

# COMPSCI 389 Introduction to Machine Learning

Days: Tu/Th. Time: 2:30 – 3:45 Building: Morrill 2 Room: 222

**Topic 10.4: PyTorch and Overfitting** 

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Note: This presentation covers (and provides additional context/information regarding) 10.5 Introduction to PyTorch.ipynb

### Autograd

- Can be slow because it executes Python code.
- Is designed for differentiating arbitrary code
  - It does not have extra functionality for machine learning

### **Deep Learning Libraries**

- There are many deep learning libraries that extend autograd to:
  - Leverage low-level compiled code for faster runtimes.
  - Enable forward and backwards passes on the GPU rather than CPU (more on this later).
  - Have built-in implementations of
    - Common loss functions
    - Common activation functions
    - Common network layers
      - Fully connected feed-forward
      - Convolutional layers
      - Pooling layers
      - Etc.

## **Deep Learning Libraries**

### • PyTorch

- The most commonly used today.
- What we will use in class.
- Tensorflow
  - Produced and maintained by Google
  - Integrates nicely with Google's cloud computing platforms
  - Steeper learning curve and more verbose syntax
- Keras, Caffe, MXNet, etc.
  - Many less popular alternatives

## PyTorch

You can install PyTorch with:

pip install torch torchvision

We will use the following imports:

## Defining a Neural Network Architecture Defining a Parametric Model

- Extend the nn.Module base class
  - The base class provides functionality for tracking trainable parameters (and their gradients), moving parameters to the GPU, saving and loading models, etc.
- Implement two functions:
  - <u>init</u> (self): Define the different layers (number of units, number of inputs) and different activation functions that will be used.
  - forward(self, x): Perform a forward pass on input x.
- You do not need to implement any gradients or the backwards pass!
  - PyTorch uses reverse mode automatic differentiation to automatically compute gradients.

**Note**: This model is bigger than needed for the GPA prediction problem. This allows us to more easily compare runtimes later, and to show a phenomenon called "overfitting".

```
class FullyConnectedNetwork(nn.Module):
   def __init__(self):
       # First call the nn.Module constructor to initialize other parts of the model. Always do this first.
       super(FullyConnectedNetwork, self).__init__()
       # Define layers. The lines below create the layers (memory is allocated for the weights here).
       self.fc1 = nn.Linear(9, 1024) # First hidden layer with 1024 neurons and 9 inputs.
       self.fc2 = nn.Linear(1024, 512) # Second hidden layer with 512 neurons and 1024 inputs.
       self.fc3 = nn.Linear(512, 128) # Third hidden layer with 128 neurons and 512 inputs.
       self.fc4 = nn.Linear(128, 1) # Output layer with 1 neuron and 128 inputs.
                                                   nn.Linear represents a linear
       # Define activation function.
       self.relu = nn.ReLU()
                                                    parametric model with no basis.
                                                    That is, each unit is a perceptron
   def forward(self, x):
                                                   without an activation function.
       # Pass data through the network
       x = self.relu(self.fc1(x))
       x = self.relu(self.fc2(x))
       x = self.relu(self.fc3(x))
       x = self.fc4(x)
                                       # No activation after the output layer
       return x
```

We can now create an instance of this model:

```
# Create an instance of the network
net = FullyConnectedNetwork()
```

# The network structure is printed as a sanity check
print(net)

FullyConnectedNetwork(

```
(fc1): Linear(in_features=9, out_features=1024, bias=True)
```

```
(fc2): Linear(in_features=1024, out_features=512, bias=True)
```

```
(fc3): Linear(in_features=512, out_features=128, bias=True)
```

```
(fc4): Linear(in_features=128, out_features=1, bias=True)
```

(relu): ReLU()

bias=True indicates that each perceptron includes an extra feature that is always equal to 1 (and hence one extra weight beyond the number of outputs from the previous layer). This is what we discussed previously when we talked about appending a 1 to the columns of a data set to implement the "y-intercept" in linear regression. For perceptrons and neural networks, this extra weight is called the bias.

Next, let's load the GPA data, split it into training and testing, and standardize it. + Code + Markdown

```
df = pd.read_csv("https://people.cs.umass.edu/~pthomas/courses/COMPSCI_389_Spring2024/GPA.csv", delimiter=',')
#df = pd.read csv("data/GPA.csv", delimiter=',')
# We already loaded X and y, but do it again as a reminder
X = df.iloc[:, :-1]
y = df.iloc[:, -1]
# Split the data into training and testing sets
X train, X test, y train, y test = train test split(X, y, test size=0.2, shuffle=True)
# Standardize the features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train) # This sets the min/max values from the training data (without looking
X test = scaler.transform(X test) # This uses the min/max scaling values chosen during training! (transfo
```

Python

PyTorch has its own objects for storing data, called PyTorch tensors. These are simply multidimensional arrays. Let's convert our data to these tensor objects. Note that the **tensor** constructor is not compatible with **pandas.Series** objects, so we call **y\_train.values** and **y\_test.values** to convert these to **numpy.ndarray** objects.

```
# Convert data to PyTorch tensors
X_train_tensor = torch.tensor(X_train, dtype=torch.float32)
y_train_tensor = torch.tensor(y_train.values, dtype=torch.float32).view(-1,1)
X_test_tensor = torch.tensor(X_test, dtype=torch.float32)
y_test_tensor = torch.tensor(y_test.values, dtype=torch.float32).view(-1,1)
```

### Loss Function

• PyTorch has many built-in loss functions, including MSE:

```
loss_function = nn.MSELoss()
```

# Optimizer

- PyTorch has many built-in loss optimizers, including gradient descent (SGD), and Adam (SGD with a specific adaptive step size method).
  - Several optimizers are discussed in the Jupyter notebook.
  - Adam is the most common, and what we will use.

optimizer = optim.Adam(net.parameters())

net.parameters() contains the weights, and after backwards passes will also contain the gradient information. The optimizer uses this gradient information to update the weights.



```
epochs = 100
for epoch in range(epochs):
```

# The number of epochs to run

```
# Forward pass
y_pred = net(X_train_tensor)
```

Perform a forward pass of the parametric model for each training point.

```
# Compute loss
loss = loss_function(y_pred, y_train_tensor)
```

Perform a forward pass of the loss function.

```
epochs = 100
for epoch in range(epochs):
```

```
# Forward pass
y_pred = net(X_train_tensor)
```

```
# Compute loss
loss = loss_function(y_pred, y_train_tensor)
```

# Backward pass and optimize
loss.backward()

Perform a backwards pass, computing the gradient of loss w.r.t. each model parameter (each weight)

# The number of epochs to run

```
epochs = 100
for epoch in range(epochs):
```

```
# Forward pass
y_pred = net(X_train_tensor)
```

```
# Compute loss
loss = loss_function(y_pred, y_train_tensor)
```

# Backward pass and optimize
loss.backward()
optimizer.step()

Update the weights using gradient descent with adaptive step size.

# The number of epochs to run

```
epochs = 100
for epoch in range(epochs):
```

```
# Forward pass
y_pred = net(X_train_tensor)
# Compute loss
loss = loss_function(y_pred, y_train_tensor)
# Backward pass and optimize
loss.backward()
optimizer.step()
                                            Print the loss on the training
# Print statistics
                                            set.
if epoch % 10 == 0:
```

# The number of epochs to run

print(f'Epoch [{epoch}/{epochs}], Loss: {loss.item():.4f}')

### A note about backward ()

- Each model parameter has a .grad attribute storing the gradient of the loss w.r.t. that parameter.
- Sometimes many gradients are computed before one step
  - This isn't something we have discussed
- To accommodate this, loss.backward() adds the derivative of the loss w.r.t. the model parameter to whatever is already stored in .grad
- So, after each gradient update, we need to set .grad back to zero

```
# The number of epochs to run
epochs = 100
for epoch in range(epochs):
    # Zero the gradients
                                         Set all the parameter gradients
    optimizer.zero_grad() +
                                         to zero.
    # Forward pass
    y_pred = net(X_train_tensor)
    # Compute loss
    loss = loss_function(y_pred, y_train_tensor)
    # Backward pass and optimize
    loss.backward()
    optimizer.step()
    # Print statistics
    if epoch % 10 == 0:
        print(f'Epoch [{epoch}], Loss: {loss.item():.4f}')
```

### Results

- Runtime: 36.9 seconds on my desktop.
  - This is training a much more complicated model than the simple linear model we trained using autograd.
- Next, evaluate on the test set.
  - Note: When evaluating the model we do not need to store intermediate values during a forwards pass.
  - Torch.no\_grad() tells PyTorch not to store extra information during a forwards pass.

```
# Evaluate the model with test data
with torch.no_grad():
    y_pred_test = net(X_test_tensor)
    test_loss = loss_function(y_pred_test, y_test_tensor)
    print(f'Test Loss: {test_loss.item():.4f}')
```

Epoch	[0/100],	Loss: 8	8.3346
Epoch	[10/100],	Loss:	1.3681
Epoch	[20/100],	Loss:	0.9073
Epoch	[30/100],	Loss:	0.7348
Epoch	[40/100],	Loss:	0.7225
Epoch	[50/100],	Loss:	0.6655
Epoch	[60/100],	Loss:	0.6407
Epoch	[70/100],	Loss:	0.6143
Epoch	[80/100],	Loss:	0.5949
Epoch	[90/100],	Loss:	0.5819

Test Loss: 0.5778

### Runtime

- 32.7 seconds is a significant training time for such a small data set.
- My work desktop has an Intel i9-9900k with 16 cores (CPU).
- It also has an RTX 2070 GPU
  - This has 2304 cores! (An RTX 4090 has 18,432 CUDA cores and 512 special "Tensor" cores)
- These GPU cores are limited in comparison to CPU cores.
  - No branch prediction
  - Limited cache
  - Shorter pipeline (typically)
    - Slower clock (1.605 GHz vs 5 MHz)
  - Not designed for parallel processing (many processes running at once)
- Designed to perform many simple operations like dot products efficiently and in parallel
  - These operations are useful for displaying graphics (e.g., applying simple functions to each pixel on the screen between every frame, changing things like lighting)
  - They are also useful for ML! Running an ANN means computing a *lot* of dot products (and some non-linearities).

### PyTorch and CUDA

- The Jupyter Notebook associated with this lecture includes instructions for installing NVIDIA CUDA, which is necessary to use PyTorch to train models on the GPU.
- Note that PyTorch is compatible with CUDA 12.1, not the latest CUDA 12.4.
- Notice that you need to custom-install the version of PyTorch that is compatible with the version of CUDA that you installed.
- Some ML libraries and tools are only compatible with specific versions of CUDA, and so you may need to use different versions of CUDA and PyTorch for different applications.

### Training on the GPU

• Check if CUDA (GPU support) is available.

device = torch.device("cuda" if torch.cuda.is\_available() else "cpu")

• Move the network to the GPU.

net.to(device)

• Move the training data to the GPU.

X\_train\_tensor = X\_train\_tensor.to(device)

y\_train\_tensor = y\_train\_tensor.to(device)

• When we are done training the model, we can then move it back to the CPU:

net.to('cpu')

<pre>net = FullyConnectedNetwork()</pre>	# Create a new network to train from scratch
<pre>optimizer = optim.Adam(net.parameters())</pre>	# Create the optimizer for this network
<pre>device = torch.device("cuda" if torch.cuda</pre>	.is_available() else "cpu")
<pre>display(device)</pre>	# Confirm that the GPU is being used
not to (dovice)	# Move the network to CDU if eveilable
het.to(device)	# Move the network to GPU IT available
X_train_tensor = X_train_tensor.to(device)	# Also move the tensors to the chosen device
<pre>y_train_tensor = y_train_tensor.to(device)</pre>	
epochs = 100	# Number of epochs
for epoch in range(epochs):	
ontimizer zero grad()	# Zero the gradients
v prod = pot(X train tonson)	# Convend pace
y_pred = net(x_train_tensor)	# Forward pass
loss = loss_function(y_pred, y_train_to	ensor) # Compute the loss for printing/plotting
loss.backward()	# Backwards pass
optimizer.step()	# Update the weights using the optimizer
if epoch % 10 == 0:	# Print statistics
<pre>print(f'Epoch [{epoch}/{epochs}],</pre>	<pre>Loss: {loss.item():.4f}')</pre>
<pre>net.to('cpu')</pre>	# Move the model back to the CPU
Move the model beak to the OF	I Lifvou will rup it or monipulate it on the ODU (e.g., equing the
שטעפ נחפ חוסטפנ שמכא נס נחפ כף	To it you will full it of manipulate it on the CPU (e.g., saving the

model/weights to a file). Leave on the GPU if you will only run it on the GPU.

#### device(type='cuda')

Epoch	[0/100],	_oss:	8.4130
Epoch	[10/100],	Loss:	1.5344
Epoch	[20/100],	Loss:	0.8190
Epoch	[30/100],	Loss:	0.7992
Epoch	[40/100],	Loss:	0.7053
Epoch	[50/100],	Loss:	0.6705
Epoch	[60/100],	Loss:	0.6278
Epoch	[70/100],	Loss:	0.6009
Epoch	[80/100],	Loss:	0.5837
Epoch	[90/100],	Loss:	0.5744



### Mini-Batches (GPU)

- Typically, mini-batches are computed on the CPU.
- They are then passed to the GPU to perform a gradient update.
- PyTorch's DataLoader object facilitates passing data efficiently (using multiple CPU cores) between the CPU and GPU.
- Often GPUs have limited memory, so entire data sets may not fit on the GPU.
  - RTX 2070: **8 GB memory**, 2304 CUDA cores, ~\$350
  - RTX 4090: 24 GB memory, 16384 CUDA cores, ~\$1,500
  - A100: 80 GB memory, 6912 CUDA cores, ~\$8,000
    - Custom made for deep learning with large models.
- Mini-batches can be created using the PyTorch DataLoader.
  - DataLoader works with PyTorch's own data set object: TensorDataset.

```
net = FullyConnectedNetwork()
                               optimizer = optim.Adam(net.parameters())
                               device = torch.device("cuda" if torch.cuda.is available() else "cpu")
                               net.to(device)
Convert the training data
                               # Create a TensorDataset and DataLoader
into a TensorDataset, so
                               train dataset = TensorDataset(X train tensor, y train tensor)
that it is compatible with
                               train loader = DataLoader(dataset=train dataset, batch size=100, shuffle=True)
DataLoader.
                               epochs = 100
                               for epoch in range(epochs):
Note: batch size = 100
                                   total loss = 0.0 # To sum the loss over all batches
                                   num batches = 0  # A lazy way to get the number of batches: count them
                                   for X batch, y batch in train loader:
                                                                                                  # Iterate over mini-batches
                                      X batch, y batch = X batch.to(device), y batch.to(device) # Move batches to GPU
                                      optimizer.zero grad()
                                      y_{pred} = net(X_{batch})
                                      loss = loss function(y pred, y batch)
                                      total loss += loss.item()
                                      num batches += 1
                                      loss.backward()
                                      optimizer.step()
                                   # Calculate the average loss over all mini-batches in this epoch
                                   average loss = total loss / num batches
                                   if epoch % 10 == 0: # Print statistics
                                       print(f'Epoch [{epoch}], Average Loss: {average loss:.4f}')
                               net.to('cpu') # Move the model back to CPU if needed
```

```
net = FullyConnectedNetwork()
optimizer = optim.Adam(net.parameters())
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
net.to(device)
```

```
# Create a TensorDataset and DataLoader
train_dataset = TensorDataset(X_train_tensor, y_train_tensor)
train loader = DataLoader(dataset=train dataset, batch size=100, shuffle=True)
```

```
epochs = 100
for epoch in range(epochs):
   total loss = 0.0 # To sum the loss over all batches
   num batches = 0  # A lazy way to get the number of batches: count them
   for X batch, y batch in train loader:
                                                                   # Iterate over mini-batches
       X batch, y batch = X batch.to(device), y batch.to(device) # Move batches to GPU
       optimizer.zero grad()
       y pred = net(X batch)
       loss = loss function(y pred, y batch)
       total loss += loss.item()
       num batches += 1
       loss.backward()
       optimizer.step()
   # Calculate the average loss over all mini-batches in this epoch
   average loss = total loss / num batches
```

```
if epoch % 10 == 0: # Print statistics
    print(f'Epoch [{epoch}/{epochs}], Average Loss: {average_loss:.4f}')
net.to('cpu') # Move the model back to CPU if needed
```

Update tracking of losses to compute the average loss per mini-batch each epoch

```
net = FullyConnectedNetwork()
                              optimizer = optim.Adam(net.parameters())
                              device = torch.device("cuda" if torch.cuda.is available() else "cpu")
                              net.to(device)
                              # Create a TensorDataset and DataLoader
                              train dataset = TensorDataset(X train tensor, y train tensor)
                              train loader = DataLoader(dataset=train dataset, batch size=100, shuffle=True)
                              epochs = 100
                              for epoch in range(epochs):
                                  total loss = 0.0 # To sum the loss over all batches
                                  num batches = 0  # A lazy way to get the number of batches: count them
Loop over batches using the
                                  for X batch, y batch in train loader:
                                                                                                 # Iterate over mini-batches
DataLoader, sending
                                      X batch, y batch = X batch.to(device), y batch.to(device) # Move batches to GPU
batches to the GPU.
                                      optimizer.zero grad()
                                      y pred = net(X batch)
                                      loss = loss function(y pred, y batch)
                                      total_loss += loss.item()
                                      num batches += 1
                                      loss.backward()
                                      optimizer.step()
                                  # Calculate the average loss over all mini-batches in this epoch
                                  average loss = total loss / num batches
                                  if epoch % 10 == 0: # Print statistics
                                      print(f'Epoch [{epoch}], Average Loss: {average loss:.4f}')
```

```
net.to('cpu') # Move the model back to CPU if needed
```

```
net = FullyConnectedNetwork()
optimizer = optim.Adam(net.parameters())
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
net.to(device)
```

```
# Create a TensorDataset and DataLoader
train_dataset = TensorDataset(X_train_tensor, y_train_tensor)
train loader = DataLoader(dataset=train dataset, batch size=100, shuffle=True)
```

```
epochs = 100
```

```
for epoch in range(epochs):
```

<pre>total_loss = 0.0 # To sum the loss over all batches</pre>		
<pre>num_batches = 0 # A lazy way to get the number of batches:</pre>	count them	
for X_batch, y_batch in train_loader:	# Iterate	over mini-batches
<pre>X_batch, y_batch = X_batch.to(device), y_batch.to(device)</pre>	# Move bat	ches to GPU
optimizer.zero_grad()		
<pre>y_pred = net(X_batch)</pre>		
<pre>loss = loss_function(y_pred, y_batch)</pre>		
<pre>total_loss += loss.item()</pre>		
num_batches += 1		
loss.backward()		
<pre>optimizer.step()</pre>		

# Calculate the average loss over all mini-batches in this epoch average\_loss = total\_loss / num\_batches

```
if epoch % 10 == 0: # Print statistics
    print(f'Epoch [{epoch}], Average Loss: {average_loss:.4f}')
net.to('cpu') # Move the model back to CPU if needed
```

We do **not** need to "remove" the batches from GPU memory. This is done automatically.

### What do we expect to happen?

• Recall, 100 epochs before:

Epoch [0/100], Loss: 8.4130 Epoch [10/100], Loss: 1.5344 Epoch [20/100], Loss: 0.8190 Epoch [30/100], Loss: 0.7992 Epoch [40/100], Loss: 0.7053 Epoch [50/100], Loss: 0.6705 Epoch [60/100], Loss: 0.6278 Epoch [70/100], Loss: 0.6009 Epoch [80/100], Loss: 0.5837 Epoch [90/100], Loss: 0.5744

• Now we run 100 epochs using mini-batches of size 100

Epoch	[0/100], /	Average l	_oss: (	0.7102
Epoch	[10/100],	Average	Loss:	0.5707
Epoch	[20/100],	Average	Loss:	0.5621
Epoch	[30/100],	Average	Loss:	0.5527
Epoch	[40/100],	Average	Loss:	0.5417
Epoch	[50/100],	Average	Loss:	0.5260
Epoch	[60/100],	Average	Loss:	0.5058
Epoch	[70/100],	Average	Loss:	0.4798
Epoch	[80/100],	Average	Loss:	0.4524
Epoch	[90/100],	Average	Loss:	0.4282

#### We have never seen sample MSEs so low!

### Evaluate on the test set

• Remember to use torch.no\_grad() for faster evaluation

```
# Evaluate the model with test data (optional)
with torch.no_grad():
    y_pred_test = net(X_test_tensor)
    test_loss = loss_function(y_pred_test, y_test_tensor)
    print(f'Test Loss: {test_loss.item():.4f}')
```

- Note:
  - The net model was moved back to the CPU.
  - The testing data is on the CPU.
  - We could have left the  ${\tt net}$  model on the GPU and moved the testing data to the GPU.

Epoch [0/100], Average Loss: 0.7102 Epoch [10/100], Average Loss: 0.5707 Epoch [20/100], Average Loss: 0.5621 Epoch [30/100], Average Loss: 0.5527 Epoch [40/100], Average Loss: 0.5417 Epoch [50/100], Average Loss: 0.5260 Epoch [60/100], Average Loss: 0.5058 Epoch [70/100], Average Loss: 0.4798 Epoch [80/100], Average Loss: 0.4524 Epoch [90/100], Average Loss: 0.4282

Test Loss: 0.7296

### No method has achieved a test loss so… **high**! **Question**: Why is the test loss so much higher than the training loss? **Answer**: The network has **overfit** to the training data.

### Overfitting

- Recall that the *training* error for *nearest neighbor* (NN) was zero, but the testing error was large.
  - NN essentially "memorized" the training data, and gave good predictions for the training data.
  - The model did not **generalize** to new inputs: it had high errors for points not in the training data.
- When this happens using parametric models, it is called **overfitting**.

### 10 points from y = x + N(0,1)



### Least Squares fit, 10<sup>th</sup> Degree Polynomial

- Linear parametric model using 10<sup>th</sup> degree polynomial basis.
- The model perfectly predicts every training point!
- The model will have significant error for new points.



### Least Squares fit, 10<sup>th</sup> Degree Polynomial

- Linear parametric model using 10<sup>th</sup> degree polynomial basis.
- The model perfectly predicts every training point!
- The model will have significant error for new points.
- A linear fit (with no basis) would provide better predictions for new points!



Linear and 10th Degree Polynomial Fit to Points with Gaussian Noise

### Overfitting

- When training parametric models with gradient descent, initially the loss decreases on the training **and** testing sets.
  - The model is learning general trends in the data that generalize to new points.
- Eventually, the model starts to learn specific trends in the training data that do **not** generalize to new points.
  - This typically results in lower loss on the training data, but higher loss (or no change in loss) for the testing data.

### Plotting Training vs Testing Loss (General Case)

**Idea**: Stop training when the testing loss starts increasing.



### Plotting Training vs Testing Loss (GPA Data)

• With a *relatively* simple problem, overfitting begins within the first epoch!



### **Overfitting and Model Complexity/Capacity**

- Notice that we can't overfit this data using a line!
- The model complexity or model capacity refers to a parametric model's ability to represent general functions.
  - Models with higher complexity/capacity can represent more functions.
  - Models with higher complexity/capacity are more prone to over-fitting.



Linear and 10th Degree Polynomial Fit to Points with Gaussian Noise

## Avoiding Over-Fitting (Overview of Strategies)

- 1. Early stopping: Stop training when testing error increases.
  - Typically split data into training, validation, and testing
  - Stop training when the error on the *validation* set begins to increase
  - This ensures that the training process never looks at the testing data
- 2. Include a "regularization" term in the loss function
  - Complete details are beyond the scope of this course.
  - Regularization terms increase the loss the farther the weight vector is from zero:  $L_{\text{new}}(w, D) = L(w, D) + \lambda ||w||$ 
    - Often using the L1 norm,  $||w|| = \sum_j |w_j|$  or the L2 norm  $||w|| = \sqrt{\sum_j w_j^2}$ .
- 3. Other strategies (e.g., dropout)
- 4. Use a large network!

↓ ||·|| denotes a **norm** (a notion of "length")

### "Use a large network": Double Descent

- Large networks seem like they should be particularly prone to overfitting.
- When trained sufficiently on large amounts of data, empirical evidence suggests that deep (large) networks tend not to over-fit!

This phenomenon, called *double descent*, is an active research topic!



# End

