

Running a forward pass

INTRODUCTION TO DEEP LEARNING WITH PYTORCH



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What is a forward pass?

- Input data is **passed forward** or **propagated** through a network
- Computations performed at each layer
- Outputs of each layer passed to each subsequent layer
- **Output** of final layer: "prediction"
- Used for both **training** and prediction

Some possible outputs:

- **Binary classification**
 - Single probability between 0 and 1
- **Multiclass classification**
 - Distribution of probabilities summing to 1
- **Regression values**
 - Continuous numerical predictions

Is there also a backward pass?

- **Backward pass**, or **backpropagation** is used to update weights and biases during training
- In the "training loop", we:
 1. **Propagate** data forward
 2. **Compare** outputs to true values (ground-truth)
 3. **Backpropagate** to update model weights and biases
 4. **Repeat** until weights and biases are tuned to produce useful outputs

Binary classification: forward pass

```
# Create input data of shape 5x6
input_data = torch.tensor(
    [[-0.4421,  1.5207,  2.0607, -0.3647,  0.4691,  0.0946],
     [-0.9155, -0.0475, -1.3645,  0.6336, -1.9520, -0.3398],
     [ 0.7406,  1.6763, -0.8511,  0.2432,  0.1123, -0.0633],
     [-1.6630, -0.0718, -0.1285,  0.5396, -0.0288, -0.8622],
     [-0.7413,  1.7920, -0.0883, -0.6685,  0.4745, -0.4245]])
```

```
# Create binary classification model
model = nn.Sequential(
    nn.Linear(6, 4), # First linear layer
    nn.Linear(4, 1), # Second linear layer
    nn.Sigmoid() # Sigmoid activation function
)
```

```
# Pass input data through model
output = model(input_data)
```

Binary classification: forward pass

```
print(output)
```

```
tensor([[0.5188], [0.3761], [0.5015], [0.3718], [0.4663]],  
        grad_fn=<SigmoidBackward0>)
```

- **Outputs:**
 - five probabilities between zero and one
 - one value for each sample (row) in data
- **Classification:**
 - Class = 1 for first and third values: 0.5188 , 0.5015
 - Class = 0 for second, fourth and fifth values: 0.3761 , 0.3718 , 0.4633

Multi-class classification: forward pass

```
# Specify model has three classes
n_classes = 3

# Create multiclass classification model
model = nn.Sequential(
    nn.Linear(6, 4), # First linear layer
    nn.Linear(4, n_classes), # Second linear layer
    nn.Softmax(dim=-1) # Softmax activation
)

# Pass input data through model
output = model(input_data)
print(output.shape)
```

```
torch.Size([5, 3])
```

Multi-class classification: forward pass

```
print(output)
```

```
tensor([[0.4969, 0.3606, 0.1425],  
        [0.5105, 0.3262, 0.1633],  
        [0.3253, 0.3174, 0.3572],  
        [0.5499, 0.3361, 0.1141],  
        [0.4117, 0.3366, 0.2517]], grad_fn=<SoftmaxBackward0>)
```

- **Outputs:**
 - The output dimension is 5×3
 - Each row sums to one
 - Value with highest probability is assigned predicted label in each row
 - Row 1 = class 1 (mammal), row 2 = class 1 (mammal), row 3 = class 3 (reptile)

Regression: forward pass

```
# Create regression model
model = nn.Sequential(
    nn.Linear(6, 4), # First linear layer
    nn.Linear(4, 1) # Second linear layer
)

# Pass input data through model
output = model(input_data)

# Return output
print(output)
```

```
tensor([[0.3818],
        [0.0712],
        [0.3376],
        [0.0231],
        [0.0757]],
        grad_fn=<AddmmBackward0>)
```


Let's practice!

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Using loss functions to assess model predictions

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Why do we need a loss function?

Loss function:

- Gives feedback to model during training
- Takes in model prediction \hat{y} and ground truth y
- Outputs a float

Why do we need a loss function?

| hair | feathers | eggs | milk | airborne | aquatic | predator | toothed | backbone | breathes | venomous | fins | legs | tail | domestic | catsize | class |
|------|----------|------|------|----------|---------|----------|---------|----------|----------|----------|------|------|------|----------|---------|-------|
| 1 | 0 | 0 | 1 | 0 | 0 | 1 | 1 | 1 | 1 | 0 | 0 | 4 | 0 | 0 | 1 | 0 |

- Predicted class = 0 -> **correct** = low loss
- Predicted class = 1 -> **wrong** = high loss
- Predicted class = 2 -> **wrong** = high loss

One-hot encoding concepts

- $loss = F(y, \hat{y})$
- y is a single **integer** (class label)
 - e.g. $y = 0$ when y is a mammal
- \hat{y} is a **tensor** (output of softmax)
 - If N is the number of classes, e.g. $N = 3$
 - \hat{y} is a tensor with N dimensions,
 - e.g. $\hat{y} = [0.57492, 0.034961, 0.15669]$

How do we compare an integer with a tensor?

One-hot encoding concepts

Transforming true label to tensor of zeros and ones

| | | | |
|---------------------|---|---|---|
| | ground truth $y = 0$ number of classes $N = 3$ | | |
| class | 0 | 1 | 2 |
| one-hot encoding | 1 | 0 | 0 |

```
one_hot_numpy = np.array([1, 0, 0])
```

Transforming labels with one-hot encoding

```
import torch.nn.functional as F
```

```
F.one_hot(torch.tensor(0), num_classes = 3)
```

```
tensor([1, 0, 0])
```

```
F.one_hot(torch.tensor(1), num_classes = 3)
```

```
tensor([0, 1, 0])
```

```
F.one_hot(torch.tensor(2), num_classes = 3)
```

```
tensor([0, 0, 1])
```

Cross entropy loss in PyTorch

```
from torch.nn import CrossEntropyLoss

scores = tensor([[ -0.1211,  0.1059]])
one_hot_target = tensor([[1, 0]])

criterion = CrossEntropyLoss()
criterion(scores.double(), one_hot_target.double())
```

```
tensor(0.8131, dtype=torch.float64)
```


Bringing it all together

Loss function takes

- **scores**
 - model predictions **before** the final softmax function
- **one_hot_target**
 - one hot encoded ground truth label

and outputs

- **loss**
 - a single **float**.

Our training goal is to minimize loss.

Let's practice!

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Using derivatives to update model parameters

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Minimizing the loss

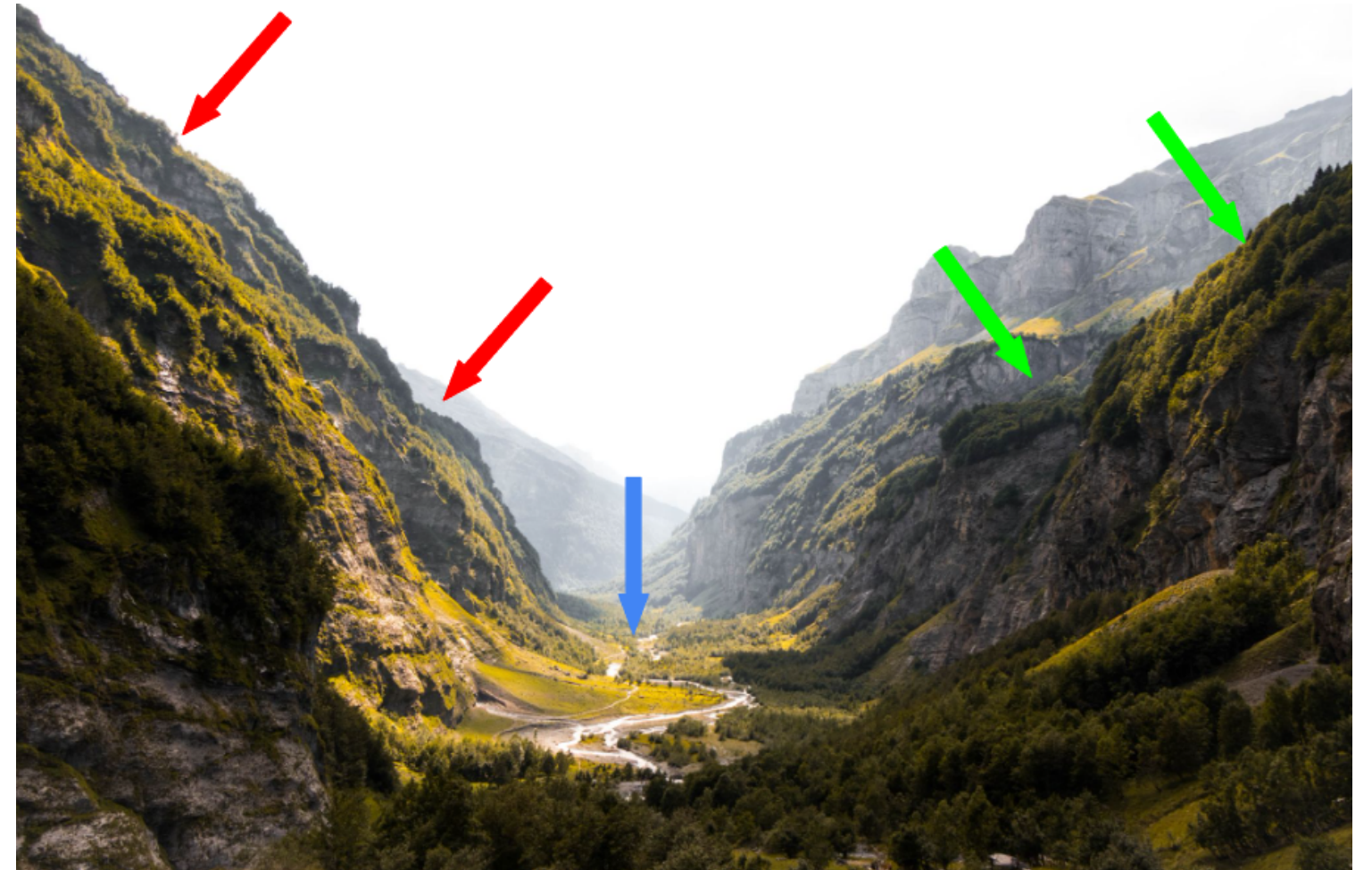
We need to minimize loss

- High loss: model prediction is wrong
- Low loss: model prediction is correct

An analogy for derivatives

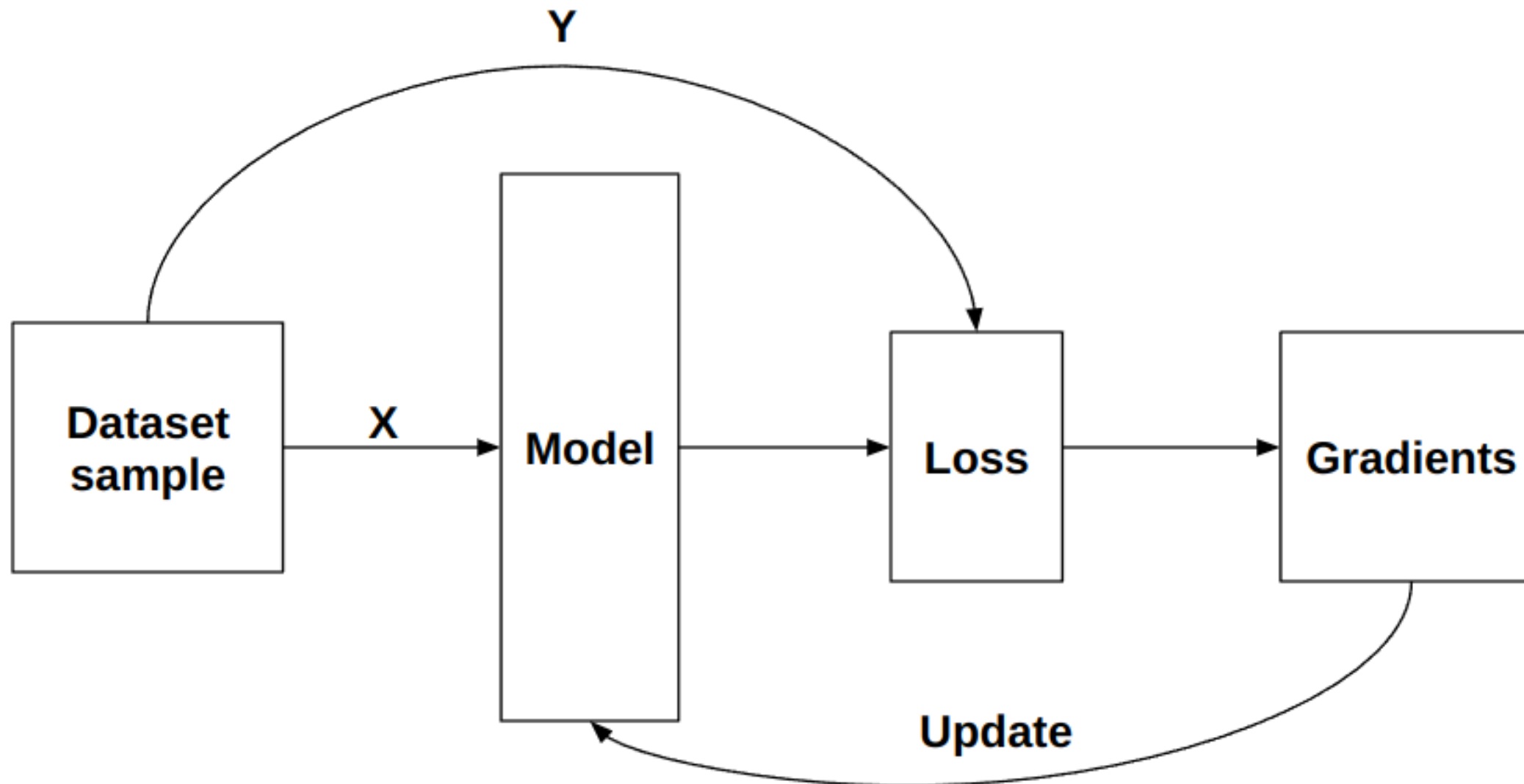
Hiking down a mountain to the valley floor:

- **steep slopes:**
 - a step makes us lose a lot of elevation = derivative is high (red arrows)
- **gentler slopes:**
 - a step makes us lose a little bit of elevation = derivative is low (green arrows)
- **valley floor:**
 - not losing elevation by taking a step = derivative is null (blue arrow)



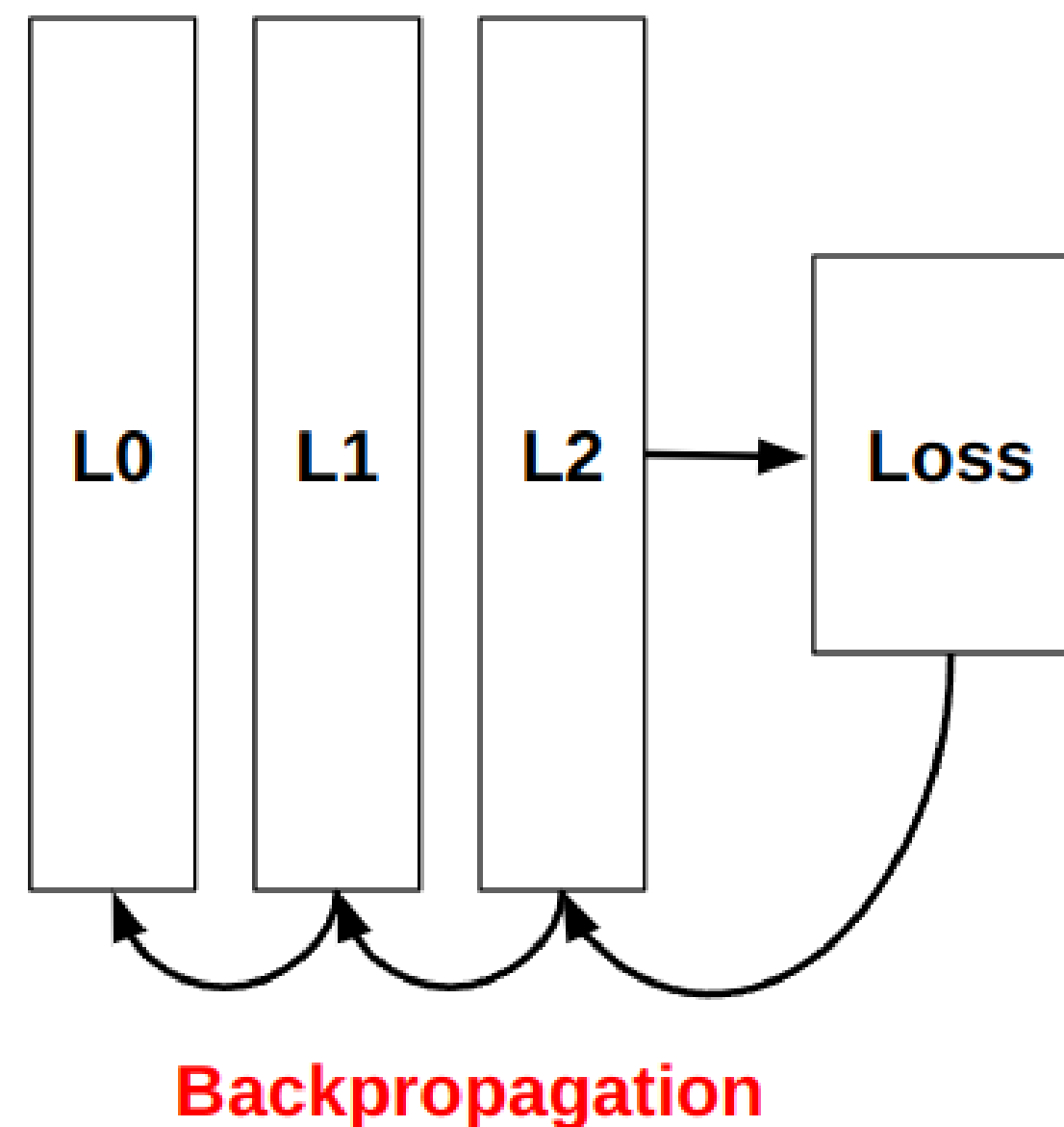
Connecting derivatives and model training

Model training: updating a model's parameters to minimize the loss.



Backpropagation concepts

- Consider a network made of three layers, $L0$, $L1$ and $L2$
 - we calculate local gradients for $L0$, $L1$ and $L2$ using **backpropagation**
 - we calculate loss gradients with respect to $L2$, then use $L2$ gradients to calculate $L1$ gradients, and so on



Backpropagation in PyTorch

```
# Create the model and run a forward pass
```

```
model = nn.Sequential(nn.Linear(16, 8),  
                      nn.Linear(8, 4),  
                      nn.Linear(4, 2))  
  
prediction = model(sample)
```

```
# Calculate the loss and compute the gradients
```

```
criterion = CrossEntropyLoss()  
loss = criterion(prediction, target)  
loss.backward()
```

```
# Access each layer's gradients
```

```
model[0].weight.grad, model[0].bias.grad  
model[1].weight.grad, model[1].bias.grad  
model[2].weight.grad, model[2].bias.grad
```


Updating model parameters

- Update the weights by subtracting local gradients scaled by the **learning rate**

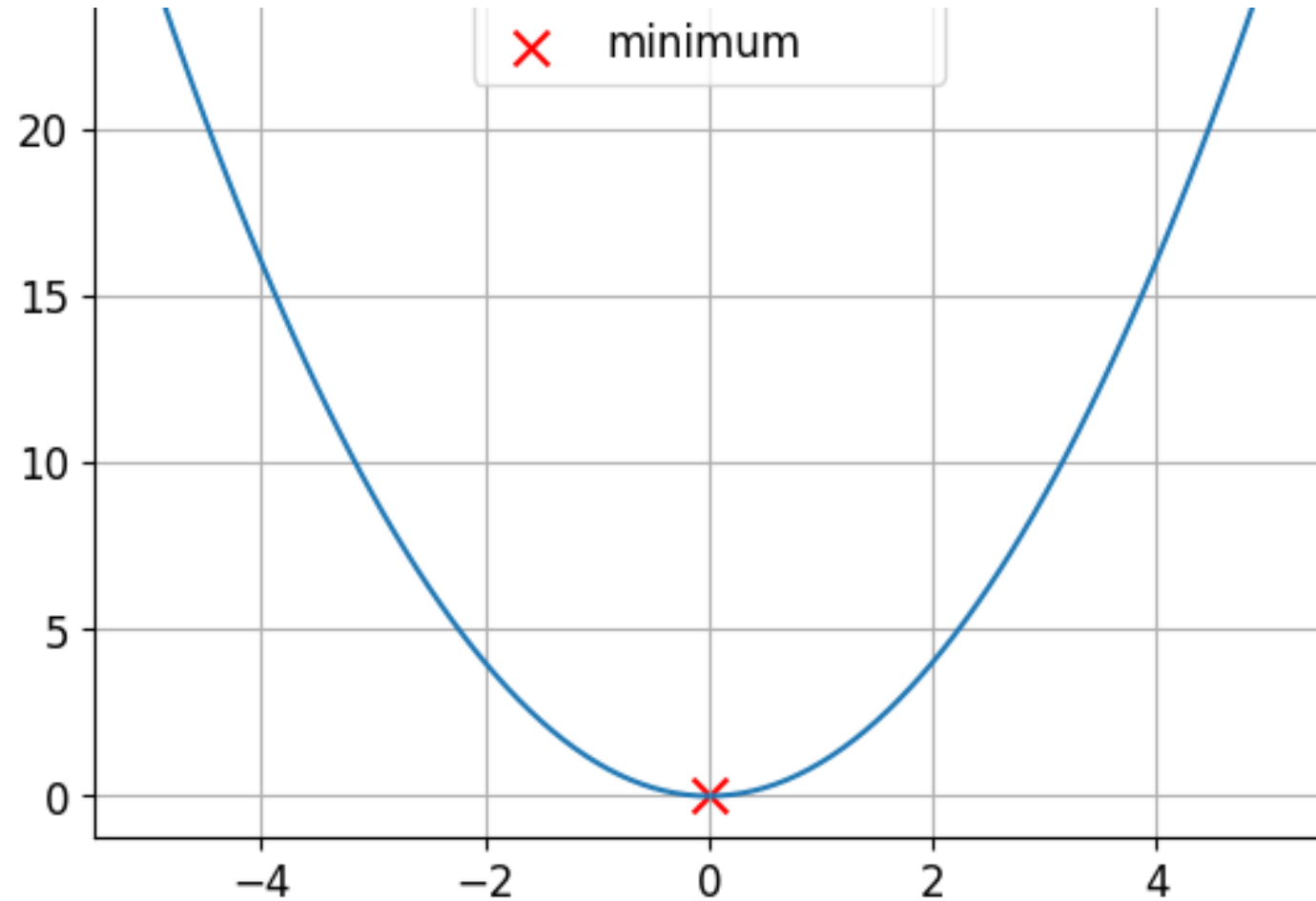
```
# Learning rate is typically small  
lr = 0.001
```

```
# Update the weights  
weight = model[0].weight  
weight_grad = model[0].weight.grad  
weight = weight - lr * weight_grad
```

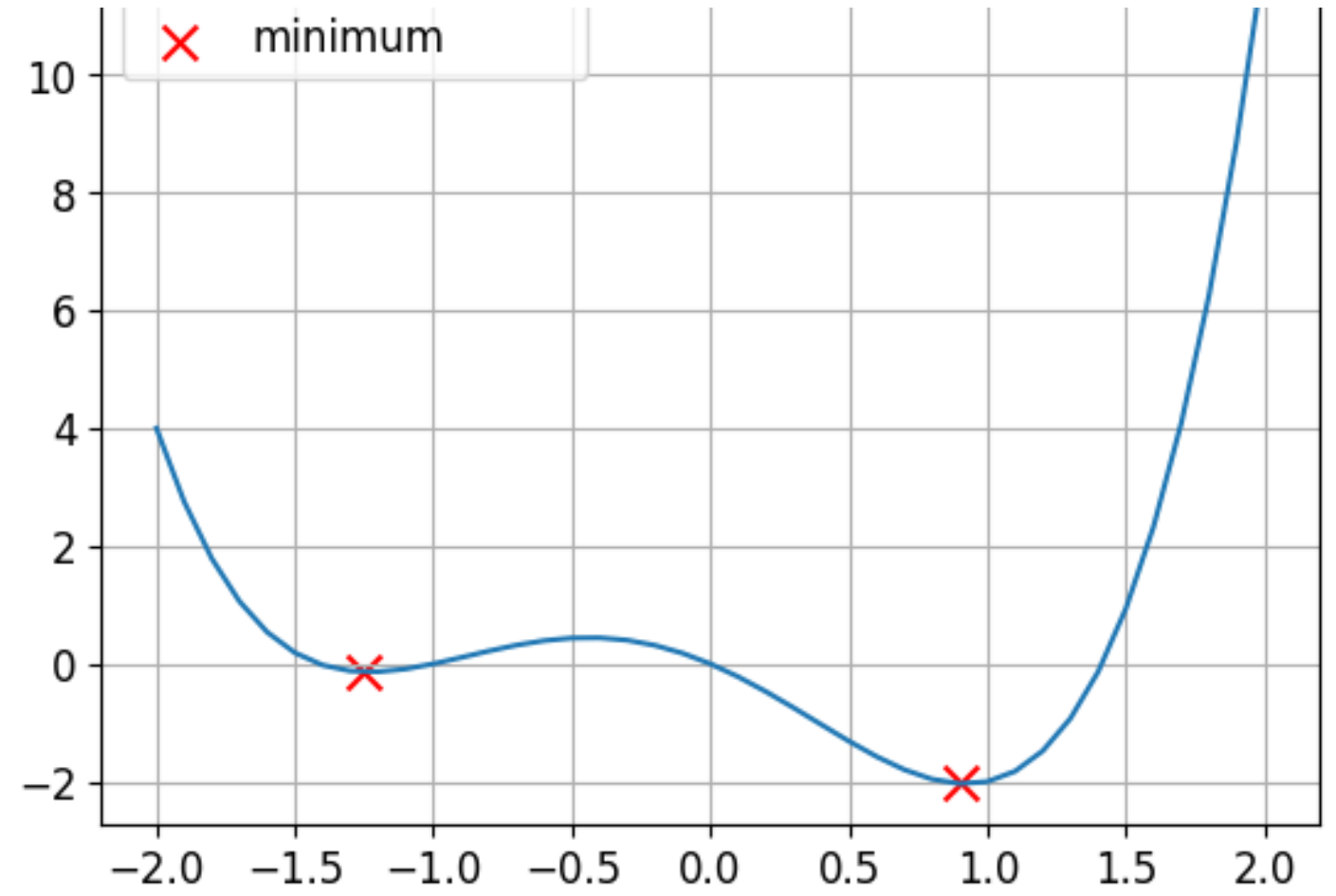
```
# Update the biases  
bias = model[0].bias  
bias_grad = model[0].bias.grad  
bias = bias - lr * bias_grad
```

Convex and non-convex functions

This is a convex function.



This is a non-convex function.



Gradient descent

- For non-convex functions, we will use an iterative process such as **gradient descent**
- In PyTorch, an **optimizer** takes care of weight updates
- The most common **optimizer** is stochastic gradient descent (SGD)

```
import torch.optim as optim

# Create the optimizer
optimizer = optim.SGD(model.parameters(), lr=0.001)
```

- Optimizer handles updating model parameters (or weights) after calculation of local gradients

```
optimizer.step()
```

Let's practice!

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Writing our first training loop

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Training a neural network

1. Create a model
2. Choose a loss function
3. Create a dataset
4. Define an optimizer
5. Run a training loop, where for each sample of the dataset, we repeat:
 - Calculating loss (forward pass)
 - Calculating local gradients
 - Updating model parameters

Introducing the Data Science Salary dataset

- This dataset contains salary data for data science-related jobs.
- The features are: `experience_level` , `employment_type` , `remote_ratio` and `company_size` . They were turned into categories.

| <code>experience_level</code> | <code>employment_type</code> | <code>remote_ratio</code> | <code>company_size</code> | <code>salary_in_usd</code> |
|-------------------------------|------------------------------|---------------------------|---------------------------|----------------------------|
| 0 | 0 | 0.5 | 1 | 0.036 |
| 1 | 0 | 1.0 | 2 | 0.133 |
| 2 | 0 | 0.0 | 1 | 0.234 |
| 1 | 0 | 1.0 | 0 | 0.076 |
| 2 | 0 | 1.0 | 1 | 0.170 |

- The target is salary in US dollars; it is **not a category but a continuous quantity**
- For regression problems, we cannot use softmax or sigmoid as last activation function
- We need a different loss function than cross-entropy

Introducing the Mean Squared Error Loss

- The mean squared error loss (MSE loss) is the squared difference between the prediction and the ground truth.

```
def mean_squared_loss(prediction, target):  
    return np.mean((prediction - target)**2)
```

- in PyTorch

```
criterion = nn.MSELoss()  
# Prediction and target are float tensors  
loss = criterion(prediction, target)
```

- This loss is used for regression problems (e.g., when trying to fit a linear regression model).

Before the training loop

```
# Create the dataset and the dataloader
```

```
dataset = TensorDataset(torch.tensor(features).float(), torch.tensor(target).float())  
dataloader = DataLoader(dataset, batch_size=4, shuffle=True)
```

```
# Create the model
```

```
model = nn.Sequential(nn.Linear(4, 2),  
                      nn.Linear(2, 1))
```

```
# Create the loss and optimizer
```

```
criterion = nn.MSELoss()  
optimizer = optim.SGD(model.parameters(), lr=0.001)
```

The training loop

```
# Loop through the dataset multiple times
for epoch in range(num_epochs):
    for data in dataloader:
        # Set the gradients to zero
        optimizer.zero_grad()
        # Get feature and target from the data loader
        feature, target = data
        # Run a forward pass
        pred = model(feature)
        # Compute loss and gradients
        loss = criterion(pred, target)
        loss.backward()
        # Update the parameters
        optimizer.step()
```

Let's practice!

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