialisation

Installation

```
pip install autogluon
```

Import

```
import autogluon as ag
from autogluon.tabular import TabularDataset, TabularPredictor
from autogluon.core.models import AbstractModel
import autogluon.common as agco
```

We import the following from autoguon:

Import Module	Module Name	Use Case Description
autogluon	ag	Main module for AutoGluon, providing AutoML capabilities.
autogluon.tabular	TabularDataset	Handles tabular data loading and preprocessing.
autogluon.tabular	TabularPredictor	Generates models for tabular data with AutoML features.
autogluon.core.models	AbstractModel	Base class for defining custom models in AutoGluon.
autogluon.common	agco	Contains utilities and common components for AutoGluon.

Hyperparameters

```
ag.tabular.models.tabular_nn.hyperparameters.parameters.get_hyper_params(framework='pytorch')
```

We see that the following parameters can be tweaked in the **NN_TORCH** model:

```
{
  "activation": "relu",
  "embedding_size_factor": 1.0,
  "embed_exponent": 0.56,
  "max_embedding_dim": 100,
  "y_range": "None",
  "y_range_extend": 0.05,
  "dropout_prob": 0.1,
  "optimizer": "adam",
  "learning_rate": 0.0003,
  "weight_decay": 1e-06,
  "proc.embed_min_categories": 4,
  "proc.impute_strategy": "median",
  "proc.max_category_levels": 100,
  "proc.skew_threshold": 0.99,
  "use_ngram_features": False,
  "num_layers": 4,
  "hidden_size": 128,
  "max_batch_size": 512,
  "use_batchnorm": false,
  "loss_function": "auto"
}
```

Abstract Model Generation

We make a custom model for hyperparameter tuning called `PyTorchWrapper` which inherits from `AbstractClass`

```
from autogluon.core.models import AbstractModel

class PyTorchWrapper(AbstractModel):
    def __init__(self, **kwargs):
        super().__init__(**kwargs)
        self.model = None
        self.num_epochs = kwargs.get('num_epochs', 5)
        self.learning_rate = kwargs.get('learning_rate', 1e-3)
        self.batch_size = kwargs.get('batch_size', 2)

    def _fit(self, X, y, **kwargs):
        # Convert data to PyTorch tensors
        X_tensor = torch.tensor(X.values, dtype=torch.float32)
        y_tensor = torch.tensor(y.values, dtype=torch.float32)

        # Initialize the model
        self.model = MLP()

        # Define loss and optimizer
        optimiser = AdamW(model.parameters(), lr=self.learning_rate)
        criteria = CrossEntropyLoss()

        # Training loop
        for epoch in range(self.num_epochs): # Adjust epochs as needed
            optimiser.zero_grad()
            outputs = self.model(X_tensor)
            loss = criteria(outputs, y_tensor)
            loss.backward()
            optimiser.step()

    def _predict(self, X, **kwargs):
        X_tensor = torch.tensor(X.values, dtype=torch.float32)
        with torch.no_grad():
            predictions = self.model(X_tensor)
        return predictions.numpy()
```

Grid Search

We will do a grid search using AutoGloun (backend: Ray Tuner and get the model parameters)

Search Space was defined aas the following

```
search_space = {
    "lr": tune.grid_search([1e-3, 1e-5]),
    "num_epochs": tune.grid_search([1,3,5]),
    "batch_size": tune.grid_search([2, 4])
}
```

Experiment Configuration: train_MLP_2025-02-26_13-21-53

Parameter	Value
Search Algorithm	BasicVariantGenerator
Scheduler	FIFOScheduler
Number of Trials	12

Output

Trial Name	Status	Learning Rate	Epochs	Batch Size	Iter	Total Time (s)	Accuracy	F1 Score
train_MLP_b82a5_00000	TERMINATED	0.001	1	2	1	5.10377	0.266667	0.421053
train_MLP_b82a5_00001	TERMINATED	0.001	1	4	1	4.71742	0.266667	0.421053
train_MLP_b82a5_00002	TERMINATED	1e-05	1	2	1	4.99102	0.266667	0.421053
train_MLP_b82a5_00003	TERMINATED	1e-05	1	4	1	4.80002	0.400000	0.571429
train_MLP_b82a5_00004	TERMINATED	0.001	3	2	1	5.39796	0.666667	0.786325
train_MLP_b82a5_00005	TERMINATED	0.001	3	4	1	5.11316	0.333333	0.500000
train_MLP_b82a5_00006	TERMINATED	1e-05	3	2	1	5.30945	0.400000	0.571429
train_MLP_b82a5_00007	TERMINATED	1e-05	3	4	1	5.08326	0.333333	0.500000
train_MLP_b82a5_00008	TERMINATED	0.001	5	2	1	5.61105	0.666667	0.769231
train_MLP_b82a5_00009	TERMINATED	0.001	5	4	1	4.98850	0.666667	0.769231
train_MLP_b82a5_00010	TERMINATED	1e-05	5	2	1	5.62792	0.266667	0.421053
train_MLP_b82a5_00011	TERMINATED	1e-05	5	4	1	5.19684	0.333333	0.500000

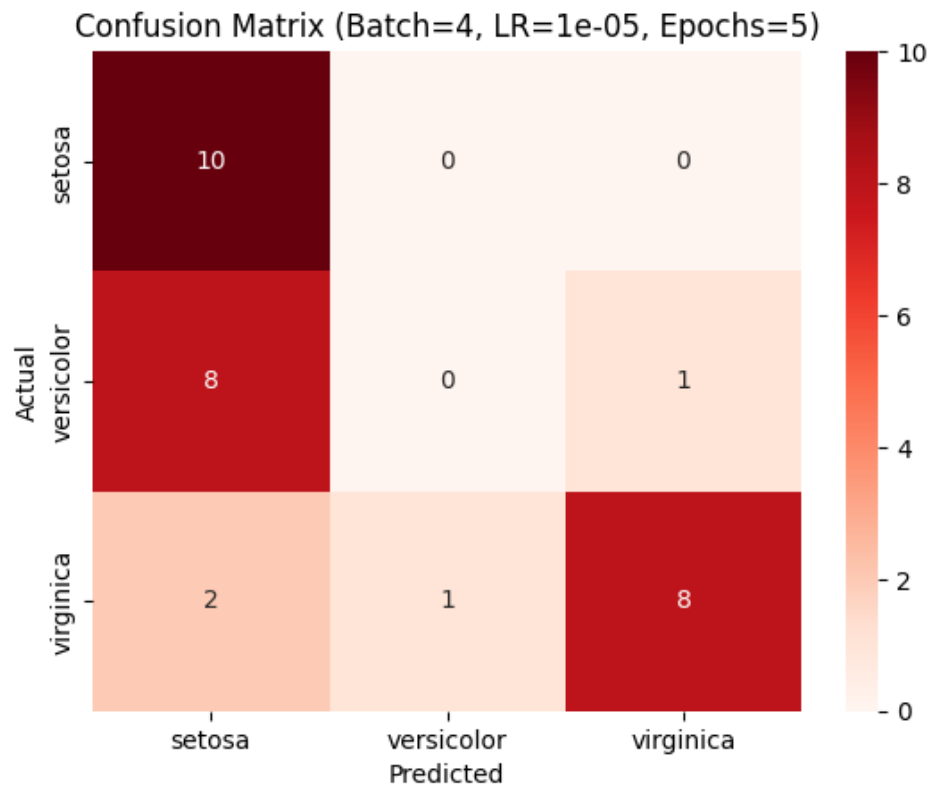
It took us a total of 61.94 secondsfor the computation in Grid Search

Best Configuration

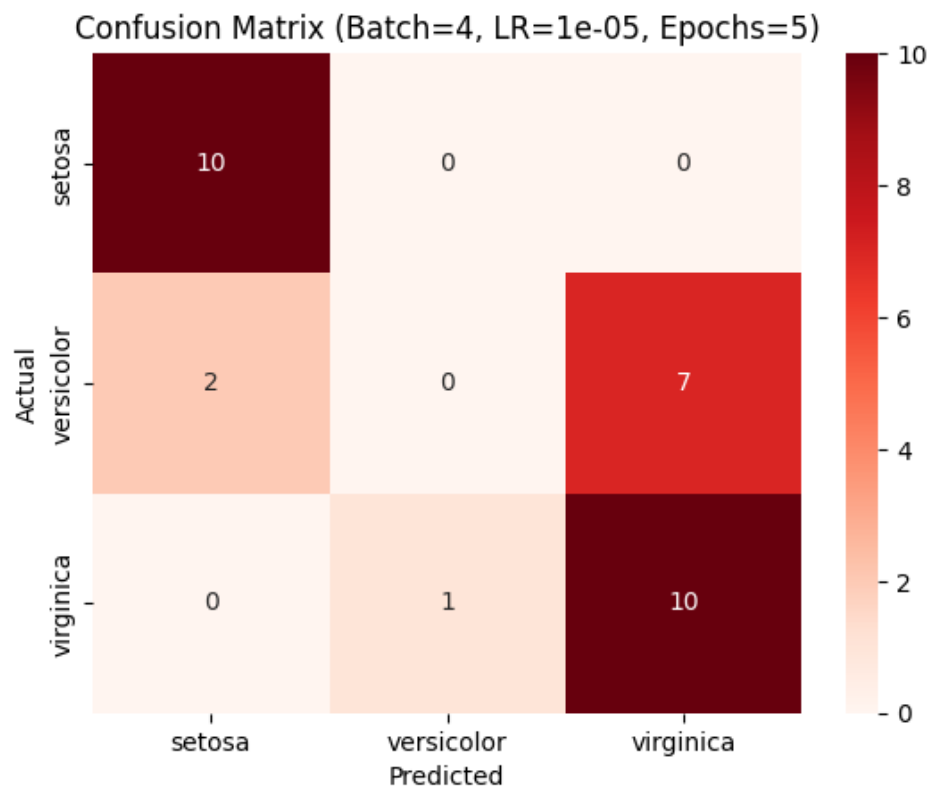
```
{  
  "lr": 0.001,  
  "num_epochs": 3,  
  "batch_size": 2  
}
```


Confusion Matrices of all models

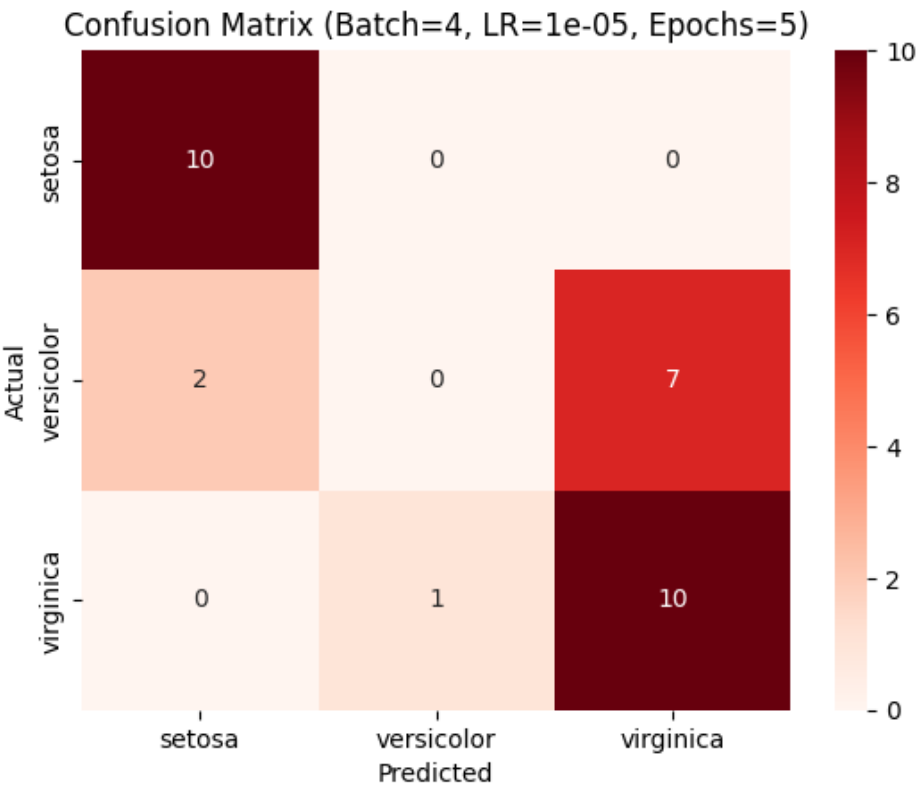
Model 1



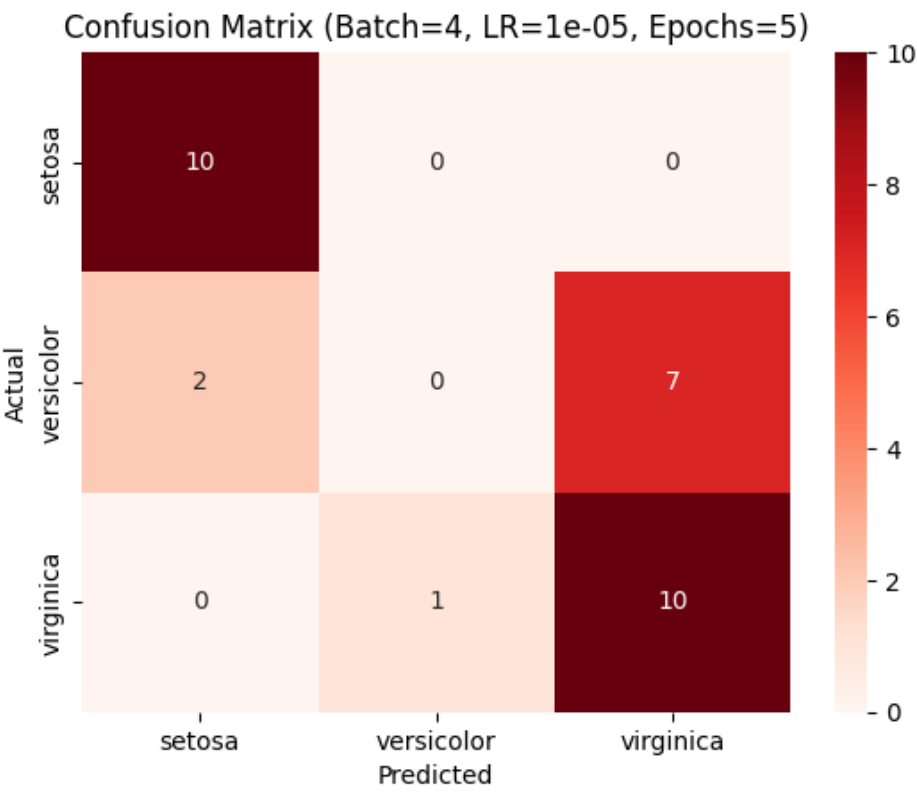
Model 2



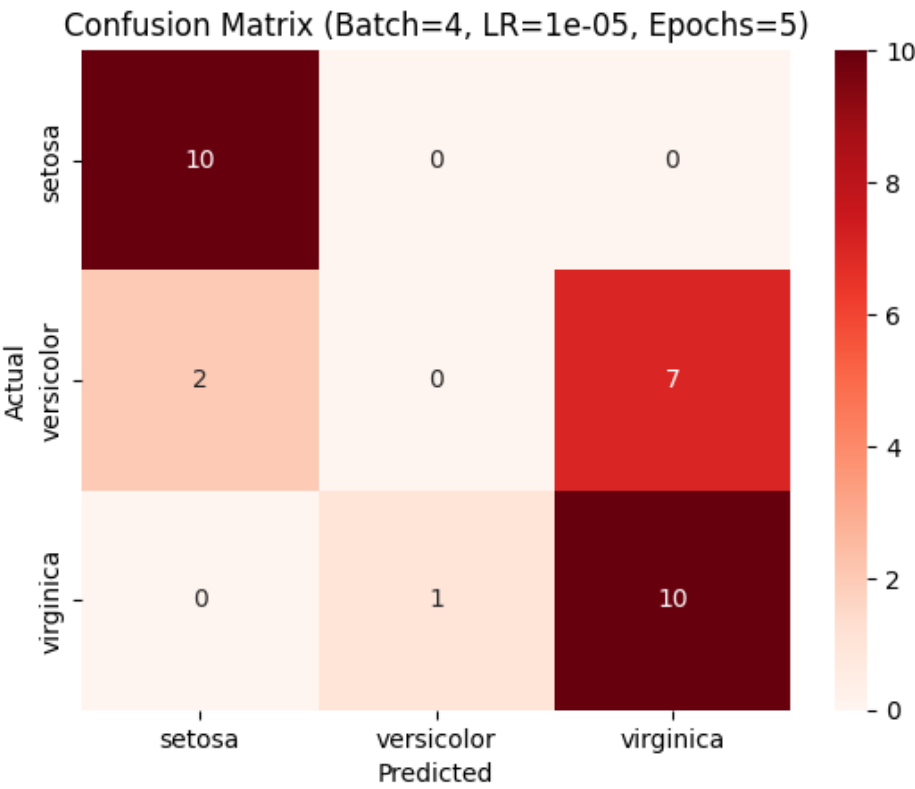
Model 3



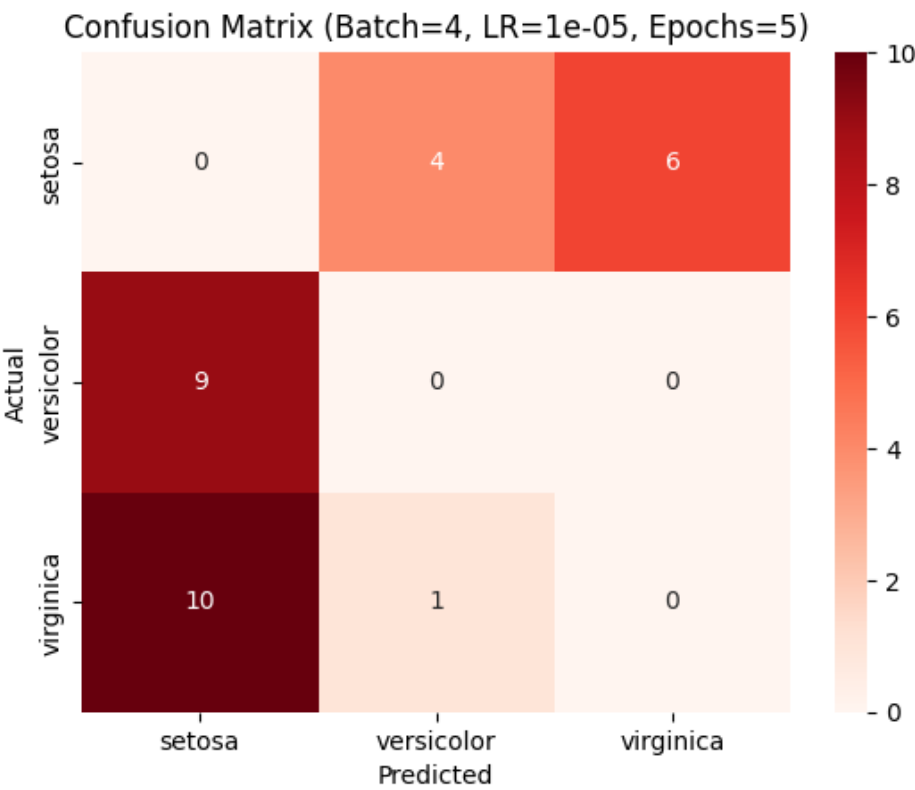
Model 4



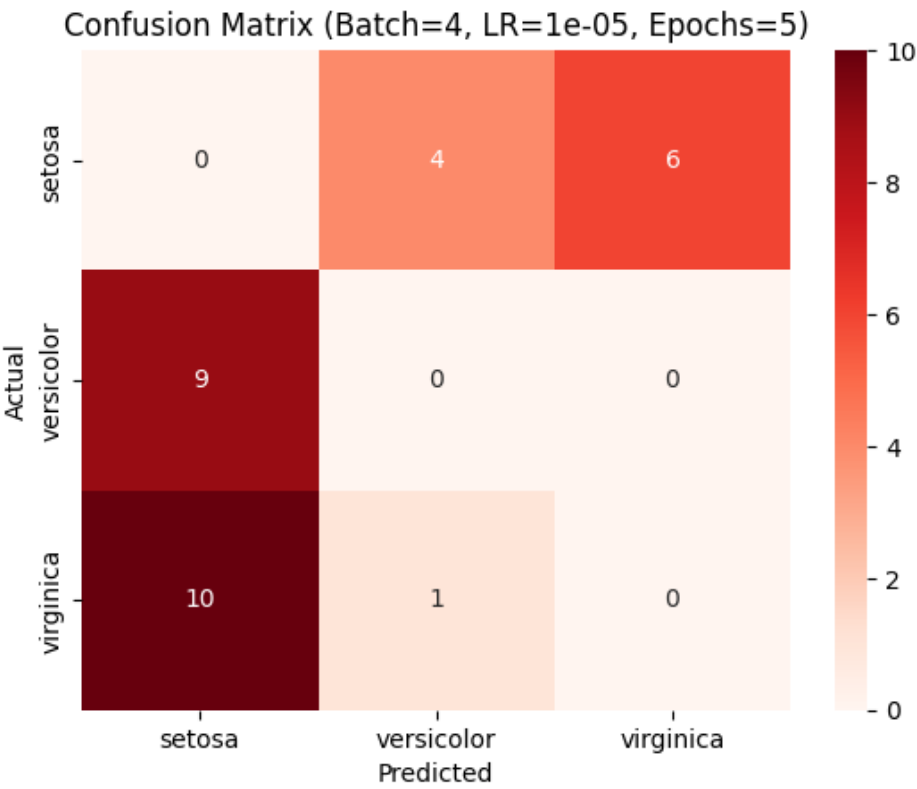
Model 5



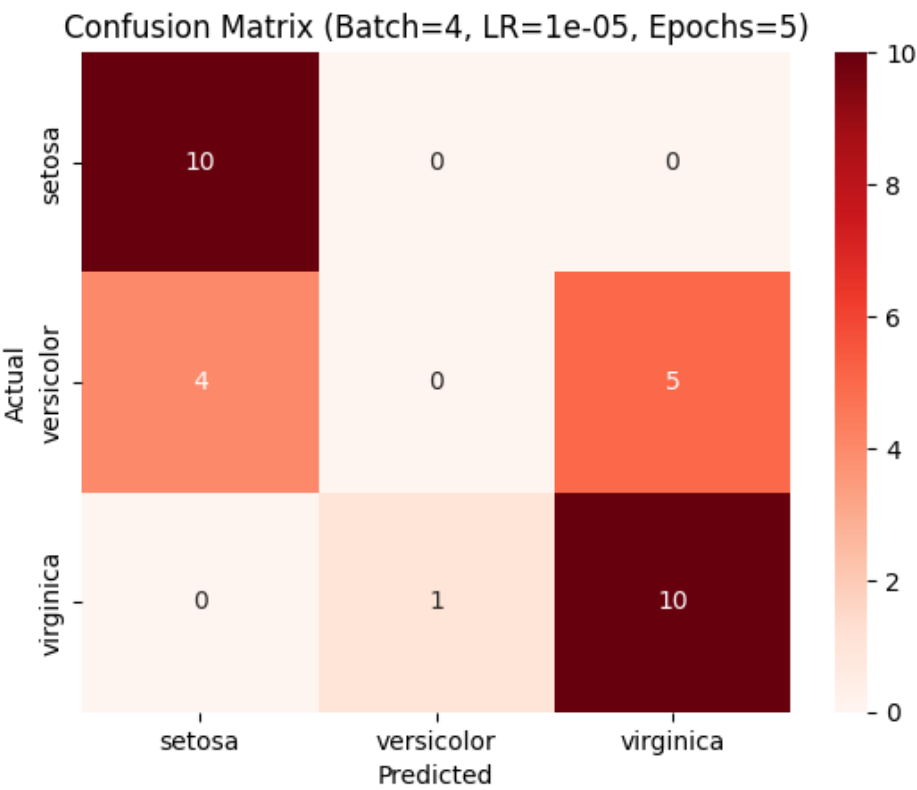
Model 6



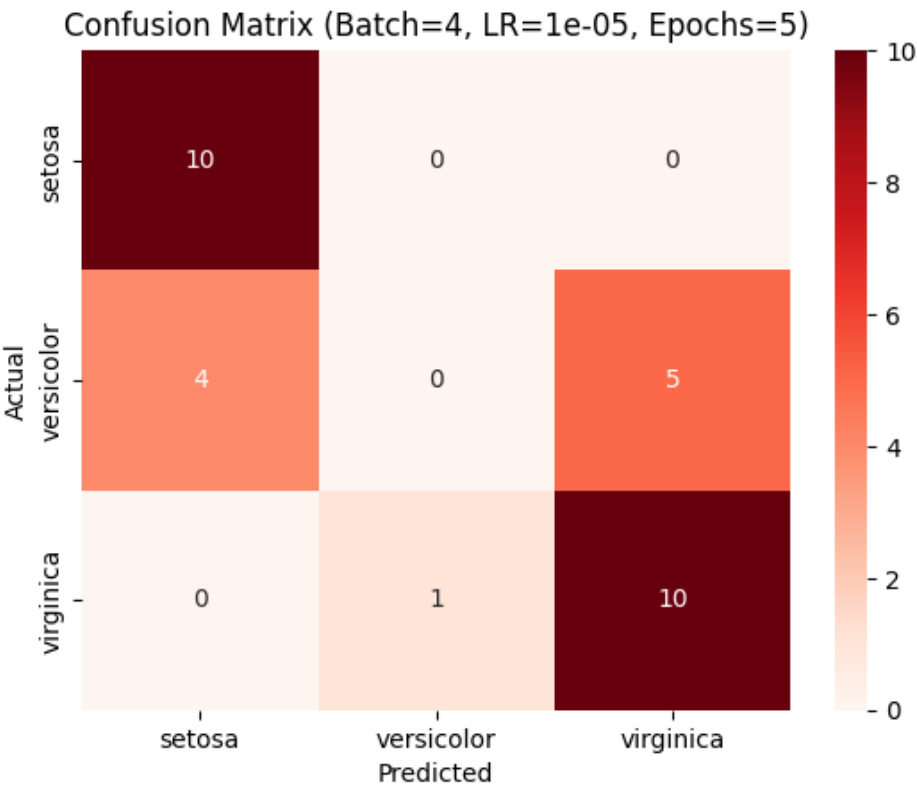
Model 7



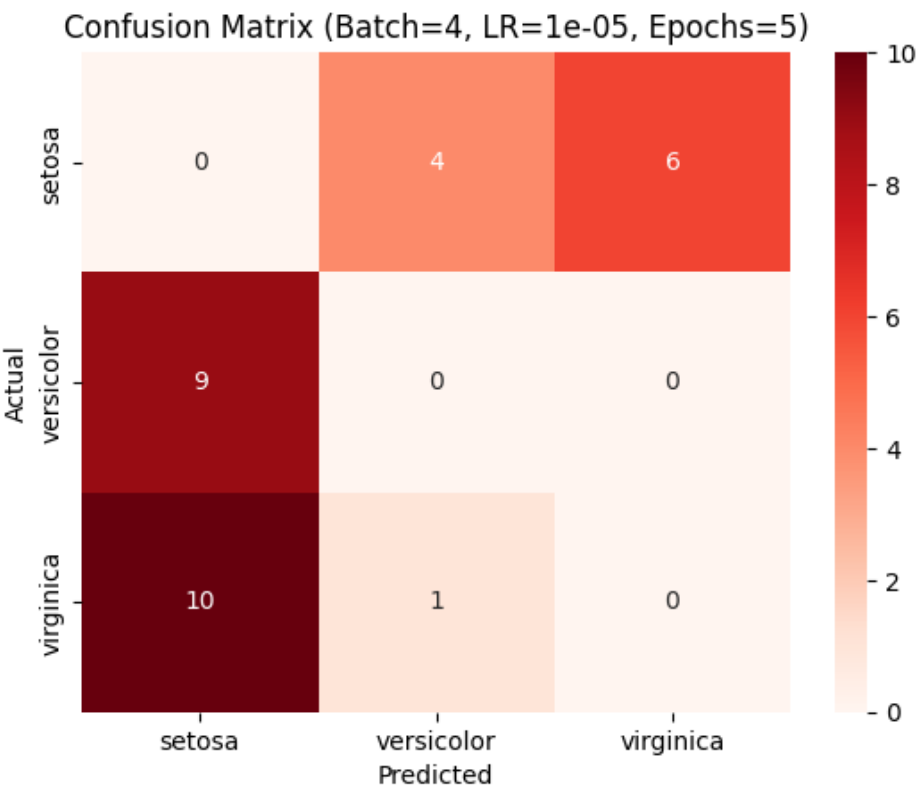
Model 8



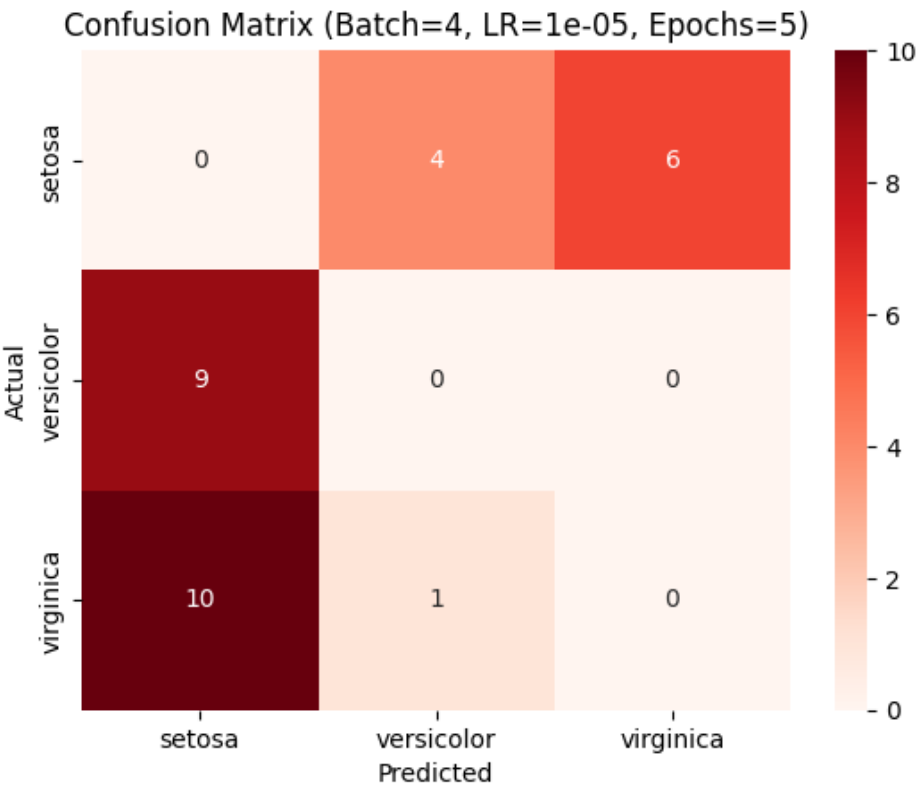
Model 9



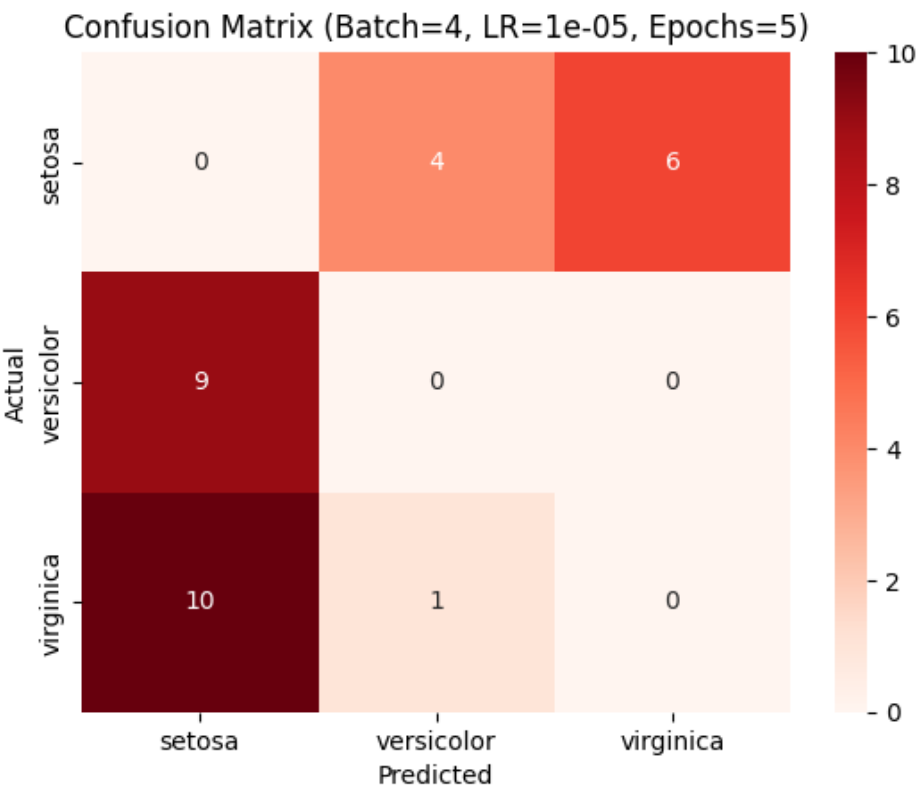
Model 10



Model 11

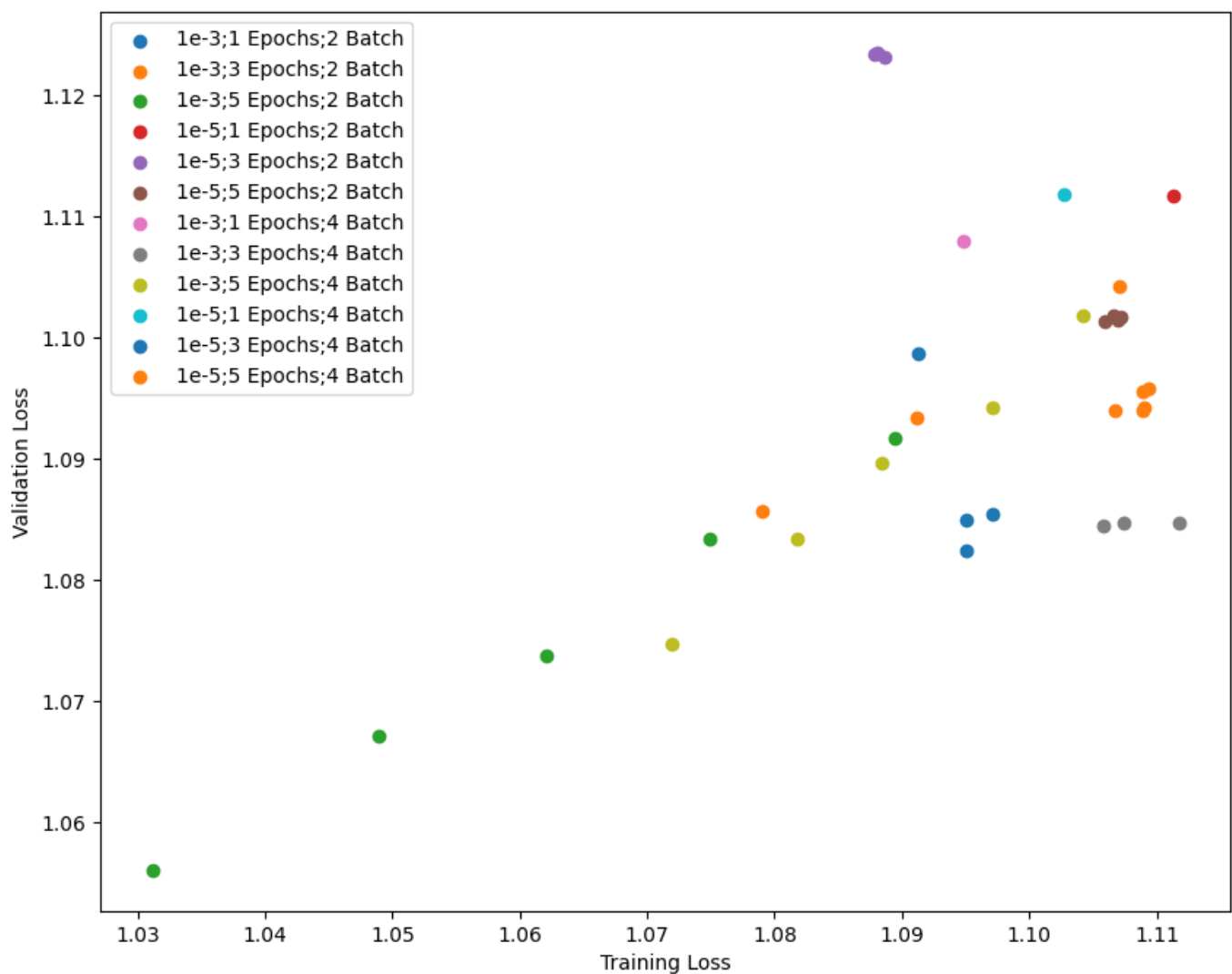


Model 12



Training Loss vs Validation Loss

Relationship between Training Loss and Validation Loss:



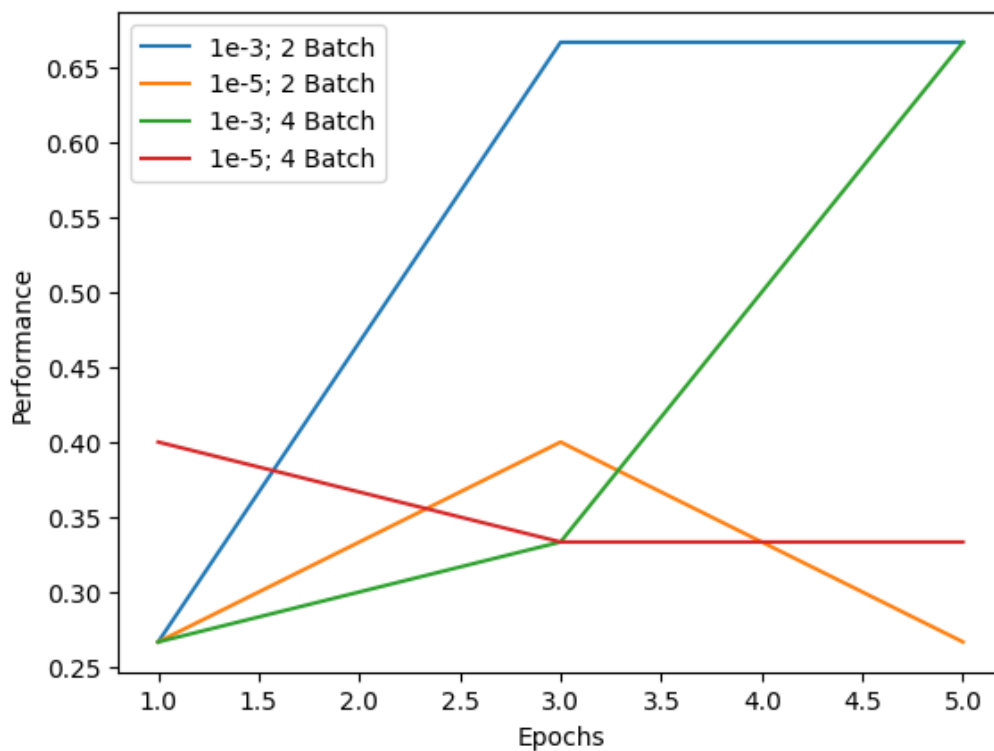
1. *Positive Correlation:* The plot suggests a general upward trend, indicating that as Training Loss increases, Validation Loss also increases.

2. *Hyperparameter Variations:*

- The legend categorizes different trials based on learning rate, number of epochs, and batch size.
- Different colors indicate different configurations, allowing for a clear comparison.

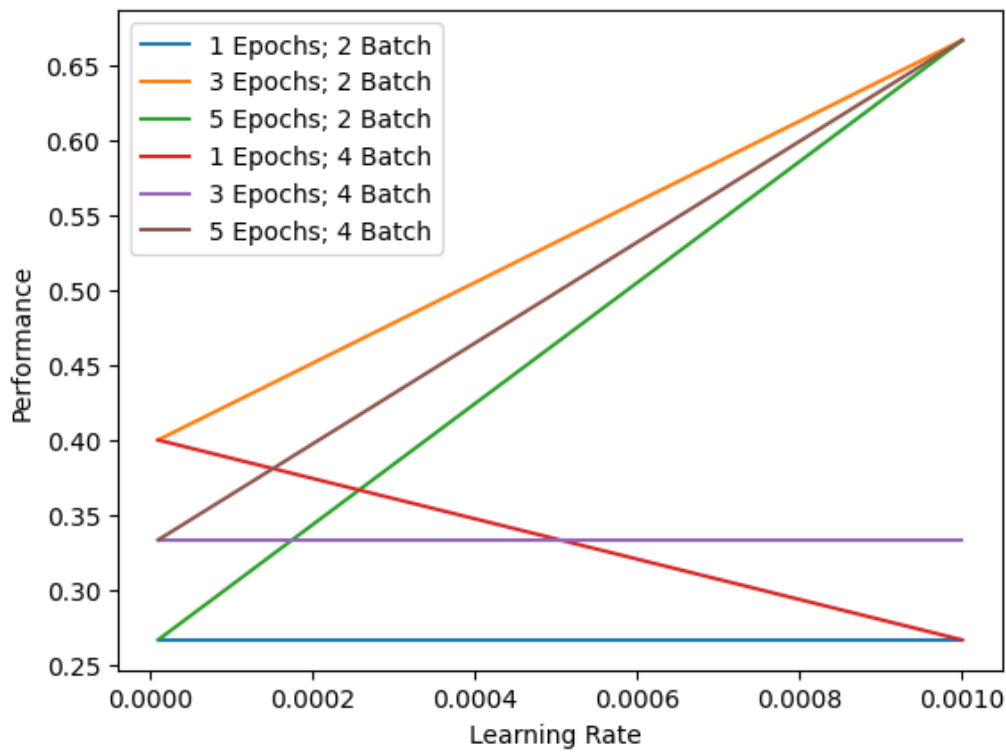
3. Trials with a higher learning rate (1e-3) and fewer epochs (1, 3) seem to have slightly lower losses compared to those with a smaller learning rate (1e-5).

Model Fluctuation with change in Epoch



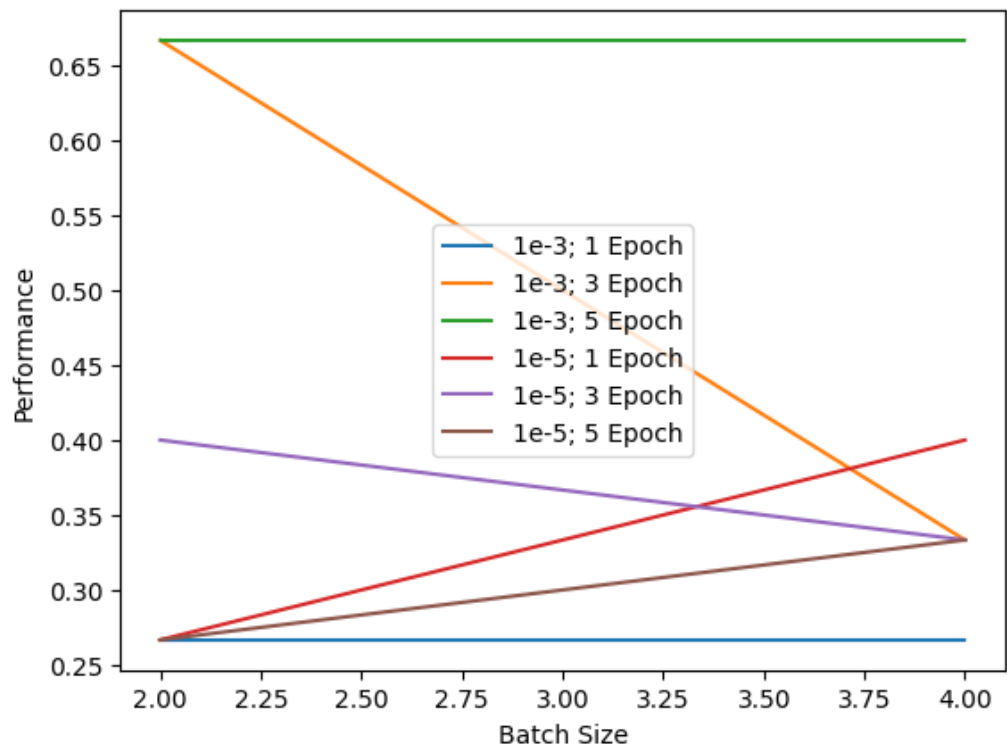
- Most configurations show an increase in performance during the initial epochs.
- This is because the model is learning key patterns from the dataset and optimizing its parameters.
- Higher learning rates (e.g., $1e-3$) lead to faster improvements in fewer epochs.
- Some models stabilize or plateau after a certain number of epochs, indicating that they have reached an optimal state for learning.

Model Fluctuation with change in Learning Rate



- **Inference:** As the learning rate increases, the performance of most configurations steadily improves.

Model Fluctuation with change in Batch Size



- **Inference:** As the batch size increases, the performance of most configurations have had **worsening**.

Random Search

We will do a random search using AutoGloun (backend: Ray Tuner and get the model parameters)

Search Space was defined as the following:

```
search_space = {
    "lr": tune.choice([1e-3, 1e-5]),
    "num_epochs": tune.choice([1,3,5]),
    "batch_size": tune.choice([2, 4])
}
```

Output

Trial Name	Status	Learning Rate	Epochs	Batch Size	Iterations	Total Time (s)	Accuracy	F1 Score
train_MLP_21169_00000	TERMINATED	1e-05	5	2	1	1.20604	0.266667	0.421053
train_MLP_21169_00001	TERMINATED	0.001	5	2	1	1.22789	0.466667	0.533333
train_MLP_21169_00002	TERMINATED	0.001	5	2	1	1.21297	0.666667	0.786325
train_MLP_21169_00003	TERMINATED	1e-05	1	2	1	1.09823	0.266667	0.421053
train_MLP_21169_00004	TERMINATED	0.001	3	2	1	1.03375	0.733333	0.828571
train_MLP_21169_00005	TERMINATED	0.001	1	2	1	0.999687	0.266667	0.421053
train_MLP_21169_00006	TERMINATED	1e-05	3	2	1	1.12087	0.266667	0.421053
train_MLP_21169_00007	TERMINATED	0.001	3	2	1	1.05694	0.4	0.56
train_MLP_21169_00008	TERMINATED	0.001	3	2	1	1.00531	0.333333	0.433333
train_MLP_21169_00009	TERMINATED	0.001	5	2	1	1.10407	0.266667	0.414815

Total Training Time: 11.066727 seconds

Best Configuration

```
{
  "lr": 0.001,
  "num_epochs": 3,
  "batch_size": 2
}
```

Hyperband Search

We will do a hyperband search using AutoGloun (backend: Ray Tuner; sheduler: HyperbandScheduler) and get the model parameters

Experiment Results

Trial Name	Status	Learning Rate	Epochs	Batch Size	Iterations	Total Time (s)	Accuracy	F1 Score
train_MLP_333f5_00000	TERMINATED	0.001	5	4	1	1.14064	0.266667	0.369231
train_MLP_333f5_00001	TERMINATED	1e-05	3	2	1	1.12037	0.266667	0.421053
train_MLP_333f5_00002	TERMINATED	1e-05	3	2	1	1.05419	0.333333	0.5
train_MLP_333f5_00003	TERMINATED	0.001	5	4	1	1.11868	0.666667	0.769231
train_MLP_333f5_00004	TERMINATED	1e-05	5	4	1	1.06551	0.733333	0.828571
train_MLP_333f5_00005	TERMINATED	1e-05	5	4	1	1.00337	0.4	0.571429
train_MLP_333f5_00006	TERMINATED	1e-05	3	2	1	1.03871	0.466667	0.577143
train_MLP_333f5_00007	TERMINATED	0.001	3	4	1	1.04353	0.333333	0.5
train_MLP_333f5_00008	TERMINATED	1e-05	5	2	1	1.31153	0.4	0.571429
train_MLP_333f5_00009	TERMINATED	1e-05	5	2	1	1.19259	0.333333	0.5
train_MLP_333f5_00010	TERMINATED	1e-05	5	4	1	1.08369	0.266667	0.421053
train_MLP_333f5_00011	TERMINATED	1e-05	1	4	1	0.930045	0.333333	0.5
train_MLP_333f5_00012	TERMINATED	0.001	5	2	1	1.23356	0.666667	0.769231
train_MLP_333f5_00013	TERMINATED	1e-05	5	2	1	1.18108	0.666667	0.769231
train_MLP_333f5_00014	TERMINATED	1e-05	1	4	1	0.904613	0.333333	0.5
train_MLP_333f5_00015	TERMINATED	0.001	1	4	1	0.992929	0.333333	0.428571
train_MLP_333f5_00016	TERMINATED	1e-05	5	2	1	1.17069	0.333333	0.5
train_MLP_333f5_00017	TERMINATED	0.001	1	2	1	1.12946	0.333333	0.5
train_MLP_333f5_00018	TERMINATED	0.001	5	2	1	1.45521	0.666667	0.769231
train_MLP_333f5_00019	TERMINATED	1e-05	5	2	1	1.18111	0.733333	0.828571

Total Training Time: 22.361398 seconds

Best Configuration

```
{
  "lr": 1e-05,
  "num_epochs": 5,
  "batch_size": 4
}
```

Baysiean Search

We will do a hyperband search using AutoGloun (backend: Ray Tuner; alogorithm: BayesOptSearch) and get the model parameters

Configuration for experiment	train_MLP_2025-02-26_13-51-12
Search algorithm	SearchGenerator
Scheduler	FIFOScheduler
Number of trials	5

Results

Trial Name	Status	Learning Rate	Num Epochs	Batch Size	Iter	Total Time (s)	Accuracy	F1 Score
train_MLP_f7c966ac	TERMINATED	5.88e-05	4	3	1	1.10065	0.266667	0.421053
train_MLP_571a3499	TERMINATED	0.000846	2	4	1	1.0377	0.533333	0.636257
train_MLP_18973f21	TERMINATED	0.000142	4	3	1	1.19837	0.266667	0.421053
train_MLP_494594e3	TERMINATED	0.000980	5	4	1	1.10084	0.266667	0.421053
train_MLP_505568a9	TERMINATED	0.000790	2	4	1	0.997634	0.666667	0.786325

Best Config:

```
{
  "lr": 0.0007897842804285067,
  "num_epochs": 2,
  "batch_size": 4
}
```

Run Time: 5.44s

Hyperparameter Tuning Results

Comparison of Different Tuning Methods

Method	Learning Rate	Num Epochs	Batch Size	Accuracy	F1 Score	Time (s)	Trials
Bayesian	0.00079	2	4	0.666667	0.786325	5.44	5
Hyperband	0.00001	5	2	0.733333	0.828571	22.36	20 (Forced)
Random	0.00100	3	2	0.733333	0.828571	11.06	10 (Forced)
Grid	0.00100	3	2	0.733333	0.828571	61.94	12

Manual Tuning vs. Automated Search

Automated search methods like **Bayesian optimization, Hyperband, and Grid Search** systematically explore hyperparameters, leading to better accuracy and efficiency.

- **Bayesian optimization** achieves high accuracy in less time, making it efficient.
- **Hyperband and Random Search** can find optimal configurations but the number of trials required is not known before hand.
- **Grid Search** is exhaustive but very time-consuming.