

LAB 2 (Part 2): MULTI-LAYER PERCEPTRONS (MLP)

University of Washington, Seattle

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OUTLINE

Part 1: Introduction to MLP

- Shallow vs Deep Networks
- Regression vs Classification
- Outputting Probabilities with Softmax Function

Part 2: Additional Data Prep Methods

- Training/Validation/Test sets
- One-hot encoding

Part 3: Stochastic Gradient Descent

- SGD, Mini-batch GD, Batch GD
- Implementing variants of Gradient Descent

Part 4: Additional Hyperparameters & Regularizers

- Activation functions
- Loss functions and Advanced Optimizers
- Regularizers
- Batch Normalization
- Weight initializations

Part 5: Training Fully Connected Deep Network

Iris Classification Example

Lab Assignment

- MNIST Classification using MLP
- Tips for Training Your Model



INTRODUCTION TO MLP

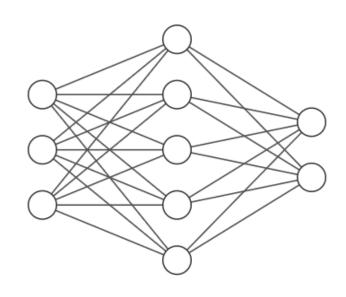
Shallow vs Deep Networks

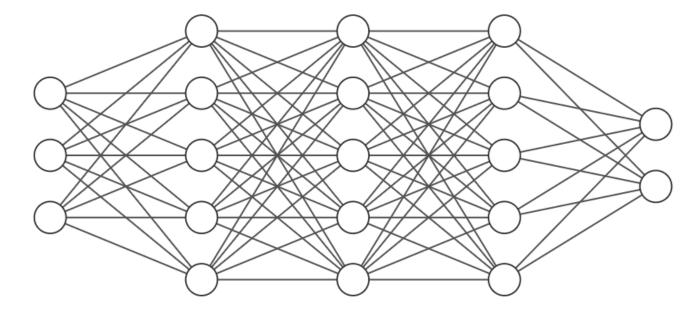
Regression vs Classification

Outputting Probabilities with Softmax Function



Shallow vs Deep Networks





Shallow Networks

One hidden layer

Universal function approximator

(with enough hidden neurons)

Easier to train

Fit for simple problems

Deep Networks

≥1 hidden layer

Upper hidden neurons reuse lower-level features

Can approximate more complex & general functions

Harder to train

Fit for more complex problems



Regression vs Classification

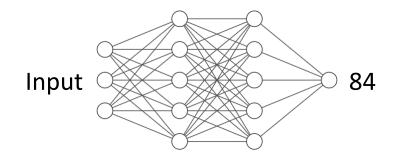
Regression



What will be the temperature tomorrow?



Fahrenheit



Classification

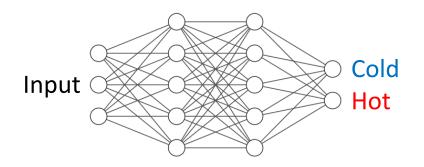


Will it be hot or cold tomorrow?



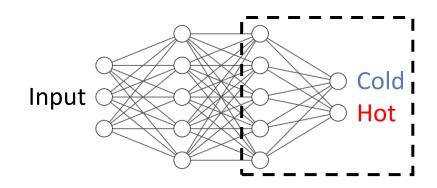
Fahrenheit

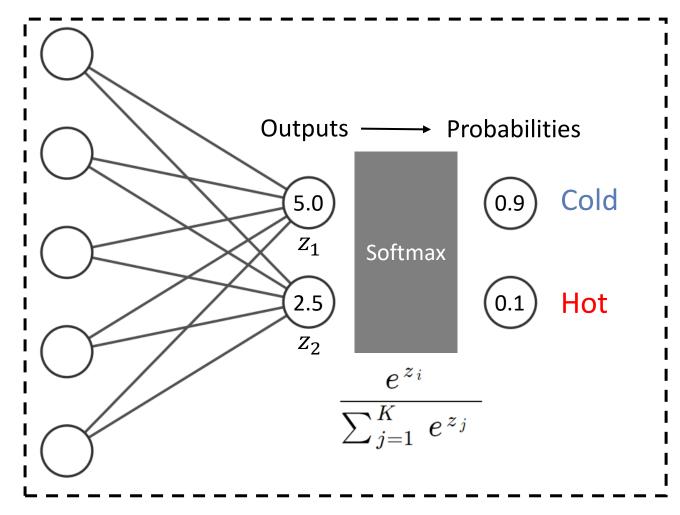
Image credit: Towards Data Science





Outputting Probabilities with Softmax Function





torch.nn.Softmax()



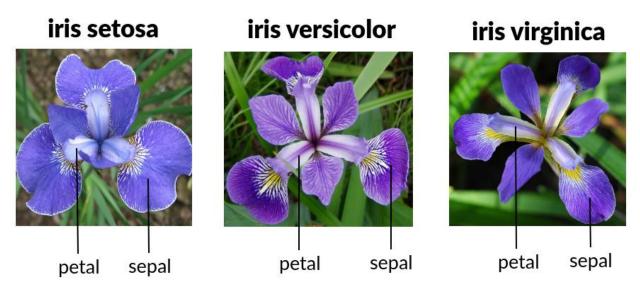
ADDITIONAL DATA PREP METHODS

Training/Validation/Test Sets

One-Hot Encoding



Iris Dataset



SepalLengthCm SepalWidthCm PetalLengthCm PetalWidthCm Species 5.1 3.5 Iris-setosa 4.9 3.0 Iris-setosa 3.2 Iris-setosa 1.5 Iris-setosa 5.0 Iris-setosa 5.4 Iris-setosa 4.6 Iris-setosa 5.0 1.5 Iris-setosa 2.9 1.4 4.4 Iris-setosa 10 3.1 4.9 1.5 Iris-setosa

Features

- 150 samples
- 4 features/sample
 - Sepal length (cm)
 - Sepal width (cm)
 - Petal length (cm)
 - Petal width (cm)
- 3 labels
 - Iris setosa (0)
 - Iris versicolor (1)
 - Iris virginica (2)

Labels (Targets)



Train/Validation/Test Split

```
1 from sklearn.datasets import load iris
  from sklearn.preprocessing import StandardScaler
   from sklearn.model_selection import train_test_split
   iris = load iris()
  X = iris['data']
   y = iris['target']
   scaler = StandardScaler()
   X scaled = scaler.fit transform(X)
12
   X_train, X_test, y_train, y_test = train_test_split(X_scaled, y,
                           Testing data ratio (0.2 = 20\%) \leftarrow test_size=0.2,
14
                        Random seed to use for splitting ← random_state=2)
15
16
   X_validation = X_train[:int(len(X_test))]
   y validation = y train[:int(len(X test))]
19
  X train = X train[int(len(X test)):]
21 y_train = y_train[int(len(X_test)):]
```

Load Iris dataset

Extract features (X) and target labels (y)

Scale features using scikit-learn provided standard scaler

Split the dataset into Training (80%) and Testing (20%)

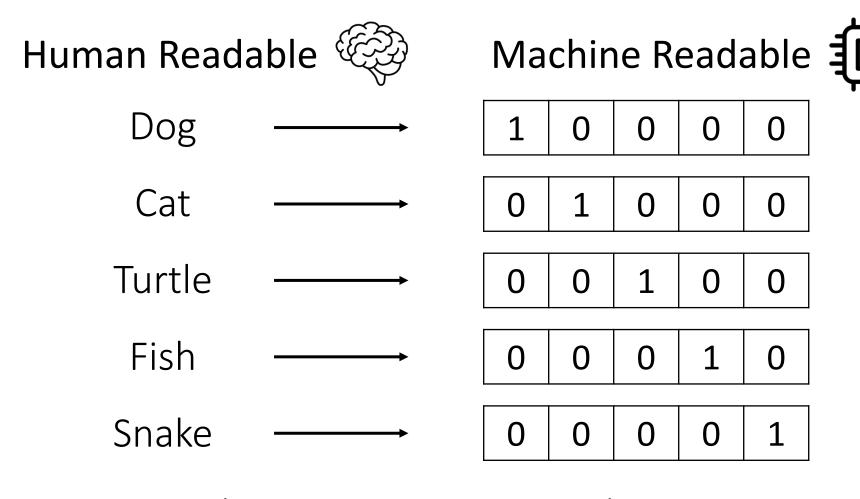
Assign subset of the training dataset as validation data (same size as testing)

Use the remaining dataset as training

Final split ratios = Training: 60%, Testing: 20%, Validation: 20%



One-hot Encoding



Categorical Data

One-hot vectors



One-hot Encoding

Official function documentation:

https://pytorch.org/docs/stable/generated/torch.nn.functional.one_hot.html

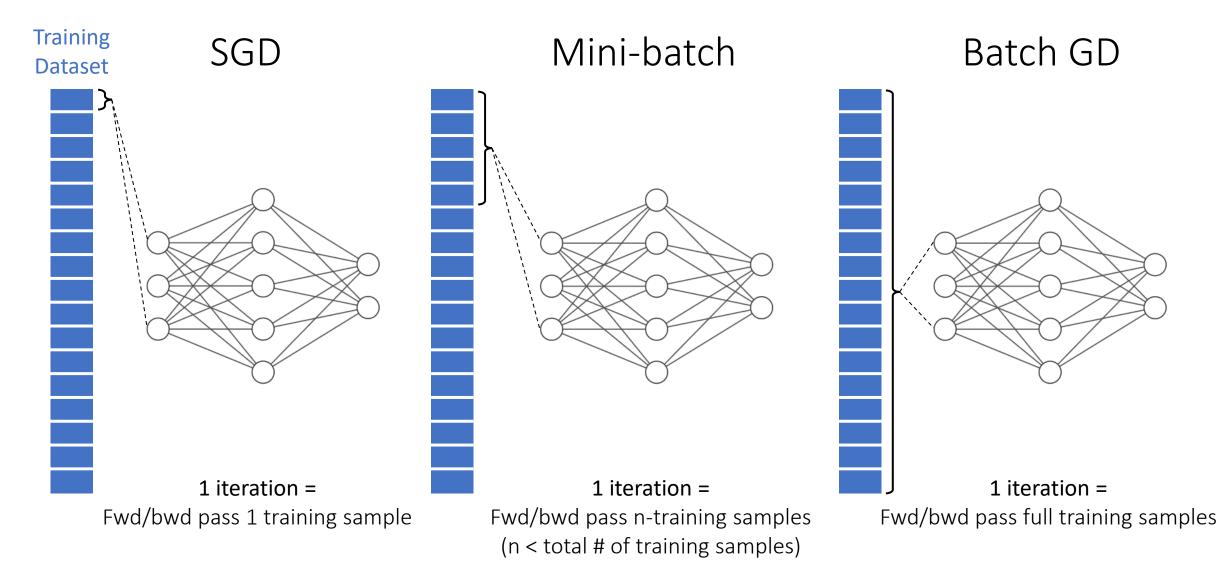


STOCHASTIC GRADIENT DESCENT

SGD, Mini-batch GD, Batch GD



Variants of Gradient Descent





Implementing Variants of Gradient Descent

SGD

For epoch in range(epochs)

For sample in train

Training loop

- zero_grad
- fwd pass input
- compute loss
- backpropagation
- update weights/biases

Mini-batch

For epoch in range(epochs)

For mini-batch in train

Training Loop

Batch GD

For epoch in range(epochs)

Training Loop

Total # of Epochs × m iterations (m =total # of samples in training)

Epochs \times R (R = m/mini-batch size)

Epochs



ADDITIONAL HYPER-PARAMETERS &

REGULARIZERS

Activation Functions

Loss Functions and Advanced Optimizers

Regularizers

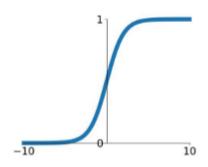
Batch Normalization

Network Initialization



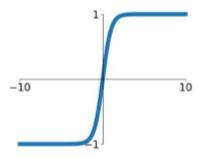
Activation Functions





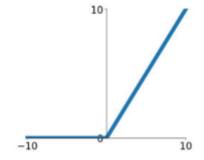
torch.nn.functional.sigmoid()

Tanh



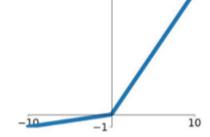
torch.nn.functional.tanh()

ReLU



torch.nn.functional.relu()

Leaky ReLU



torch.nn.functional.leaky_relu()



Activation Functions

```
class Model(torch.nn.Module):
 2
       def init (self, input dim, output dim):
            super(Model, self). init ()
            self.layer1 = torch.nn.Linear(input dim, 5)
           self.layer2 = torch.nn.Linear(5, 5)
            self.layer3 = torch.nn.Linear(5, output dim)
10
       def forward(self, x):
11
12
           out1 = torch.nn.functional.relu(self.layer1(x))
13
           out2 = torch.nn.functional.relu(self.layer2(out1))
14
           output = torch.nn.functional.softmax(self.layer3(out2), dim=1)
15
16
            return output
17
```

Apply ReLU activation function to outputs of layer1 and 2



Loss Functions

Regression

Mean Squared Error
$$MSE = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$
 torch.nn.MSELoss()

Classification

Cross Entropy
$$L_{\text{CE}} = -\sum_{i=1}^{n} t_i \log(p_i)$$
 torch.nn.CrossEntropyLoss()

NOTE: torch.nn.CrossEntropyLoss() automatically implements one-hot encoding and softmax when providing integer labels as targets.



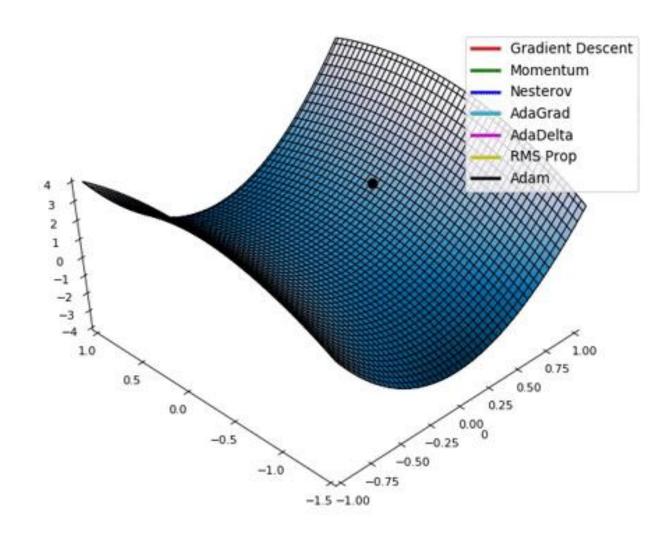
Advanced Optimizers

Gradient Descent torch.optim.SGD()

Adam torch.optim.Adam()

RMS Prop torch.optim.RMSprop()

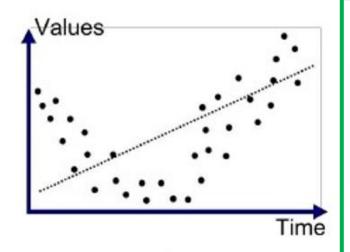
Ada Delta torch.optim.Adadelta()



More Optimizers: https://pytorch.org/docs/stable/optim.html

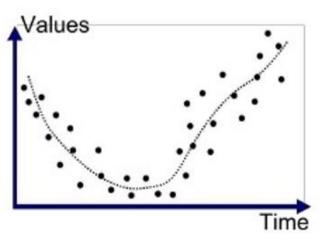


Avoiding Overfitting with Regularization



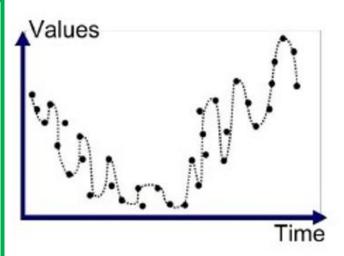
Underfitted

Bad training accuracy Bad testing accuracy



Good Fit/Robust

Good training accuracy
Good testing accuracy



Overfitted

Great training accuracy
Bad testing accuracy



L1, L2 Regularizations in PyTorch

L1 Regularization

$$Loss = Error(y, \hat{y}) + \lambda \sum_{i=1}^{N} |w_i|$$

L2 Regularization

$$Loss = Error(y, \hat{y}) + \lambda \sum_{i=1}^{N} w_i^2$$

Penalizes sum of absolute values of weights

Results in a sparse model

Not suitable for learning complex patterns

Robust to outliers

Penalizes sum of squared values of weights

Results in a dense model

Learns complex patterns

Sensitive to outliers



L1, L2 Regularizations in PyTorch

L1

```
1  l1_penalty = torch.nn.L1Loss(size_average=False)
2  reg_loss = 0
3
4  for param in model.parameters():
5     reg_loss += l1_penalty(param)
7     lambda_ = 0.9
9  loss += lambda_ * reg_loss
```

Loop through model parameters to compute L1 regularization term

Pick the lambda value

Add the L1 term to loss during training

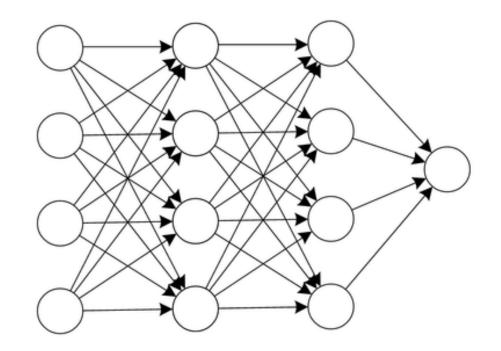
L2

```
1 optimizer = torch.optim.SGD(model.parameters(), lr=0.001, weight_decay=0.9)
```

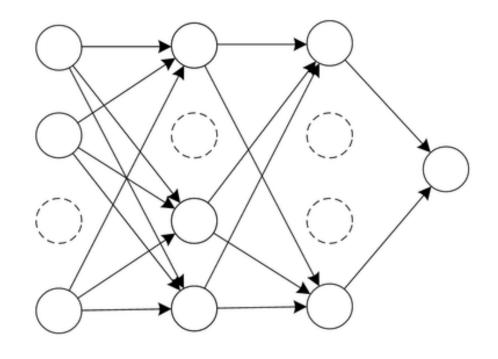
weight_decay sets lambda value for L2 regularization term



Dropout Regularization in PyTorch



Standard Neural Network



Network with Dropout

Srivastava et al 2014 (~35000 citations!)

Dropout forces the network to learn more robust features + different random subsets of other neurons



Dropout Regularization in PyTorch

```
class Model(torch.nn.Module):
       def __init__(self, input_dim, output_dim):
 3
           super(Model, self).__init__()
 5
 6
           self.layer1 = torch.nn.Linear(input_dim, 5)
           self.layer2 = torch.nn.Linear(5, output_dim)
 8
           self.dropout = torch.nn.Dropout(p = 0.25)
 9
10
11
       def forward(self, x):
12
13
           out1 = self.layer1(x)
          out1 = self.dropout(out1)
14
           output = self.layer2(out1)
15
16
           return output
17
```

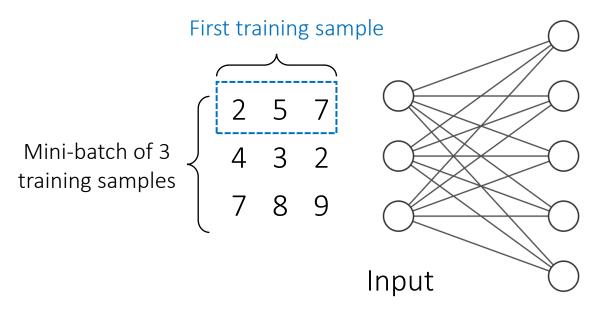
Add the dropout in __init__ with p = probability of neuron state is set to 0

Apply dropout to the output of the desired layer



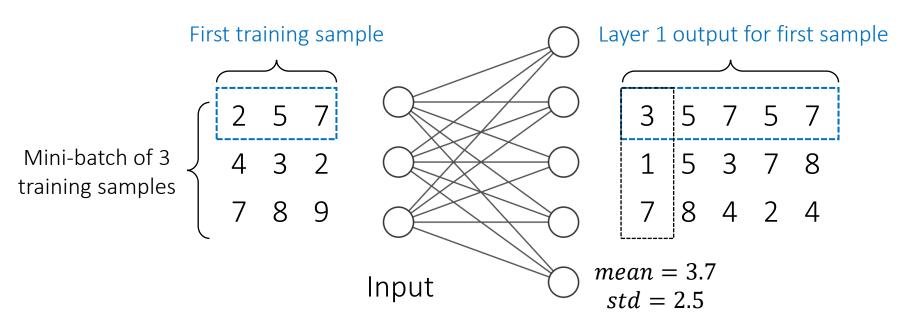
Preventing Vanishing/Exploding Gradients: Batch Normalization

Loffe et al 2015 (>35000 citations)



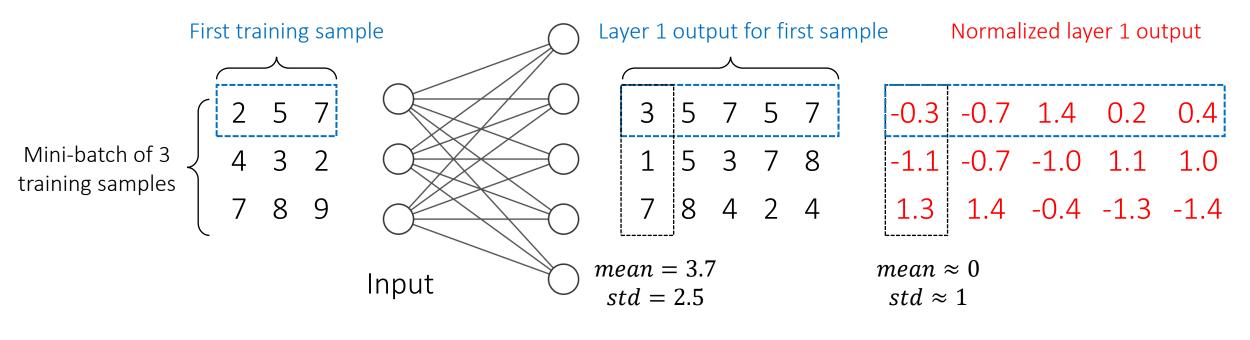
Layer 1





Layer 1





Layer 1

Batch normalization



Batch Normalization in PyTorch

```
class Model(torch.nn.Module):
         def __init__(self, input_dim, output_dim):
              super(Model, self).__init__()
              self.layer1 = torch.nn.Linear(input_dim, 5)
             self.layer2 = torch.nn.Linear(5, output_dim)
self.bn1 = torch.nn.BatchNorm1d(5)
10
         def forward(self, x):
11
12
             out1 = self.layer1(x)
out1 = self.bn1(out1)
13
14
             out1 = torch.nn.functional.relu(out1)
15
              output = self.layer2(out1)
16
17
18
              return output
```

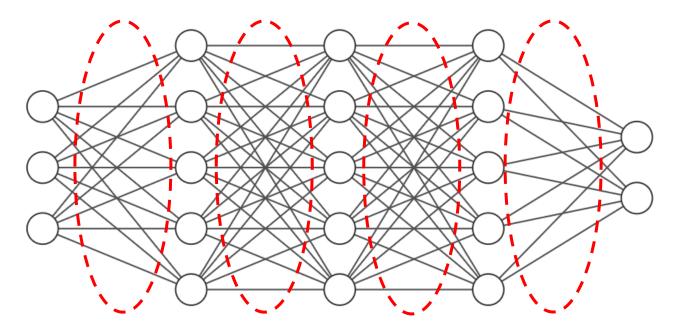
Add BatchNorm1D in ___init__ with number of features in desired layer output

Apply batch normalization to the output of the desired layer.

NOTE: Batch normalization is done BEFORE feeding into activation function



Preventing Vanishing/Exploding Gradients: Weight Initialization



Proper weight initialization plays essential roles in preventing exploding/vanishing gradients



Faster convergence



Weight Initialization Methods

Uniform

Uniform distribution

torch.nn.init.uniform_()

Normal

Gaussian distribution

torch.nn.init.normal ()

Xavier

Suitable for tanh() activation

torch.nn.init.xavier_uniform_()

Xavier et al 2010

Kaiming

Suitable for ReLU() activation

torch.nn.init.kaiming_uniform_()

He et al 2015

More initializations: https://pytorch.org/docs/stable/nn.init.html



Weight Initialization in PyTorch

```
class Model(torch.nn.Module):
       def __init__(self, input_dim, output_dim):
           super(Model, self).__init__()
           self.layer1 = torch.nn.Linear(input dim, 5)
           self.layer2 = torch.nn.Linear(5, output_dim)
           torch.nn.init.kaiming_uniform_(self.layer2.weight)
10
11
       def forward(self, x):
12
           out1 = torch.nn.functional.relu(self.layer1(x))
13
           output = torch.nn.functional.relu(self.layer2(out1))
14
15
           return output
16
```

Manually apply Kaiming He Initialization to layer2

NOTE: PyTorch already applies good default initialization for most layers. We suggest using manual initialization for experimental purposes



TRAINING MULTI-LAYER PERCEPTRONS

Iris Classification Example



Neural Network Workflow in PyTorch

Prepare Data

Define Model

Select Hyperparameter

Identify Tracked Values

Train Model

Visualization and Evaluation



Prepare Data

```
1 from sklearn.datasets import load iris
  from sklearn.preprocessing import StandardScaler
   from sklearn.model_selection import train_test_split
   iris = load iris()
 7 | X = iris['data']
   y = iris['target']
   scaler = StandardScaler()
   X_scaled = scaler.fit_transform(X)
12
   X_train, X_test, y_train, y_test = train_test_split(X_scaled, y,
                           Testing data ratio (0.2 = 20\%) \leftarrow test_size=0.2,
14
                        Random seed to use for splitting ← random_state=2)
15
16
   X_validation = X_train[:int(len(X_test))]
   y validation = y train[:int(len(X test))]
19
  X train = X train[int(len(X_test)):]
21 y_train = y_train[int(len(X_test)):]
```

Load Iris dataset

Extract features (X) and target labels (y)

Scale features using scikit-learn provided standard scaler

Split the dataset into Training (80%) and Testing (20%)

Assign subset of the training dataset as validation data (same size as testing)

Use the remaining dataset as training

Final split ratios = Training: 60%, Testing: 20%, Validation: 20%



Define Model

```
class irisClassificationFCN(torch.nn.Module):
       def __init__(self, input_dim, output_dim, hidden1_dim, hidden2_dim):
           super(irisClassificationFCN, self).__init__()
           self.layer1 = torch.nn.Linear(input_dim, hidden1_dim)
           self.layer2 = torch.nn.Linear(hidden1 dim, hidden2 dim)
           self.layer3 = torch.nn.Linear(hidden2_dim, output_dim)
 9
10
       def forward(self, x):
11
12
           out1 = torch.nn.functional.relu(self.layer1(x))
13
           out2 = torch.nn.functional.relu(self.layer2(out1))
14
           output = self.layer3(out2)
15
16
17
           return output
```

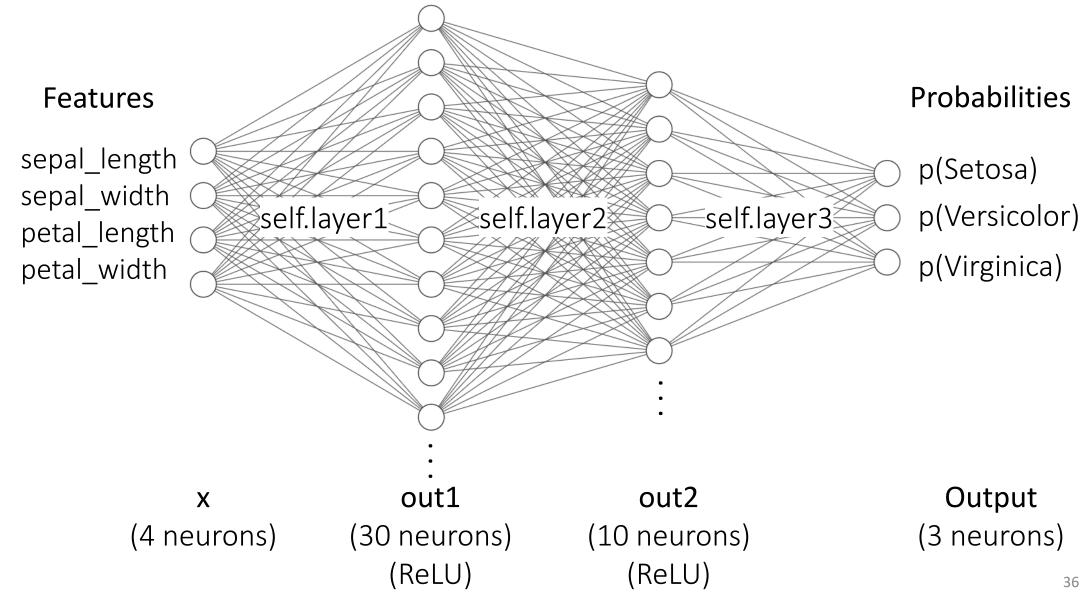
```
Input layer (input_dim = 4)
2 hidden layers (hidden1_dim = 30, hidden2_dim = 10)
output layer (output_dim = 3)
```

ReLU activation for the outputs of each hidden layer

Return raw final output



Define Model





irisClassificationFCN(

(layer1): Linear(in_features=4, out_features=30, bias=True)

(layer2): Linear(in_features=30, out_features=10, bias=True)

(layer3): Linear(in_features=10, out_features=3, bias=True)

Select Hyperparameter

```
model = irisClassificationFCN(input_dim = 4, output_dim = 3, hidden1_dim = 30, hidden2_dim = 10)

learning_rate = 0.025
epochs = 25

loss_func = torch.nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(model.parameters(), lr = learning_rate)

model

Initialize the model with input_dim = 4, output_dim = 3, hidden1_dim = 30, hidden2_dim = 10

Using learning rate of 0.025 and 25 as epochs

Using Cross Entropy Loss and Adam Optimizer

model
```

37

Model variable correctly shows our network

structure



Identify Tracked Values

```
train_loss_list = np.zeros((epochs,))
validation_accuracy_list = np.zeros((epochs,))
training
```

Create empty list or NumPy arrays to hold training loss and validation accuracy



Train Model

```
import tqdm

train_inputs = torch.from_numpy(X_train).float()
train_targets = torch.from_numpy(y_train).long()

validation_inputs = torch.from_numpy(X_validation).float()
validation_targets = torch.from_numpy(y_validation).long()

testing_inputs = torch.from_numpy(X_test).float()
testing_targets = torch.from_numpy(y_test).long()

testing_targets = torch.from_numpy(y_test).long()
```

Import tqdm to visualize the progress of your training

Convert training/validation/testing datasets into PyTorch Tensors

Convert the targets into int64 form via .long()



Train Model

```
# Training Loop
15
   for epoch in tqdm.trange(epochs):
17
18
       optimizer.zero_grad()
19
       train_outputs = model(train_inputs)
20
21
22
       loss = loss_func(train_outputs, train_targets)
23
       train_loss_list[epoch] = loss.item()
24
25
26
       loss.backward()
27
28
       optimizer.step()
29
30
       # Compute Validation Accuracy
31
32
       with torch.no grad():
33
           validation outputs = model(validation inputs)
34
35
           correct = (torch.argmax(validation_outputs, dim=1) ==
36
37
                      validation_targets).type(torch.FloatTensor)
38
           validation accuracy list[epoch] = correct.mean()
39
```

Training loop

- Empty gradient buffer
- Forward propagation
- Compute loss
- Save loss value to a list
- Backward propagation
- Update weights/biases

Compute Validation accuracy per epoch

- Forward pass validation inputs to network
- Compare the outputs (index with the highest probability)
 against the validation target
- Compute and append the validation accuracy



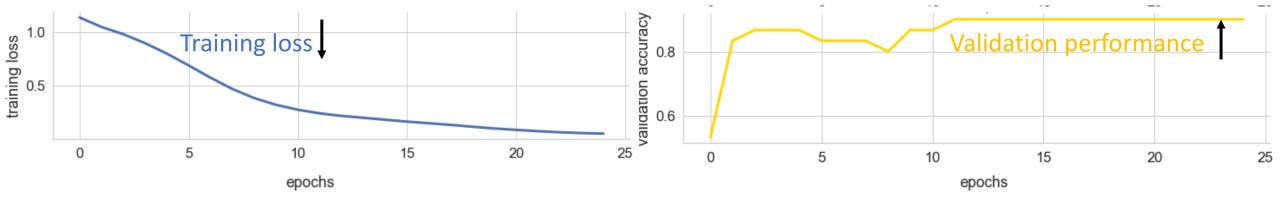
Testing Accuracy: 93.333333730697

Visualization and Evaluation

```
7 plt.subplot(2, 1, 2)
8 plt.plot(train_loss_list, linewidth = 3)
9 plt.ylabel("training loss")
10 plt.xlabel("epochs")
11 sns.despine()
```

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

plt.subplot(2, 1, 1)
plt.plot(validation_accuracy_list, linewidth = 3, color = 'gold')
plt.ylabel("validation accuracy")
```



```
with torch.no_grad():

# Pass the testing feature data (30 samples) to the network to produce model predictions
y_pred_test = model(testing_inputs)

# Use the same technique as above to commpute the testing classification accuracy
correct = (torch.argmax(y_pred_test, dim=1) == testing_targets).type(torch.FloatTensor)

print("Testing Accuracy: " + str(correct.mean().numpy()*100) + '%')
```

Testing performance

93% classification accuracy



LAB 2 ASSIGNMENT:

MNIST Classification using multi-layer perceptron



MNIST Dataset



Handwritten digits 0-9

Target labels are the correct values of the digit

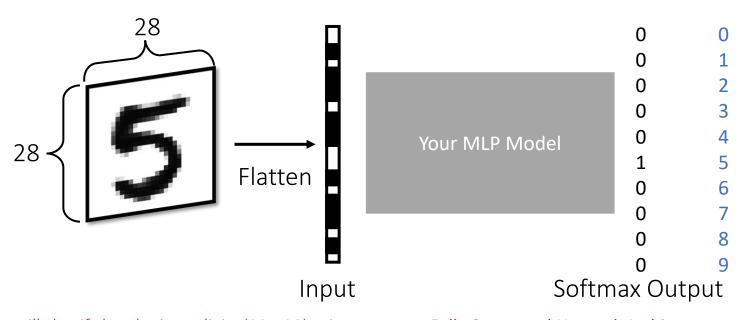
Data consists of grayscale images of fixed size (28x28) – flattens to 784

Canonical dataset for machine learning

1000 training samples, 100 testing samples



MNIST Classification with MLP



In this exercise, you will classify handwritten digits (28 x 28) using your own Fully Connected Network Architecture.

Prior to training your neural net, 1) Flatten each digit into 1D array of size 784, 2) Normalize the dataset using standard scaler and 3) Split the dataset into train/validation/test.

Design your own neural net architecture with your choice of hidden layers, activation functions, optimization method etc.

Your goal is to achieve a testing accuracy of >90%, with no restrictions on epochs.

Demonstrate the performance of your model via plotting the training loss, validation accuracy and printing out the testing accuracy.

Plot the testing samples where your model failed to classify correctly and print your model's best guess for each of them



Tips for Training Your Model

First things to decide

- Number of layers
- Neurons in each layer
- Activation function (ReLU, Tanh, sigmoid)
- Training batch size (SGD, Mini-batch, Batch Gradient)
- Learning rate
- Optimizer
 (SGD, Adam, RMS Prop etc)
- Number of training epochs

If your model is overfitting

(high training performance but low validation/testing performance)

- Add dropout layers
- Add regularization terms
- Stop training early
- Make network smaller (fewer layers or neurons)