COMP 6721 Applied Artificial Intelligence (Summer 2023)

Assignment #08: Introduction to Deep Learning and 09: CNNs and Optimization

Solutions

PyTorch is a deep learning research platform that was designed for maximum flexibility and speed.¹ To gain a basic understanding on how to implement an Artificial Neural Network using the PyTorch library, in the following questions you will implement a simple MLP and a convolutional neural network for a specific image classification task.

Question 1 Let's use PyTorch to implement a multi-layer perceptron for classifying the CIFAR10 dataset (see Figure 1).² The torchvision package³ provides data loaders for common datasets such as Imagenet, CIFAR10, MNIST, etc.

¹See https://pytorch.org/docs/stable/index.html

²For details on CIFAR10, see https://en.wikipedia.org/wiki/CIFAR-10

³https://pytorch.org/docs/stable/torchvision/index.html

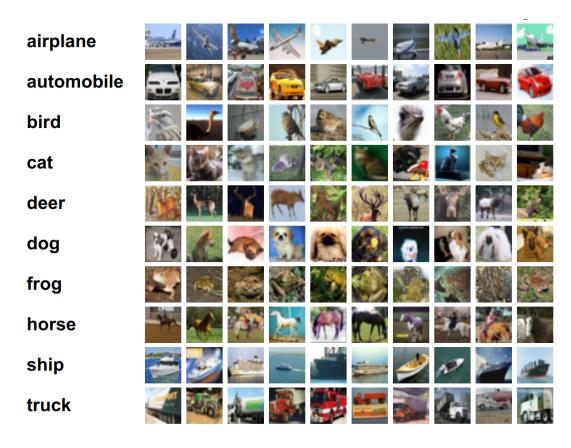


Figure 1: Some example images from the CIFAR-10 dataset

First, use the following code block, which provides Python imports and the cifar_loader function as a helper function to load the CIFAR-10 dataset. This function returns the train and the test data loaders that can be used as an iterator, so to extract the data, we can use the standard Python iterators such as enumerate. After setting the hyper-parameters, where H is the hidden dimension and D_out is the output dimension, the dataset is loaded.

(a) This is where the model definition takes place. The most straightforward way of creating a neural network structure in PyTorch is by creating a class inheriting from the nn.Module⁴ superclass within PyTorch. The nn.Module is a very useful PyTorch class that contains all you need to construct typical deep learning networks. Define the MultiLayerFCNet class, which is a four-layer, fully connected network. Use the hyper-parameter H as the number of hidden units for all hidden layers. For the activation function, apply ReLU to the hidden layers and use log_softmax in the output.

The forward function overrides the base forward function in nn.Module and is required for the nn.Module functionality to work correctly.

```
class MultiLayerFCNet(nn.Module):
    def __init__(self, D_in, H, D_out):
        super(MultiLayerFCNet, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, H)
        self.linear2 = torch.nn.Linear(H, H)
        self.linear3 = torch.nn.Linear(H, H)
        self.linear4 = torch.nn.Linear(H, D_out)

def forward(self, x):
        x = F.relu(self.linear1(x))
        x = F.relu(self.linear2(x))
        x = F.relu(self.linear3(x))
        x = self.linear4(x)
        return F.log_softmax(x)
```

⁴https://pytorch.org/docs/stable/generated/torch.nn.Module.html

(b) Now use PyTorch's CrossEntropyLoss⁵ to construct the loss function and define an optimizer using torch.optim.⁶ The first argument passed to the optimizer function are the parameters we want the optimizer to train. All you have to do is pass model.parameters() to the function, and PyTorch keeps track of all the parameters within the model, which are required to be trained.:

```
model = MultiLayerFCNet(D_in, H, D_out)

criterion = torch.nn.CrossEntropyLoss()

optimizer = torch.optim.SGD(model.parameters(), lr=0.01, momentum=0.9)
```

Next, loop over the number of epochs and within this loop, pass the model outputs and the true labels to the <code>CrossEntropyLoss</code> function, defined as <code>criterion</code>. Then perform back-propagation and an optimized training. Call <code>backward()</code> on the loss variable to perform the back-propagation. Now that the gradients have been calculated in the back-propagation, call <code>optimizer.step()</code> to perform the optimizer training step.

```
for epoch in range(num_epochs):
   avg_loss_epoch = 0
   batch_loss = 0
   total_batches = 0
   for i, (images, labels) in enumerate(train_loader):
      images = images.reshape(-1, 32 * 32 * 3)
      outputs = model(images)
      loss = criterion(outputs, labels)
      optimizer.zero_grad()
      loss.backward()
      optimizer.step()
      total_batches += 1
      batch_loss += loss.item()
   avg_loss_epoch = batch_loss / total_batches
   print('Epoch [{}/{}], Averge Loss:for epoch[{}, {:.4f}]'
       .format(epoch + 1, num_epochs, epoch + 1, avg_loss_epoch))
```

(c) Finally, we need to keep track of the *accuracy* on the test set. The predictions of the model can be determined by using the torch.max()⁷ function,

 $^{^{5}}$ https://pytorch.org/docs/stable/generated/torch.nn.CrossEntropyLoss.html

⁶https://pytorch.org/docs/stable/optim.html

⁷https://pytorch.org/docs/stable/generated/torch.max.html

which returns the index of the maximum value in a tensor. The first argument to this function is the tensor to be examined, and the second argument is the axis over which to determine the index of the maximum. Report the accuracy on the test set using the torch.max() function.

```
correct = 0
total = 0
for images, labels in test_loader:
    images = images.reshape(-1, 3 * 32 * 32)
    outputs_test = model(images)
    _, predicted = torch.max(outputs_test.data, 1)
    total += labels.size(0)

    correct += (predicted == labels).sum().item()

print('Accuracy of the network on the 10000 test images: %d %%'
    % (100 * correct / total))
```

- Question 2 Assume you have a 4x3 one-channel (BW) image with the following pixel intensities. A 2x2 filter is applied to the image followed by a ReLu (the activation function of the convolutional layer is ReLu). Find the resulting activation map (output volume) before and after pooling when
 - No padding is applied followed by 2x2 max-pooling
 - 1 pixel padding is applied, followed by 2x2 average pooling

-1	0	1
2	3	4
5	6	7
8	9	10

Table 1: 4x3 image

2	1
0	-1

Table 2: 2x2 filter (kernel)

• If there is no padding, no zero pixels are added to the image. We start from the left top corner of the image and the corner 2x2 are item-by-item multiplied by the filter, i.e.,

-1	0	2	1
2	3	0	-1

The result is -1x2+0x1+2x0+3x-1=-5 and because of the Relu activation, the output will be zero. Sliding the filter to the right, the down,

$$-0x2+1x1+3x0+4x-1 = -3 < 0 -> 0$$

$$-2x2+3x1+5x0+6x-1=1$$

$$-3x2+4x1+6x0+7x-1=3$$

$$-5x2+6x1+8x0+9x-1=7$$

$$-6x2+7x1+9x0+10x-1=9$$

Therefore, the resulting activation map will be 3x2, as follows:

$\mid 0 \mid$	$\mid 0 \mid$
1	3
7	9

Now, if this output is followed by a 2x2 max-pool, we will have

$$- \max(0,0,1,3) = 3$$

$$- \max(1,3,7,9) = 9$$

• If we apply padding, the 4x3 image will be considered as a 6x5 image, as follows:

0	0	0	0	0
0	-1	0	1	0
0	2	3	4	0
0	5	6	7	0
0	8	9	10	0
0	0	0	0	0

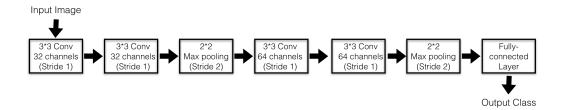
After convolution, we will obtain a 5x4 activation map as

1.0	0	0	0
0	0	0	2.0
0	1	3	8
0	7	9	14
8	25	28	20

If we apply 2x2 average pooling without sliding (non-overlapping):

0.25	0.5
2	8.5
25	28

Question 3 To improve the performance for image classification, we will use PyTorch to implement more complicated, deep learning networks. In this question, you will implement a convolutional neural network (CNN) step-by-step to classify the CIFAR-10 dataset. The CNN architecture that we are going to build can be seen in the diagram below:



(a) First, use the following code block, which provides the Python imports, the cifar_loader to load the dataset, and the hyper-parameters definition:

```
from torch.utils.data import DataLoader
import torch
import torch.nn as nn
import torchvision.transforms as transforms
import torchvision.datasets
num_epochs = 4
num_classes = 10
learning_rate = 0.001
transform = transforms.Compose(
   [transforms.ToTensor(),
   transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))])
trainset = torchvision.datasets.CIFAR10(root='./data', train=True,
                              download=True, transform=transform)
train_loader = torch.utils.data.DataLoader(trainset, batch_size=32,
                                shuffle=True, num_workers=2)
testset = torchvision.datasets.CIFAR10(root='./data', train=False,
                             download=True, transform=transform)
test_loader = torch.utils.data.DataLoader(testset, batch_size=1000,
                                shuffle=False, num_workers=2)
classes = ('plane', 'car', 'bird', 'cat',
        'deer', 'dog', 'frog', 'horse', 'ship', 'truck')
```

(b) Now create a class inheriting from the nn.Module to define different layers of the network based on provided network architecture above. The first step is to use the nn.Sequential module⁸ to create sequentially ordered

⁸https://pytorch.org/docs/stable/generated/torch.nn.Sequential.html

layers in the network. It's a handy way of creating a convolution + ReLU + pooling sequence. In each convolution layer, use LeakyRelu for the activation function and BatchNorm2d⁹ to accelerate the training process.

```
class CNN(nn.Module):
   def __init__(self):
      super(CNN, self).__init__()
      self.conv_layer = nn.Sequential(
         nn.Conv2d(in_channels=3, out_channels=32, kernel_size=3, padding=1),
         nn.BatchNorm2d(32),
         nn.LeakyReLU(inplace=True),
         nn.Conv2d(in_channels=32, out_channels=32, kernel_size=3, padding=1),
         nn.BatchNorm2d(32),
         nn.LeakyReLU(inplace=True),
         nn.MaxPool2d(kernel_size=2, stride=2),
         nn.Conv2d(in_channels=32, out_channels=64, kernel_size=3, padding=1),
         nn.BatchNorm2d(64),
         nn.LeakyReLU(inplace=True),
         nn.Conv2d(in_channels=64, out_channels=64, kernel_size=3, padding=1),
         nn.BatchNorm2d(64),
         nn.LeakyReLU(inplace=True),
         nn.MaxPool2d(kernel_size=2, stride=2),
      self.fc_layer = nn.Sequential(
         nn.Dropout(p=0.1),
         nn.Linear(8 * 8 * 64, 1000),
         nn.ReLU(inplace=True),
         nn.Linear(1000, 512),
         nn.ReLU(inplace=True),
         nn.Dropout(p=0.1),
         nn.Linear(512, 10)
      )
   def forward(self, x):
     # conv layers
     x = self.conv_layer(x)
     # flatten
     x = x.view(x.size(0), -1)
     # fc layer
```

https://pytorch.org/docs/stable/generated/torch.nn.BatchNorm2d.html#torch.nn.BatchNorm2d

```
x = self.fc_layer(x)
return x
```

(c) Before training the model, you have to first create an instance of the **Convolution** class you defined in previous part, then define the loss function and optimizer:

```
model = CNN()

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

The following steps are similar to what you've done in previous questions: Loop over the number of epochs and within this loop, pass the model outputs and true labels to the <code>CrossEntropyLoss</code> function, defined as <code>criterion</code>. Then, perform back-propagation and an optimized training. Call <code>backward()</code> on the loss variable to perform the back-propagation. Now that the gradients have been calculated in the back-propagation, call <code>optimizer.step()</code> to perform the optimizer training step.

```
total_step = len(train_loader)
loss_list = []
acc_list = []
for epoch in range(num_epochs):
   for i, (images, labels) in enumerate(train_loader):
      # Forward pass
      outputs = model(images)
      loss = criterion(outputs, labels)
      loss_list.append(loss.item())
      # Backprop and optimisation
      optimizer.zero_grad()
      loss.backward()
      optimizer.step()
      # Train accuracy
      total = labels.size(0)
      _, predicted = torch.max(outputs.data, 1)
      correct = (predicted == labels).sum().item()
      acc_list.append(correct / total)
      if (i + 1) % 100 == 0:
         print('Epoch [{}/{}], Step [{}/{}], Loss: {:.4f}, Accuracy: {:.2f}%'
              .format(epoch + 1, num_epochs, i + 1, total_step, loss.item(),
                    (correct / total) * 100))
```

(d) Now keep track of the accuracy on the test set. The predictions of the model can be determined by using torch.max().¹⁰

```
model.eval()
with torch.no_grad():
    correct = 0
    total = 0
    for images, labels in test_loader:
        outputs = model(images)
        _, predicted = torch.max(outputs.data, 1)
        total += labels.size(0)
        correct += (predicted == labels).sum().item()

print('Test Accuracy of the model on the 10000 test images: {} %'
        .format((correct / total) * 100))
```

(e) In PyTorch, the learnable parameters (i.e., weights and biases) of a model are contained in the model's parameters. A state_dict is simply a Python dictionary object that maps each layer to its parameter tensor. Because state_dict objects are Python dictionaries, they can be easily saved, updated, altered, and restored.¹¹

Saving the model's state_dict with the torch.save() function will give you the most flexibility for restoring the model later. To load the models, first initialize the models and optimizers, then load the dictionary locally using torch.load().

Inspect the PyTorch documentation to understand how you can use these functionalities.

To save a model:

```
torch.save(modelA.state_dict(), PATH)

To restore a model:

modelB = TheModelBClass(*args, **kwargs)
modelB.load_state_dict(torch.load(PATH), strict=False)
```

 $^{^{10}}$ https://pytorch.org/docs/stable/generated/torch.max.html

 $^{^{11} \}verb|https://pytorch.org/tutorials/beginner/saving_loading_models.html|$

- Question 4 The goal of skorch¹² is to make it possible to use PyTorch with scikit-learn. This is achieved by providing a wrapper around PyTorch that has a scikit-learn interface. Additionally, skorch abstracts away the training loop, a simple net.fit(X, y) is enough. It also takes advantage of scikit-learn functions, such as predict.
 - (a) In this section, we will train the same CNN model you developed in the previous question using skorch with fewer lines of code.

Let's install skorch first:

```
pip install skorch
```

Once the library is installed, we can import the libraries. The next step is to prepare the dataset before training.

```
import matplotlib.pyplot as plt
import numpy as np
import torch
import torch.nn as nn
import torch.optim as optim
import torchvision.datasets
import torchvision.transforms as transforms
from sklearn.metrics import accuracy_score
from sklearn.metrics import plot_confusion_matrix
from skorch import NeuralNetClassifier
from torch.utils.data import random_split
num_epochs = 4
num_classes = 10
learning_rate = 0.001
transform = transforms.Compose(
   [transforms.ToTensor(),
   transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))])
trainset = torchvision.datasets.CIFAR10(root='./data', train=True,
                              download=True, transform=transform)
testset = torchvision.datasets.CIFAR10(root='./data', train=False,
                             download=True, transform=transform)
m = len(trainset)
train_data, val_data = random_split(trainset, [int(m - m * 0.2), int(m * 0.2)])
DEVICE = torch.device("cpu")
y_train = np.array([y for x, y in iter(train_data)])
classes = ('plane', 'car', 'bird', 'cat',
        'deer', 'dog', 'frog', 'horse', 'ship', 'truck')
```

skorch.NeuralNetClassifier¹³ is a Neural Network class used for classification tasks. Initialize the NeuralNetClassifier class then train the CNN

¹²https://skorch.readthedocs.io/en/stable/index.html

¹³https://skorch.readthedocs.io/en/stable/classifier.html

model using the method fit. Finally print the accuracy score and confusion matrix. Note that CNN is the model you already developed from the previous question using torch.

```
torch.manual_seed(0)
net = NeuralNetClassifier(
   CNN.
   max_epochs=1,
   iterator_train__num_workers=4,
   iterator_valid__num_workers=4,
   lr=1e-3,
   batch_size=64,
   optimizer=optim.Adam,
   criterion=nn.CrossEntropyLoss,
   device=DEVICE
)
net.fit(train_data, y=y_train)
y_pred = net.predict(testset)
y_test = np.array([y for x, y in iter(testset)])
accuracy_score(y_test, y_pred)
plot_confusion_matrix(net, testset, y_test.reshape(-1, 1))
plt.show()
```

(b) Now let's evaluate the score using K-fold cross-validation. Before the evaluation, we need to make the training set sliceable using the class SliceDataset, which wraps a torch dataset to make it work with scikit-learn. Use the function $cross_val_score(estimator, X, y=None, cv=None)$ of the scikit-learn library to evaluate the validation accuracy obtained using K=5 folds for K-fold cross-validation.

To achieve this, replace the training process from the previous section with a K-fold cross-validation.

Here is a possible solution:

- Question 5 As discussed in the course, one of the techniques that helped us to mitigate the drawback of need for lots of labeled data in Deep Learning (DL) was *Transfer Learning*. In Transfer learning, we use a pretrained model so that the "optimal" encoder weights have already been determined, and we may just do further fine tuning using our own data.
 - (a) Fine Tuning: Pretrained weights are not frozen, but they change with a very low learning rate when we train the model with our data. We expect to converge faster compared to training from scratch.
 - (b) Freezing the rates: We fix the pretrained rates, but we may add a few new layers or replace the few last layers with ours and train the whole model using our data. This approach could be considered "less adaptive" but faster than updating all weights.

The PyTorch tutorial can be followed here https://pytorch.org/tutorials/beginner/transfer_learning_tutorial.html. We use resnet18 pretrained model on the CIFAR10 dataset.

Steps to load the data are the same as before (We did in the first question).

```
data_transforms = {
   'train': transforms.Compose([
      transforms.RandomResizedCrop(224),
      transforms.RandomHorizontalFlip(),
      transforms.ToTensor(),
      transforms.Normalize([0.485, 0.456, 0.406], [0.229, 0.224, 0.225])
   ]),
   'val': transforms.Compose([
      transforms.Resize(256),
      transforms.CenterCrop(224),
      transforms.ToTensor(),
      transforms.Normalize([0.485, 0.456, 0.406], [0.229, 0.224, 0.225])
   ]),
}
trainset = torchvision.datasets.CIFAR10(root='./data', train=True,
                              download=True, transform=data_transforms['train'])
train_loader = torch.utils.data.DataLoader(trainset, batch_size=32,
                                shuffle=True, num_workers=2)
testset = torchvision.datasets.CIFAR10(root='./data', train=False,
                             download=True, transform=data_transforms['val'])
test_loader = torch.utils.data.DataLoader(testset, batch_size=1000,
                                shuffle=False, num_workers=2)
dataloaders={'train':train_loader, 'val':test_loader}
dataset_sizes = {'train': len(trainset),'val': len(testset) }
```

However, the model that will be passed to the training will change as follows:

```
from torchvision import models
model_ft = models.resnet18(weights='IMAGENET1K_V1')
num_ftrs = model_ft.fc.in_features

# Alternatively, it can be generalized to ``nn.Linear(num_ftrs, len(class_names))``.
model_ft.fc = nn.Linear(num_ftrs, len(class_names))

model_ft = model_ft.to(device)
```

You could find the notebook attached. As discussed, it is just the modified version of the notebook here https://pytorch.org/tutorials/beginner/transfer_learning_tutorial.html.

Question 6 As discussed in the lecture, the main hyperparameters in a deep neural network are architectural hyperparameters such as the number of hidden layers and the number of neurons per layer.

There are other parameters that affect the performance and speed of training such as the number of epochs, batch size and the initial learning rate (or the way that it is updated). The choice of optimizer can also be considered a parameter significantly affecting the speed of training, as different optimizers may have different performance rates, depending on the type of data and structure of the network. There is no optimizer that is necessarily consistently superior to all the other optimizers for every problem.

Every optimizer may have its own parameters that need further adjustments, so it is difficult to compare several optimizers even for the same problem. However, we want to simply compare three known optimizers for the problem we saw in Question 1.

For Question 1, how can you change the optimizer and try others such as 'Adam' and 'RMSprop'?

The optimizer definition will change as follows.

```
torch.optim.Adam(model.parameters(), lr=learning_rate)
torch.optim.RMSprop(model.parameters(), lr=learning_rate)
```

You could find a notebook attached which compare these three optimizers (Disclaimer: Training time is long, so what we see is only for a few number of epochs, which may not be representative enough). Details about different optimizers in PyTorch can be found here https://pytorch.org/tutorials/beginner/basics/optimization_tutorial.html.