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Classifying the Iris Data Set with PyTorch

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In this short article we will have a look on how to use [PyTorch](#) with the Iris data set. We will create and train a neural network with [Linear](#) layers and we will employ a [Softmax](#) activation function and the [Adam](#) optimizer.



Data Preperation

To prepare the data, we will use a `StandardScaler` to remove the mean and scale the features to unit variance. Finally we want to perform a `train test split` to compare our results later on.

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

plt.style.use('ggplot')

from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

iris = load_iris()
X = iris['data']
y = iris['target']
names = iris['target_names']
feature_names = iris['feature_names']

# Scale data to have mean 0 and variance 1
# which is importance for convergence of the neural network
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)

# Split the data set into training and testing
X_train, X_test, y_train, y_test = train_test_split(
    X_scaled, y, test_size=0.2, random_state=2)
```

Visualize the Data

Let's take a look at our data to see what we are dealing with.

```
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(16, 6))
for target, target_name in enumerate(names):
    X_plot = X[y == target]
    ax1.plot(X_plot[:, 0], X_plot[:, 1],
             linestyle='none',
             marker='o',
             label=target_name)
ax1.set_xlabel(feature_names[0])
ax1.set_ylabel(feature_names[1])
ax1.axis('equal')
ax1.legend();

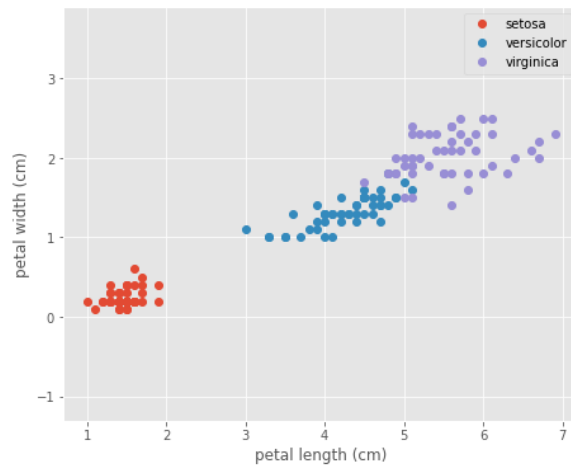
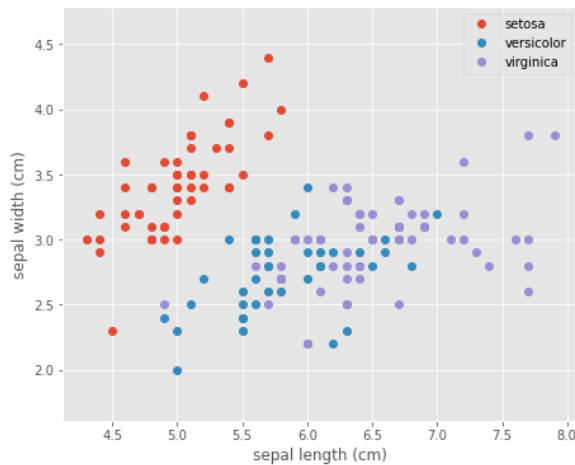
for target, target_name in enumerate(names):
    X_plot = X[y == target]
    ax2.plot(X_plot[:, 2], X_plot[:, 3],
```



```

        linestyle='none',
        marker='o',
        label=target_name)
ax2.set_xlabel(feature_names[2])
ax2.set_ylabel(feature_names[3])
ax2.axis('equal')
ax2.legend();

```



Configure Neural Network Models

```

import torch
import torch.nn.functional as F
import torch.nn as nn
from torch.autograd import Variable

```

```

class Model(nn.Module):
    def __init__(self, input_dim):
        super(Model, self).__init__()
        self.layer1 = nn.Linear(input_dim, 50)
        self.layer2 = nn.Linear(50, 50)
        self.layer3 = nn.Linear(50, 3)

    def forward(self, x):
        x = F.relu(self.layer1(x))
        x = F.relu(self.layer2(x))
        x = F.softmax(self.layer3(x), dim=1)
        return x

```

```

model = Model(X_train.shape[1])
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
loss_fn = nn.CrossEntropyLoss()
model

```

```

Model(
  (layer1): Linear(in_features=4, out_features=50, bias=True)
  (layer2): Linear(in_features=50, out_features=50, bias=True)

```



```
(layer3): Linear(in_features=50, out_features=3, bias=True)
)
```

Train the Model

Now its time to run the training. In order to track progress more efficiently, we can use `tqdm`, which is a great and easy to use progress bar for our training epochs.

```
import tqdm

EPOCHS = 100
X_train = Variable(torch.from_numpy(X_train)).float()
y_train = Variable(torch.from_numpy(y_train)).long()
X_test = Variable(torch.from_numpy(X_test)).float()
y_test = Variable(torch.from_numpy(y_test)).long()

loss_list = np.zeros((EPOCHS,))
accuracy_list = np.zeros((EPOCHS,))

for epoch in tqdm.trange(EPOCHS):
    y_pred = model(X_train)
    loss = loss_fn(y_pred, y_train)
    loss_list[epoch] = loss.item()

    # Zero gradients
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    with torch.no_grad():
        y_pred = model(X_test)
        correct = (torch.argmax(y_pred, dim=1) == y_test).type(torch.FloatTensor)
        accuracy_list[epoch] = correct.mean()
```

```
100%|██████████| 100/100 [00:00<00:00, 407.99it/s]
```

Plot Accuracy and Loss from Training

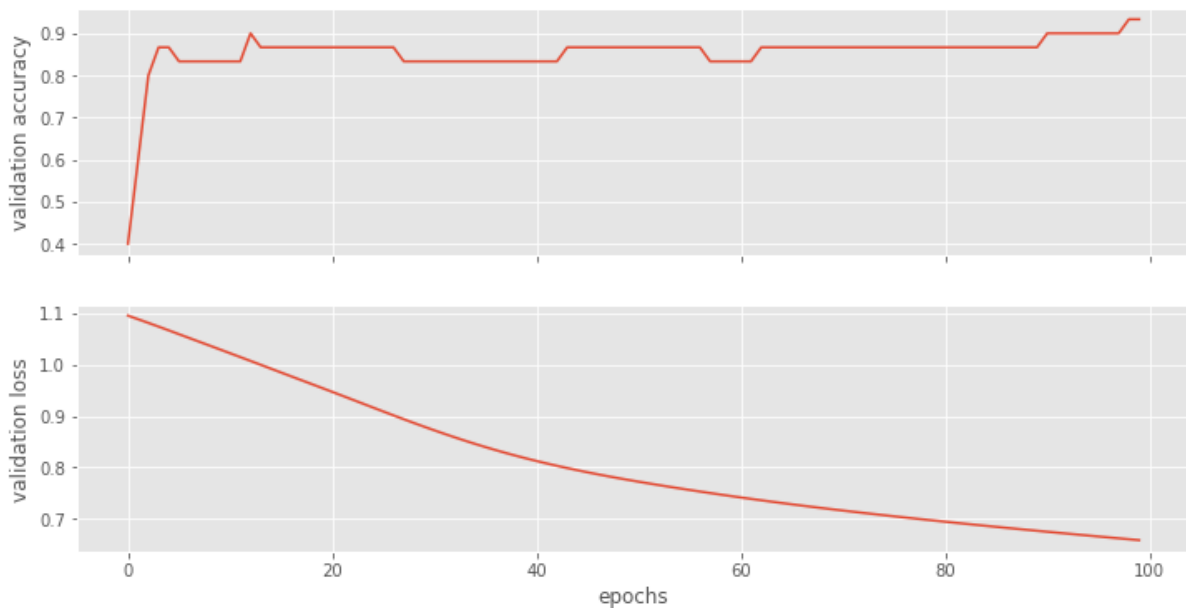
Let's have a look how our models perform. We can clearly see that adding more nodes makes the training perform better.

```
fig, (ax1, ax2) = plt.subplots(2, figsize=(12, 6), sharex=True)

ax1.plot(accuracy_list)
```



```
ax1.set_ylabel("validation accuracy")
ax2.plot(loss_list)
ax2.set_ylabel("validation loss")
ax2.set_xlabel("epochs");
```



Show ROC Curve

We have previously split the data and we can compare now with the **Receiver Operating Characteristic (ROC)** how well the models perform. The ROC plot compares the false positive rate with the true positive rate. We additionally compute for each model the **Area under the curve (AUC)**, where $auc = 1$ is perfect classification and $auc = 0.5$ is random guessing (for a two class problem). To prepare the test data, we need to use the **OneHotEncoder** to encode the integer features into a **One-hot** vector which we then flatten with `numpy.ravel()` for `sklearn.metrics.roc_curve()`.

```
from sklearn.metrics import roc_curve, auc
from sklearn.preprocessing import OneHotEncoder

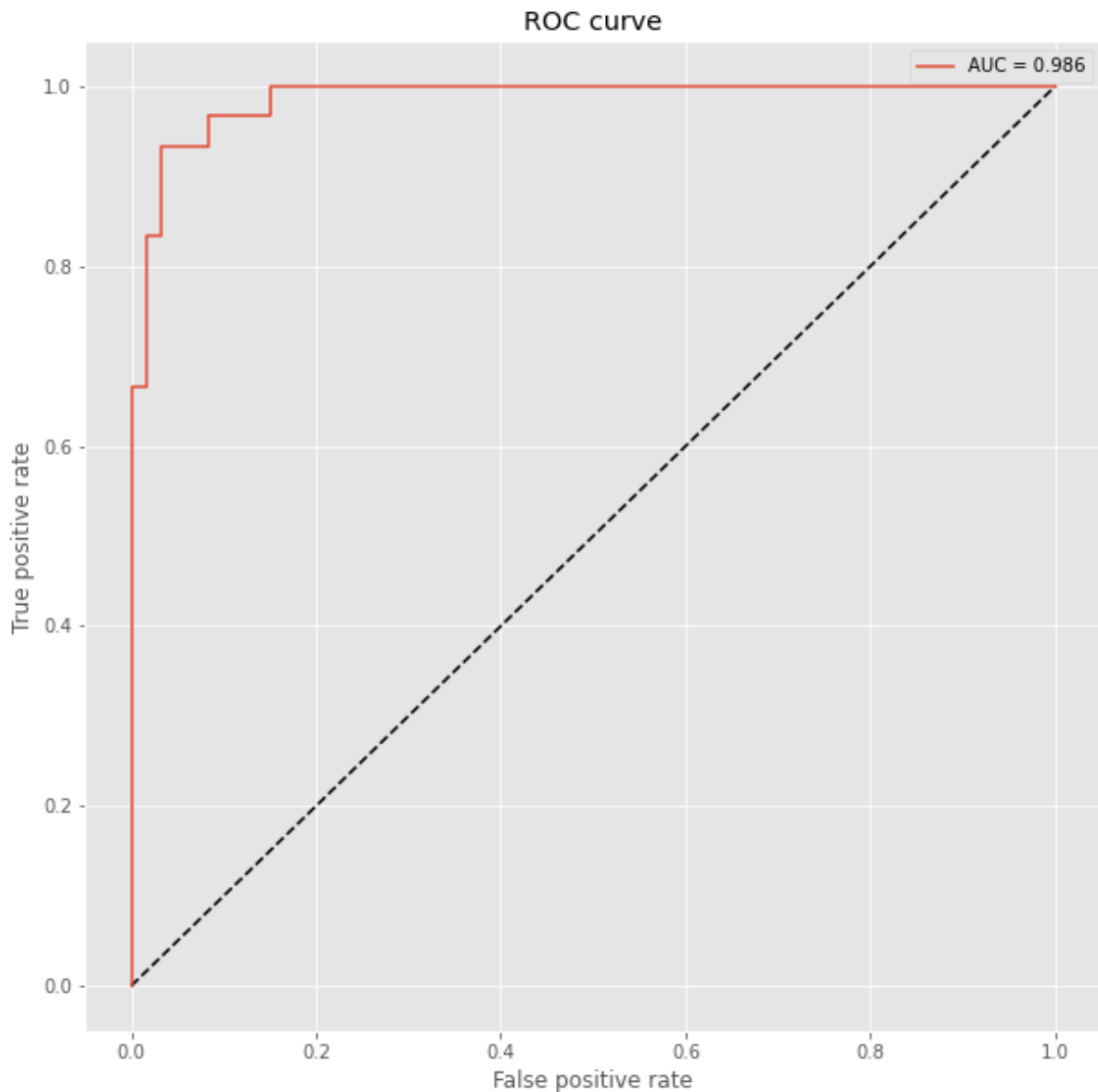
plt.figure(figsize=(10, 10))
plt.plot([0, 1], [0, 1], 'k--')

# One hot encoding
enc = OneHotEncoder()
Y_onehot = enc.fit_transform(y_test[:, np.newaxis]).toarray()

with torch.no_grad():
    y_pred = model(X_test).numpy()
    fpr, tpr, threshold = roc_curve(Y_onehot.ravel(), y_pred.ravel())
```



```
plt.plot(fpr, tpr, label='AUC = {:.3f}'.format(auc(fpr, tpr)))  
plt.xlabel('False positive rate')  
plt.ylabel('True positive rate')  
plt.title('ROC curve')  
plt.legend();
```



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