CS498: Algorithmic Engineering

Lecture 22: Neural Networks & PyTorch

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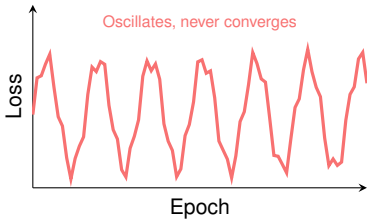
Week 12

Outline

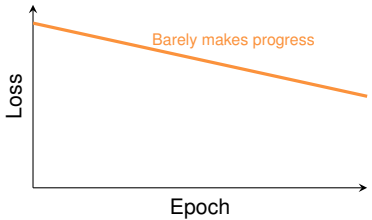
Why Not a Constant Learning Rate?

What happens if we just pick one learning rate and keep it forever?

η too high



η too low



Too high: the optimizer overshoots and oscillates. Too low: the optimizer crawls and never reaches a good solution.

Key insight: we want a learning rate that *changes* over training.

Linear Warmup and Cosine Decay

At the start of training, weights are **random** and gradients are noisy. Adam's moment estimates need several steps to calibrate.

If we take big steps with bad gradients, the model can land in a bad region early and never recover.

Linear warmup: start with $\eta \approx 0$ and linearly increase to $\eta_{\max}$ over T_w steps.

After warmup, we want η to **decrease**. Early in training, big steps explore; late in training, small steps fine-tune.

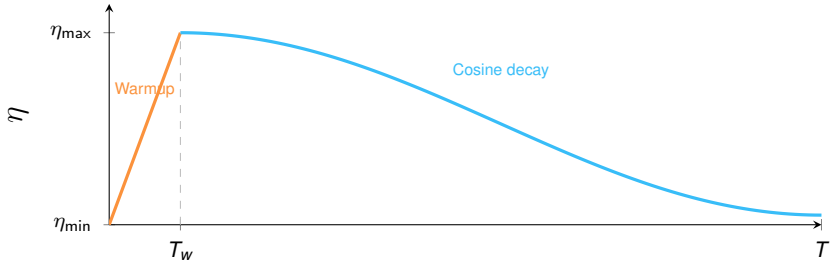
Cosine decay formula:

$$\eta_t = \frac{1}{2}\eta_{\max}\left(1 + \cos\left(\frac{\pi\,(t - T_w)}{T - T_w}\right)\right)$$

Starts at $\eta_{\max}$, smoothly decays to 0. The cosine shape gives a gradual transition.

What Does the Full Schedule Look Like?

Combine warmup + cosine decay into a single schedule:



Typical values:

- Warmup: 1%–5% of total training steps.
- $\eta_{\max}$ depends on model size: 10^{-3} for small models, 10^{-4} for large.
- This schedule is used in most modern training run (GPT, LLaMA, ...)

A Puzzle About Model Size

In Lecture 21, the bias-variance tradeoff told us:

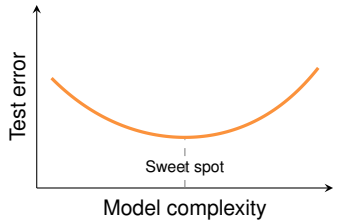
- More complexity $\rightarrow$ lower bias, higher variance.
- There is a sweet spot. Past it, test error goes up.

But: modern neural networks have *billions* of parameters, far more than training data points, and they work spectacularly well.

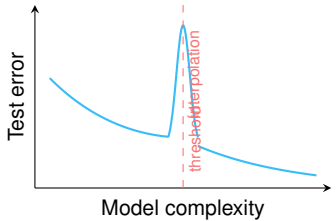
How is that possible? Shouldn't they overfit catastrophically?

Classical View vs. What Actually Happens

Classical U-shape



Double descent (reality)



Test error goes up, then **spikes** at the interpolation threshold, then comes back **down**. This is **double descent**.

The interpolation threshold is the smallest model that can perfectly fit the training data.

Why Does the Spike Happen, Then Resolve?

At the interpolation threshold, the model has *just barely* enough capacity to fit every training point. It is forced to pass through every point exactly, including noisy ones, producing wild oscillations.

Think of fitting a degree-$(n-1)$ polynomial through n noisy points: perfect interpolation but extreme oscillation.

In words: just enough capacity to memorize $=$ worst generalization.

Beyond the threshold, the model is **overparameterized**: many parameter settings fit the data perfectly. SGD's **implicit regularization** (from Lecture 21) selects flat, smooth solutions.

More parameters $\rightarrow$ smoother interpolation $\rightarrow$ better generalization.

Takeaway: overparameterization + SGD's implicit bias combine to produce well-generalizing solutions.

What Does Double Descent Mean in Practice?

The classical rule “more parameters = more overfitting” is **wrong** in the overparameterized regime. This is why billion-parameter models generalize well.

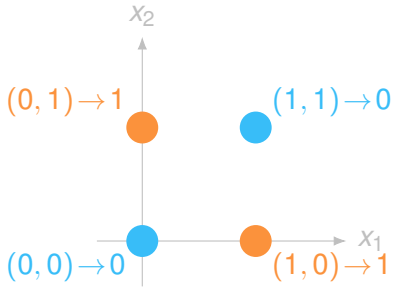
Double descent was empirically demonstrated by Belkin et al. (2019).

Practical implications:

- If your model is near the interpolation threshold, make it *bigger*, not smaller.
- Modern practice: use very large models and rely on implicit regularization.

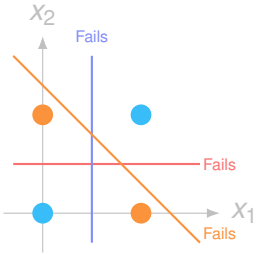
Can a Line Separate These Points?

Consider the XOR function. Four data points, two classes:



No Linear Boundary Works

Let us try three different lines:



What If We Could Transform the Inputs?

Key insight: if we map inputs into a new space where the classes *are* separable, a linear classifier on top would work.

Example: define $h = |x_1 - x_2|$.

x_1	x_2	$h = \lvert x_1 - x_2 \rvert$	y
0	0	0	0
0	1	1	1
1	0	1	1
1	1	0	0

Now a simple threshold $h > 0.5$ separates perfectly. But we hand-designed this feature.

What if we *parameterize* the transformation and optimize it with gradient descent? This is exactly what a neural network does.

What Is the Neural Network Idea?

Instead of hand-engineering features, stack **learned transformations**:

1. Take input $\mathbf{x}$.
2. Apply a **linear transform**: $\mathbf{z} = W_1\mathbf{x} + \mathbf{b}_1$.
3. Apply a **nonlinear activation**: $\mathbf{h} = \sigma(\mathbf{z})$, element-wise.
4. Apply another linear transform: $\hat{y} = W_2\mathbf{h} + \mathbf{b}_2$.

In one line:

$$f_\theta(\mathbf{x}) = W_2\,\sigma(W_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2$$

Why the nonlinearity?

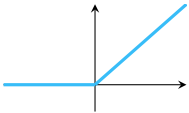
Without σ, composing two linear transforms gives another linear transform: $W_2(W_1\mathbf{x}) = (W_2W_1)\mathbf{x}$.

The nonlinearity breaks this collapse and lets the model represent nonlinear boundaries.

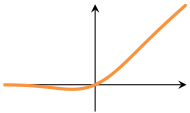
What Are the Common Activation Functions?

The nonlinearity σ is applied element-wise. Three common choices:

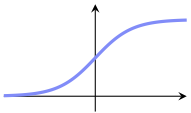
ReLU: $\max(0, z)$



GELU (smooth ReLU)

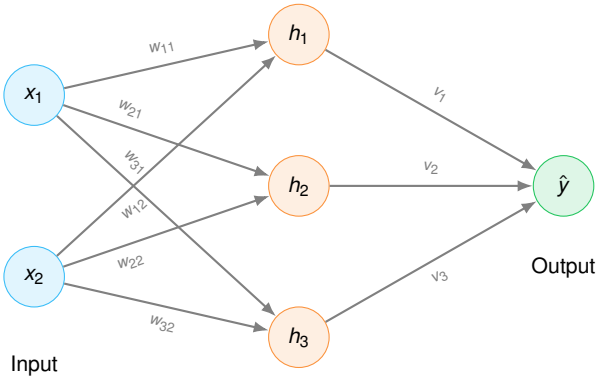


Sigmoid: $\frac{1}{1+e^{-z}}$



ReLU: gradient is 0 or 1. Simple, fast, widely used.
GELU: smooth approximation of ReLU. Standard in transformers (GPT, BERT).
Sigmoid: squashes to $[0, 1]$. Good for probabilities.

How Does a 2-Layer Network Look?



Formula: $\hat{y} = v_1 h_1 + v_2 h_2 + v_3 h_3 + b_2$, where $h_i = \text{ReLU}(w_{i1} x_1 + w_{i2} x_2 + b_{1,i})$.
This is a 2-layer network with 3 hidden neurons. Let us use it to solve XOR.

Solving XOR: Setting Up and Testing Weights

Choose

$$W_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \mathbf{b}_1 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \qquad \mathbf{v} = \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}, \qquad b_2 = 0.$$

Compute

$$\mathbf{z} = W_1\mathbf{x} + \mathbf{b}_1, \qquad \mathbf{h} = \mathrm{ReLU}(\mathbf{z}), \qquad \hat{y} = \mathbf{v}^\top \mathbf{h} + b_2.$$

Input $(0,0)$**, target** $y = 0$**:** $\mathbf{z} = (0,0,-1)^\top, \mathbf{h} = (0,0,0)^\top, \hat{y} = 0$. ✓
Input $(0,1)$**, target** $y = 1$**:** $\mathbf{z} = (0,1,0)^\top, \mathbf{h} = (0,1,0)^\top, \hat{y} = 1$. ✓
Input $(1,0)$**, target** $y = 1$**:** $\mathbf{z} = (1,0,0)^\top, \mathbf{h} = (1,0,0)^\top, \hat{y} = 1$. ✓
Input $(1,1)$**, target** $y = 0$**:** $\mathbf{z} = (1,1,1)^\top, \mathbf{h} = (1,1,1)^\top, \hat{y} = 1 + 1 - 2 = 0$. ✓

All four inputs are classified correctly.

Solving XOR: Why This Works

Key insight (On Binary Inputs):

$$h_1 = \mathrm{ReLU}(x_1) = x_1, \qquad h_2 = \mathrm{ReLU}(x_2) = x_2, \qquad h_3 = \mathrm{ReLU}(x_1 + x_2 - 1) = x_1 x_2.$$

On binary inputs, $h_3 = 1$ exactly when both inputs are 1, so

$$\hat{y} = h_1 + h_2 - 2h_3 = x_1 + x_2 - 2x_1 x_2,$$

which is exactly XOR.

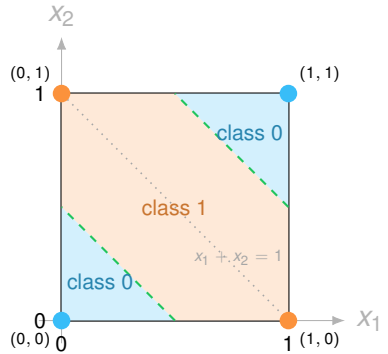
Neural Networks can learn the transformations automatically. The goal is to find good parameters using an optimizer.

What Region of the Input Space Maps to Class 1?

Our network computes

$$\hat{y}(x_1, x_2) = \mathrm{ReLU}(x_1) + \mathrm{ReLU}(x_2) - 2\,\mathrm{ReLU}(x_1 + x_2 - 1).$$

On the XOR domain $(x_1, x_2) \in [0, 1]^2$, if we predict class 1 when $\hat{y} > \frac{1}{2}$, then



Going Deeper and Universal Approximation

Stack more layers, each with its own learned transform and nonlinearity:

$$\begin{aligned}
\mathbf{h}_1 &= \sigma_1(W_1\mathbf{x} + \mathbf{b}_1) \\
\mathbf{h}_2 &= \sigma_2(W_2\mathbf{h}_1 + \mathbf{b}_2) \\
&\vdots \\
\hat{y} &= W_{L+1}\mathbf{h}_L + \mathbf{b}_{L+1}
\end{aligned}$$

Each layer refines the representation. Early layers learn simple features, later layers compose them into complex ones.
This is a **Multi-Layer Perceptron** (MLP), aka a feedforward neural network.

Going Deeper and Universal Approximation

Universal Approximation Theorem (Cybenko 1989, Hornik 1991):

Statement

A neural network with a single hidden layer of sufficient width can approximate any continuous function on a compact domain to arbitrary precision.

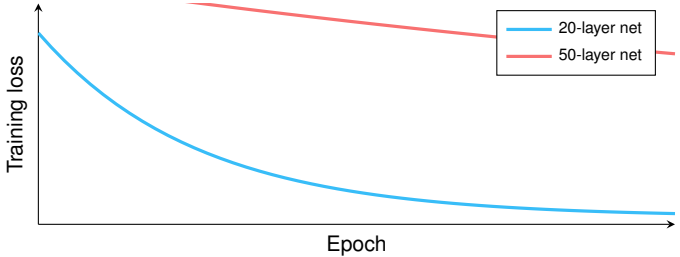
This is an *existence* result: it says the model *can* represent the function, not that SGD will find those weights.

It also says nothing about how wide the layer needs to be. The required width could be exponentially large.

The Universal Approximation Theorem says one wide layer suffices in theory. **In practice:** deeper networks are far more parameter-efficient.

What Goes Wrong in Deep Networks?

Let us try training very deep networks:



The 50-layer net trains **worse**. This should not happen: it contains all 20-layer nets as a special case (set extra layers to identity).

The question is: what prevents the deeper network from learning?

Why Do Gradients Vanish?

By the chain rule, the gradient passes through every layer:

$$\frac{\partial \mathcal{L}}{\partial W_1} = \frac{\partial \mathcal{L}}{\partial \mathbf{h}_L} \cdot \frac{\partial \mathbf{h}_L}{\partial \mathbf{h}_{L-1}} \cdots \frac{\partial \mathbf{h}_2}{\partial \mathbf{h}_1} \cdot \frac{\partial \mathbf{h}_1}{\partial W_1}$$

This is a product of L Jacobian matrices. If each has spectral norm < 1:

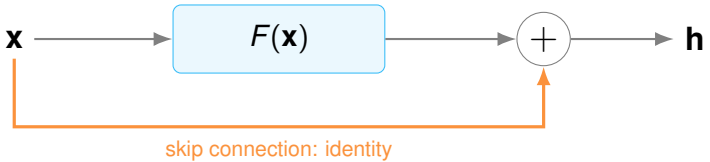
$$\left\| \frac{\partial \mathcal{L}}{\partial W_1} \right\| \leq \prod_{k=1}^{L} \left\| \frac{\partial \mathbf{h}_{k+1}}{\partial \mathbf{h}_k} \right\| \cdot \left\| \frac{\partial \mathcal{L}}{\partial \mathbf{h}_L} \right\|$$

If each factor is 0.9, then with 50 layers: $0.9^{50} \approx 0.005$. **The gradient shrinks exponentially with depth.** Early layers barely update. This is the **vanishing gradient problem**.

What Are Residual Connections?

Instead of learning $\mathbf{h} = F(\mathbf{x})$, learn the **residual**:

$$\mathbf{h} = F(\mathbf{x}) + \mathbf{x}$$



The gradient: $\frac{\partial \mathbf{h}}{\partial \mathbf{x}} = \frac{\partial F(\mathbf{x})}{\partial \mathbf{x}} + I$

The $+I$ means the gradient can never vanish to zero. It flows directly through the skip connection.

Why Do Residual Connections Work So Well?

The network only needs to learn the *residual* $F(\mathbf{x}) = \text{desired output} - \mathbf{x}$.

This is the key innovation of ResNet (He et al., 2015).

Before ResNet: training networks deeper than $\sim$20 layers was very difficult.
After ResNet: networks with 100+ layers trained successfully.

Today, **every** major architecture uses residual connections: transformers, modern CNNs, diffusion models.

Normalization: LayerNorm and RMSNorm

As data flows through many layers, activation distributions can shift dramatically, making training unstable.

Layer Normalization normalizes across features at each layer:

$$\text{LayerNorm}(\mathbf{h}) = \gamma \odot \frac{\mathbf{h} - \mu}{\sqrt{\sigma^2 + \varepsilon}} + \beta$$

where μ, σ^2 are the mean and variance of $\mathbf{h}$, and γ, β are **learned** scale/shift parameters.

RMSNorm (used in LLaMA, Qwen, Gemma) is a simpler variant that skips the mean subtraction:

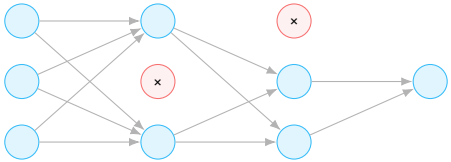
$$\text{RMSNorm}(\mathbf{h}) = \gamma \odot \frac{\mathbf{h}}{\text{RMS}(\mathbf{h})}, \quad \text{RMS}(\mathbf{h}) = \sqrt{\frac{1}{d}\sum_i h_i^2}$$

RMSNorm is simpler, slightly faster, and works just as well.

How Does Dropout Prevent Overfitting?

With millions of parameters, a network can **memorize** the training data: near-zero training loss, high test loss.

Dropout (Srivastava et al., 2014): during training, randomly set each neuron's output to 0 with probability p.



× = dropped (output set to 0)

Each forward pass uses a different random subnetwork. No single neuron can be too important.

At test time: use the full network (no dropout).

Building Blocks Summary

Problem	Solution	Mechanism
Vanishing gradients	Residual connections	$\mathbf{h} = F(\mathbf{x}) + \mathbf{x}$
Unstable activations	LayerNorm / RMSNorm	Normalize each layer
Overfitting	Dropout	Random neuron zeroing

Every modern neural network uses some combination of these three. Transformers use all three: residual connections around every block, layer normalization before each block, and dropout on attention weights and hidden states.

How Do We Define a Neural Network in PyTorch?

Every neural network in PyTorch inherits from `nn.Module`.

Two methods: `__init__` declares layers, `forward` defines the computation.

```
import torch
import torch.nn as nn

class MLP(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim):
        super().__init__()
        self.layer1 = nn.Linear(input_dim, hidden_dim)
        self.relu = nn.ReLU()
        self.layer2 = nn.Linear(hidden_dim, output_dim)

    def forward(self, x):
        x = self.layer1(x)
        x = self.relu(x)
        x = self.layer2(x)
        return x
```

PyTorch automatically tracks all parameters declared in `__init__` for `.backward()`.

nn.Sequential and Model Inspection

For simple stacked architectures, use `nn.Sequential`:

```
model = nn.Sequential(
    nn.Flatten(),           # 28x28 image -> 784 vector
    nn.Linear(784, 256),    # first hidden layer
    nn.ReLU(),
    nn.Linear(256, 128),    # second hidden layer
    nn.ReLU(),
    nn.Linear(128, 10)      # output: 10 digit classes
)
```

Use `nn.Sequential` for simple architectures; use `nn.Module` for more complex networks.

```
total = sum(p.numel() for p in model.parameters())
print(f"Total parameters: {total:,}")  # 235,146
```

Breakdown: Layer 1: $784 \times 256 + 256 = 200{,}960$. Layer 2: $256 \times 128 + 128 = 32{,}896$. Layer 3: $128 \times 10 + 10 = 1{,}290$. **Total: 235,146.**

How Do We Load Data?

MNIST: 60,000 training images of handwritten digits (28×28 pixels, 10 classes).

```
from torchvision import datasets, transforms
from torch.utils.data import DataLoader

transform = transforms.Compose([
    transforms.ToTensor(),            # PIL image -> tensor
    transforms.Normalize((0.1307,), (0.3081,))  # mean, std
])

train_data = datasets.MNIST('.', train=True, download=True,
                            transform=transform)
test_data = datasets.MNIST('.', train=False, transform=transform)

train_loader = DataLoader(train_data, batch_size=64, shuffle=True)
test_loader = DataLoader(test_data, batch_size=1000, shuffle=False)
```

`DataLoader` handles:

- **Batching**: groups data into mini-batches of size 64.
- **Shuffling**: randomizes order each epoch (important for SGD).
- **Parallel loading**: can use multiple workers to load data in the background.

What Does the Training Loop Look Like?

The core of training is just six lines inside the inner loop:

```
optimizer = torch.optim.AdamW(model.parameters(), lr=1e-3)

for epoch in range(10):
    for images, labels in train_loader:
        logits = model(images)                          # 1. Forward pass
        loss = nn.functional.cross_entropy(logits, labels)  # 2. Compute loss
        optimizer.zero_grad()                           # 3. Zero old gradients
        loss.backward()                                 # 4. Backprop
        optimizer.step()                                # 5. Update weights
```

Line by line:

1. Forward pass: run the batch through the model, get logits.
2. Compute loss. Then zero old gradients (PyTorch accumulates by default).
3. Backpropagation: compute gradients. Optimizer step: update parameters.

What Is Cross-Entropy Loss?

The model outputs **logits** $z_1, \ldots, z_n$: raw, unnormalized scores for each class.

Softmax converts logits to probabilities:

$$p_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

Cross-entropy measures how far the prediction is from the true label.

Example: logits $\mathbf{z} = (2.0, 0.5, -1.0)$, true class is 0.

Softmax:

$$(0.786,\ 0.175,\ 0.039)$$

Cross-entropy:

$$-\log p_{\text{true}} = -\log(0.786) \approx 0.241$$

How Do We Evaluate the Model?

Switch to evaluation mode and disable gradient computation:

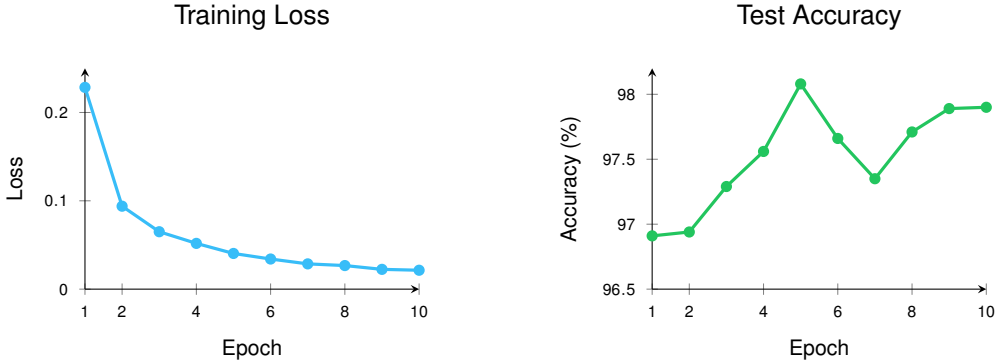
```
model.eval()   # switches off dropout, changes BatchNorm behavior
correct = 0
total = 0

with torch.no_grad():   # saves memory: no gradient tracking
    for images, labels in test_loader:
        logits = model(images)
        preds = logits.argmax(dim=1)    # highest-scoring class
        correct += (preds == labels).sum().item()
        total += labels.size(0)

accuracy = correct / total
print(f"Test accuracy: {accuracy:.1%}")  # ~98.0%
```

Key points:

- `model.eval()`: critical for correct dropout/BatchNorm behavior.
- `torch.no_grad()`: saves memory by not building the computation graph.
- `.argmax(dim=1)`: picks the class with the highest logit.

What Do the Training Curves Look Like?

Training our 235K-parameter MLP on MNIST for 10 epochs:

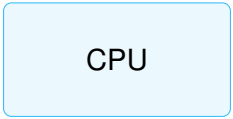


Training loss falls steadily from 0.2284 to 0.0214. Test accuracy reaches about 98%, with the best value 98.08% at epoch 5.

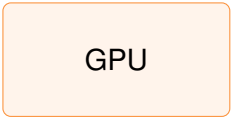
The MLP flattens images to a vector, losing all spatial structure. A 2-pixel shift

Why GPUs?

NN training is dominated by **matrix multiplications**, which can be parallelized.



8–16 fast cores
Sequential, high per-core speed



Thousands of slower cores
Parallel, massive throughput

An A100 GPU performs $\sim$312 TFLOPS in FP16.

Training that takes hours on CPU takes minutes on GPU.

What Is NCSA Delta?

NCSA Delta is the GPU cluster for this course.

Your allocation: 500 A100 GPU-hours per student (can extend to 1k). Plenty for homeworks and the final project.

How to connect:

`ssh ncsa_netid@dt-login03.delta.ncsa.illinois.edu` (not necessarily netid).

You land on a login node. **Do not run training on the login node** (shared, no GPU).

`cd /projects/bgvu/ncsa_netid` (bgvu is this class project).

Submit a **SLURM job** to request a compute node with a GPU.

SLURM is a job scheduler: you describe what resources you need and what to run, and SLURM handles the rest.

Writing and Submitting a SLURM Job

After SSH-ing into Delta and cd into project directory: Create a file `train.sh`:

```
#!/bin/bash
#SBATCH --account=bgvu-delta-gpu
#SBATCH --partition=gpuA100x4
#SBATCH --nodes=1
#SBATCH --gpus-per-node=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=16g
#SBATCH --time=00:05:00
#SBATCH --job-name=mnist_train
#SBATCH --output=mnist_%j.out
module purge
module reset
module load pytorch-conda/2.8
nvidia-smi && python train_mnist.py
```

Submit, monitor, and cancel:

```
sbatch train.sh          # Output sth like: Submitted batch job 17437859
squeue -u $USER          # check status
scancel 17437859          # cancel a job with id 17437859
cat mnist_17437859.out    # read output of job 17437859
```

The GPU Training Script

```
import torch
import torch.nn as nn
from torchvision import datasets, transforms
from torch.utils.data import DataLoader

device = torch.device('cuda')  # use GPU

transform = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((0.1307,), (0.3081,))
])
train_data = datasets.MNIST('.', train=True, download=True,
                            transform=transform)
train_loader = DataLoader(train_data, batch_size=64, shuffle=True)
```

The GPU Training Loop

```
model = nn.Sequential(
    nn.Flatten(), nn.Linear(784, 256), nn.ReLU(),
    nn.Linear(256, 128), nn.ReLU(), nn.Linear(128, 10)
).to(device)   # move model to GPU

optimizer = torch.optim.AdamW(model.parameters(), lr=1e-3)

for epoch in range(10):
    total_loss = 0
    for images, labels in train_loader:
        images = images.to(device)   # move data to GPU
        labels = labels.to(device)   # move labels to GPU

        logits = model(images)
        loss = nn.functional.cross_entropy(logits, labels)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        total_loss += loss.item()

    print(f"Epoch {epoch}: loss={total_loss/len(train_loader):.4f}")
```

What's the damage?

```
[eharb@dt-login03 eharb]$ jobcharge
Charges for user eharb and account all from 2026-03-08-23:48:11 through 2026-04-08-23:48:11.
Account           Charge (SU)
--------------  -------------
bgvu-delta-gpu           0.20


[eharb@dt-login03 eharb]$ accounts
Project Summary for User 'eharb':

Account                        Balance(Hours)   Deposited(Hours)  Project
-----------------------------  ---------------  ----------------  ----------------------
bgvu-delta-gpu                           2999              3000  gpu-accelerated llm...
```

For more details, see
https://docs.ncsa.illinois.edu/systems/delta/en/latest/index.html