MessMaster: the Curse of the Muffin-Faced Dog (part 2)

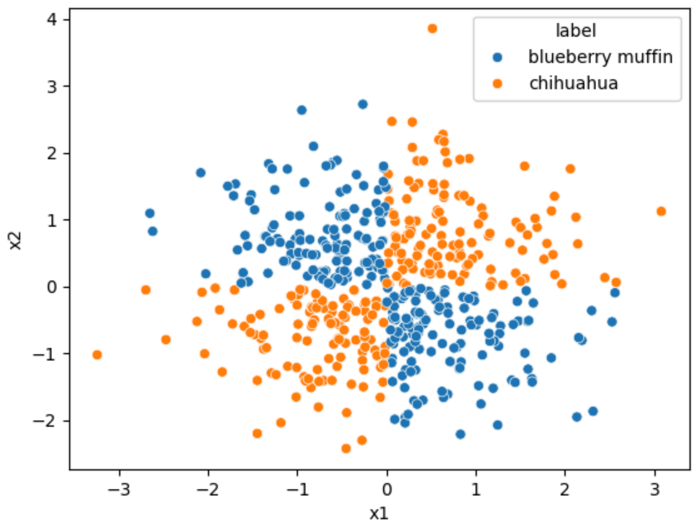
Welcome back to the quest of MessMaster!

This week, we will continue to help Boltzmann differentiate Chihuahuas and blueberry muffins, but with fancier models (no longer just linear)!

Specifically we will use the following concepts:

- Backprop: implementation and visualization
- MLP: decision boundary and contrast with linear models
- Optimization: Comparing SGD v.s. Adam

A friend has helped us found a separable 2D embedding of Chihuahuas and blueberry muffins. However, it is not linearly separable!



We will train a MLP to help with this!

1. ManualGrad: handcrafted gradients, artisanal machine learning

Backprop is the process of computing the gradient of the loss function w.r.t. all the parameters from multiple stages of nonlinear transformations of the input.

It is efficient both in terms of computation and memory and is universally used for computing the gradient and in well-implemented in many widely used tools (e.g., `torch.autograd`).

Today, we will implement backprop by hand for a 2-layer MLP because it's a good exercise for understanding backprop :)

First we will load the data and split it into train/val/test sets.

Q1a. Why is it important to have validation and test sets?

Answer:

In [21]:
```
# For reproducibility
RANDOM_SEED = 10011  # postal code of CDS <3

import torch
from sklearn.model_selection import train_test_split
import pandas as pd

# load data
df = pd.read_csv("secret/data/xor_pattern.csv")
X = df[["x1", "x2"]].values  # Extract features
y = df["y"].values  #
```

```
# train-val-test split
X_train, X_val_test, y_train, y_val_test = train_test_split(X, y, test_size=
X_val, X_test, y_val, y_test = train_test_split(X_val_test, y_val_test, test
# TODO: what is the train-val-test split ratio?

# convert to tensors
X_train_tensor = torch.tensor(X_train, dtype=torch.float32)
y_train_tensor = torch.tensor(y_train, dtype=torch.long)
X_val_tensor = torch.tensor(X_val, dtype=torch.float32)
y_val_tensor = torch.tensor(y_val, dtype=torch.long)
X_test_tensor = torch.tensor(X_test, dtype=torch.float32)
y_test_tensor = torch.tensor(y_test, dtype=torch.long)
```

Next, we define the loss function as the cross entropy loss. When we update the weights, we use the gradient of the loss function w.r.t. the weights.

Q1b. Implement the CEL loss function for binary classification. What is its connection to energy?

Answer:

In [22]:
```
def loss_fn(p_y_hat: torch.Tensor, y: torch.Tensor) -> torch.Tensor:
    """
    Compute the cross-entropy loss (negative log likelihood) of a predictior
    p_y_hat: probability of each class, shape (N, 2)
    y: true class, shape (N,)
    returns: loss, shape (1,)
    """
    # TODO: implement the loss function
    # step 1: fine the probability of the correct class
    correct_class_loc = ??? # TODO: FILL IN
    correct_class_prob = p_y_hat[correct_class_loc]
    # step 2: compute the mean of the negative log likelihood across all exa
    nll = ??? # TODO: FILL IN
    return nll
```

Before we dive into implementing the gradients, let's do a brief calculus review to make sure we have the background knowledge.

Q1c.

i. What does derivative/gradient tells us about a function? (What does positive/negative gradient mean?)

ii. Why is it useful for optimization?

iii. What is chain rule and why is it relevant to backprop?

Answer:

Q1d.

We are going to implement a two-layer MLP with ReLU activation and softmax output.

First layer: $z_1 = h_1(x) = \sigma(W_1 x + b_1) = \sigma(a_1)$

Second layer: $z_2 = h_2(x) = W_2 z_1 + b_2$

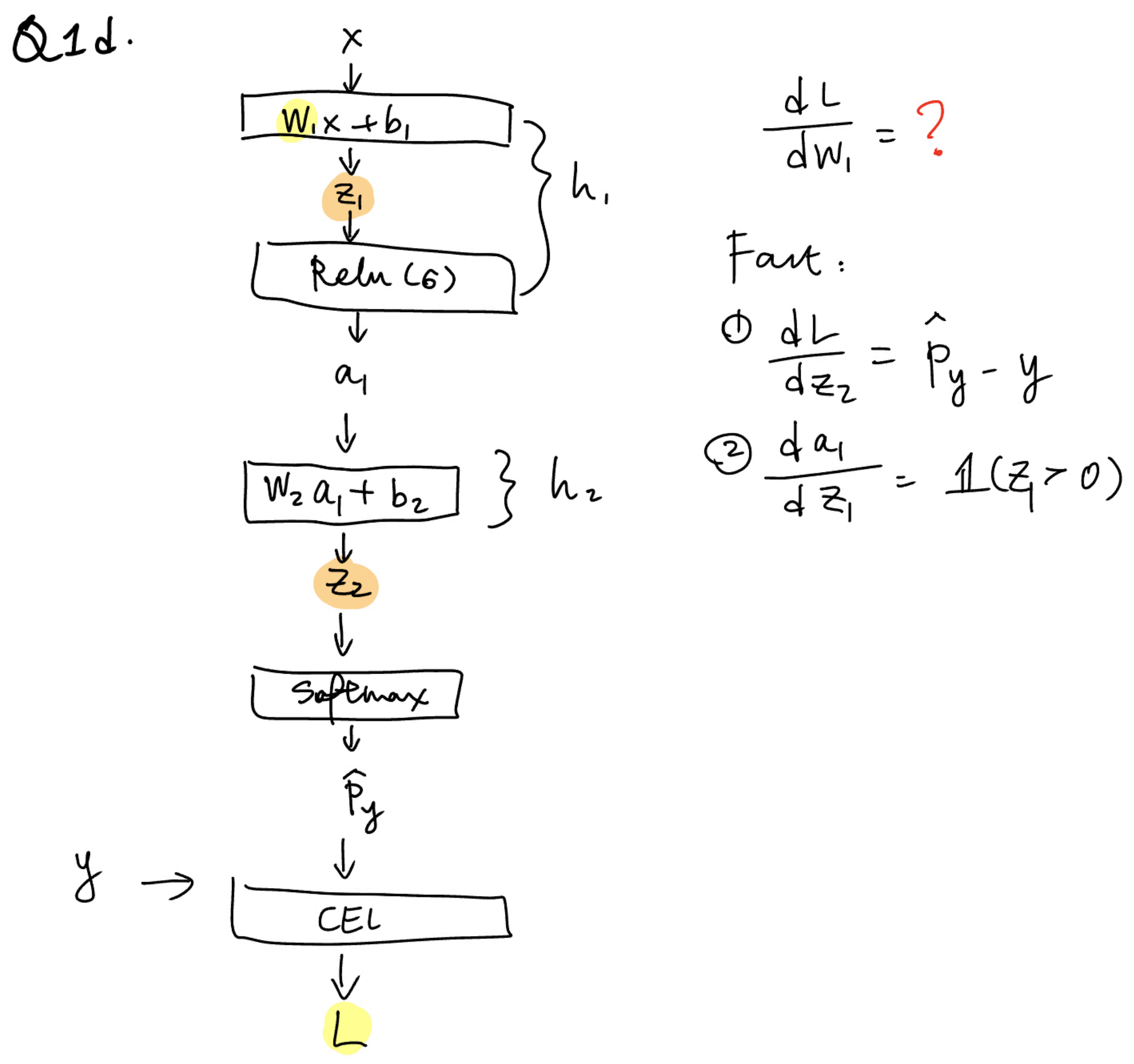
Softmax: $\hat{p} = \mathrm{softmax}(z_2) = \frac{e^{z_2}}{\sum_{j=1}^{2} e^{z_{2j}}}$

Loss function: $L(y, p_{\hat{y}}) = \mathrm{L}_{\mathrm{ce}}(y, p_{\hat{y}}) = -\log \hat{p}(\hat{y} = y)$

Consider computing the gradient of the loss function with respect to the parameters.

Let's focus on the first layer. What is $\frac{\partial L}{\partial W_1}$?

You may use the fact that $\frac{\partial L}{\partial z_2} = \hat{p} - y$ and that $\sigma'(a) = 1(\sigma(a) > 0)$, where $1(\cdot)$ is the indicator function.



(Note: I should have used ∂ (partial derivative) instead of d in the figure since loss is a multivariable function, but it's too late to change it now.)

Answer:

Q1e. Verification of gradients implementation

Check the gradients and gradient updates. Anything looks wrong? If you find something wrong, try to fix it.

In [ ]:
```python
# Initialize weights
h = 10
k = 2
W1 = torch.randn(k, h, requires_grad=False) * 0.01
b1 = torch.zeros(h, requires_grad=False)
W2 = torch.randn(h, k, requires_grad=False) * 0.01
```

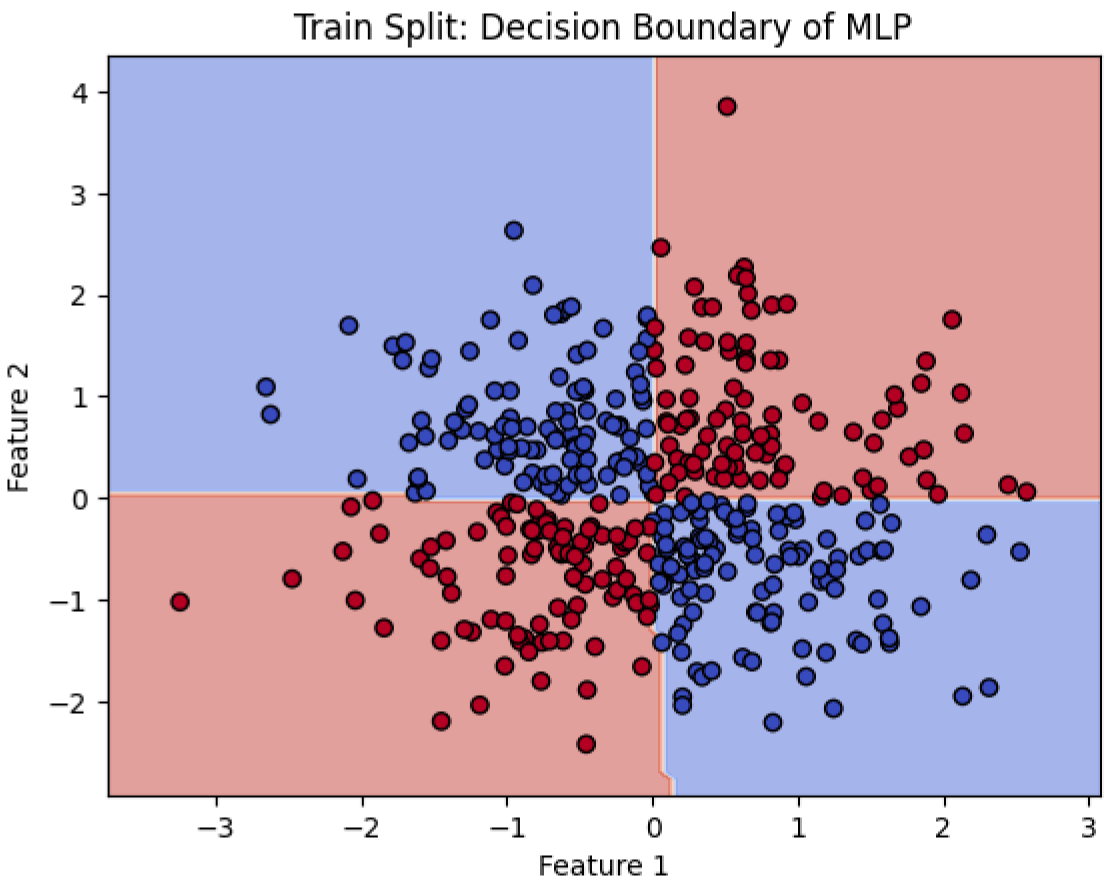
```
b2 = torch.zeros(k, requires_grad=False)

learning_rate = 0.1
epochs = 10000

for epoch in range(epochs):
    # ==================== Forward pass ====================
    # First layer: z1 = W1 * X + b1
    z1 = X_train_tensor @ W1 + b1  # Shape: (N, h)  [batch_size, hidden_dim]

    # Apply activation function: a1 = ReLU(z1)
    a1 = torch.relu(z1)  # Shape: (N, h)

    # Second layer: z2 = W2 * a1 + b2
    z2 = a1 @ W2 + b2  # Shape: (N, k)  [batch_size, num_classes]

    # Apply softmax to get probabilities: p_hat = softmax(z2)
    p_hat = torch.softmax(z2, dim=1)   # Shape: (N, k)

    # ==================== Compute Loss ====================
    # PyTorch's CrossEntropyLoss automatically applies softmax inside,
    # so we should pass raw logits (z2), not softmax probabilities (p_hat)
    loss = loss_fn(p_hat, y_train_tensor)  # Scalar loss value

    # ==================== Backpropagation ====================

    # Step 1: Compute gradient of loss w.r.t. logits (z2)
    # Cross-entropy loss with softmax:
    #   L = - (1/N) * sum(y * log(p_hat))
    # Derivative:
    #   dL/dz2 = (p_hat - y) / N
    # Shape: (N, k) [Same as z2]
    y_one_hot = torch.nn.functional.one_hot(y_train_tensor, num_classes=p_ha
    dL_dz2 = (p_hat - y_one_hot) / y_train_tensor.shape[0]  # Normalize by b

    # Step 2: Compute gradient of loss w.r.t. W2 and b2
    # Using chain rule: dL/dW2 = (dL/dz2) * (dz2/dW2)
    #   dz2/dW2 = a1^T
    #   dL/dW2 = a1^T @ dL/dz2
    # Shape: (h, k) [Same as W2]
    dL_dW2 = a1.T @ dL_dz2

    # Gradient of loss w.r.t. b2:
    #   dL/db2 = sum(dL/dz2) along batch axis
    # Shape: (k,) [Same as b2]
    dL_db2 = torch.sum(dL_dz2, dim=0)

    # Step 3: Compute gradient of loss w.r.t. activations (a1)
    #   dL/da1 = (dL/dz2) * (dz2/da1)
    #   dz2/da1 = W2^T
    #   dL/da1 = dL/dz2 @ W2^T
    # Shape: (N, h) [Same as a1]
    dL_da1 = dL_dz2 @ W2.T

    # Step 4: Compute gradient of loss w.r.t. pre-activation (z1)
    # Using chain rule: dL/dz1 = (dL/da1) * (da1/dz1)
    # ReLU derivative:
    #   da1/dz1 = 1 if z1 > 0, else 0
    # Shape: (N, h) [Same as z1]
    dL_dz1 = dL_da1 * (z1 > 0).float()

    # Step 5: Compute gradient of loss w.r.t. W1 and b1
    # Using chain rule: dL/dW1 = (dL/dz1) * (dz1/dW1)
    #   dz1/dW1 = X^T
    #   dL/dW1 = X^T @ dL/dz1
    # Shape: (d, h) [Same as W1]
    # TODO: check if this is correct
    dL_dW1 = X_train_tensor.T @ dL_dz1

    # Gradient of loss w.r.t. b1:
    #   dL/db1 = sum(dL/dz1) along batch axis
    # Shape: (h,) [Same as b1]
    dL_db1 = torch.sum(dL_dz1, dim=0)

    # Gradient update (SGD step)
    # TODO: check here
    W1 += learning_rate * dL_dW1
    b1 += learning_rate * dL_db1
    W2 += learning_rate * dL_dW2
    b2 += learning_rate * dL_db2

    if epoch % 10 == 0:
        print(f"Epoch {epoch}: Loss = {loss.item():.4f}")
```

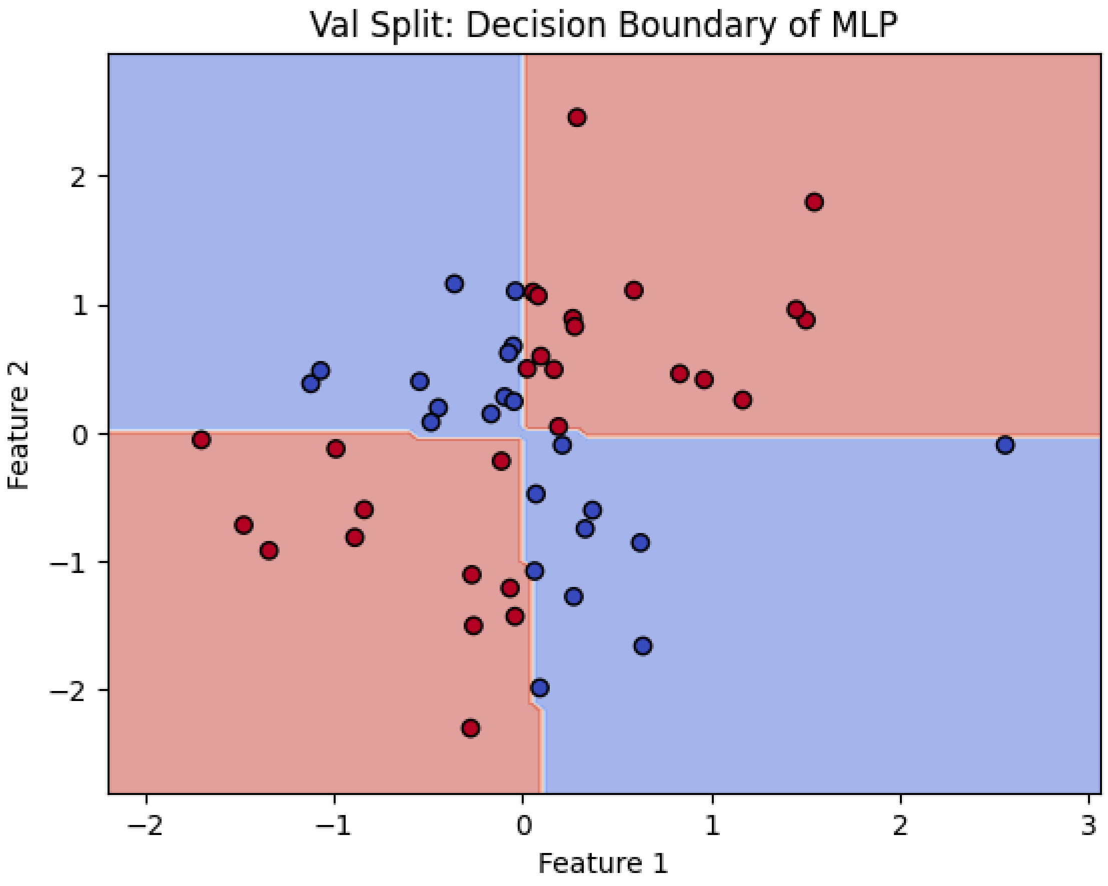
Visualization

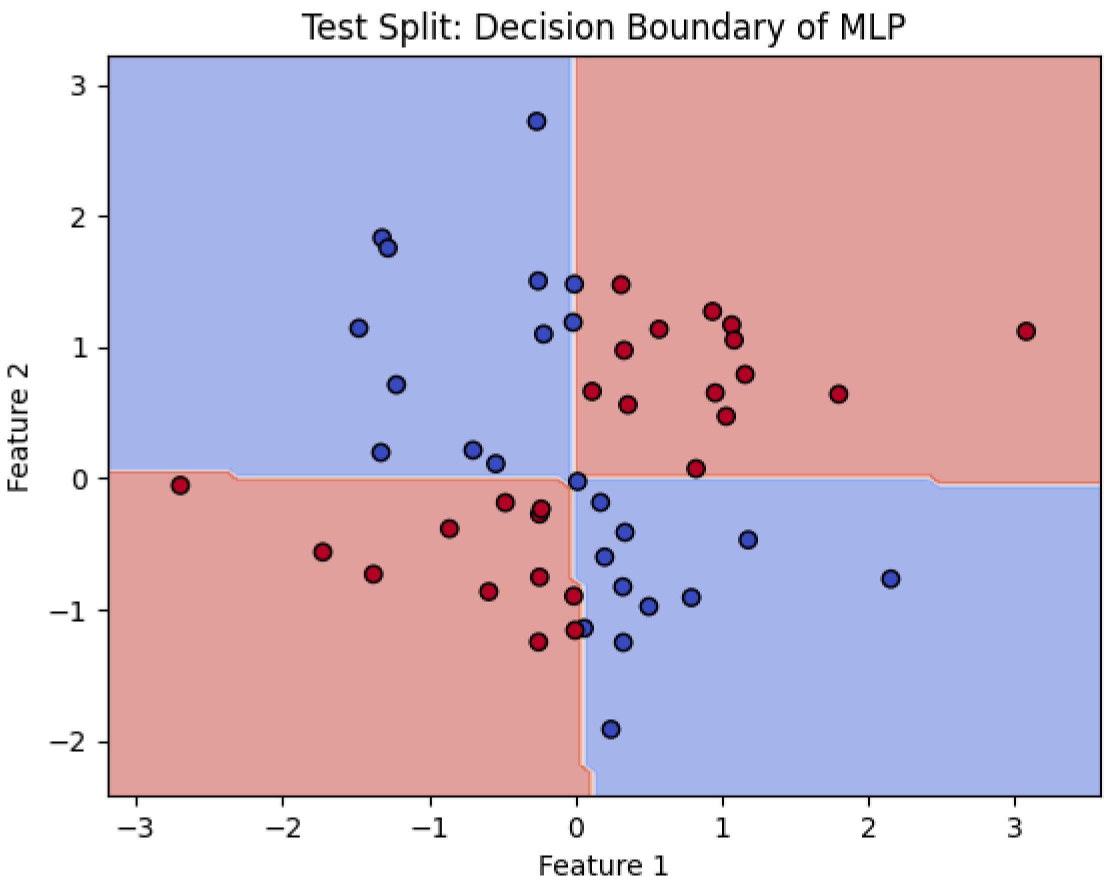
Now let's visualize the decision boundary of the trained MLP.

Can linear models learn this decision boundary?

In [19]:
```
from util import plot_decision_boundary
# Example usage:
plot_decision_boundary(W1, b1, W2, b2, X_train_tensor.numpy(), y_train_tensc
plot_decision_boundary(W1, b1, W2, b2, X_val_tensor.numpy(), y_val_tensor.nu
plot_decision_boundary(W1, b1, W2, b2, X_test_tensor.numpy(), y_test_tensor.
```


Train Split: Decision Boundary of MLP
Feature 2
Feature 1
4
3
2
1
0
−1
−2
−3
−2
−1
0
1
2
3


Val Split: Decision Boundary of MLP
Feature 2
Feature 1
2
1
0
−1
−2
−2
−1
0
1
2
3



2. Optimizers: Adam v.s. SGD

Great that the MLP worked! However, we can further accelerate the training process by dynamically adjusting the learning rate.

Q2a. What was the learning rate scheduler we used above?

Answer:

In class, we learned about the Adam optimizer, which uses exponential smoothing to reduce the variance of the gradient estimate and normalizes the update using an estimate of the second moment of the gradient.

$$\theta_t^i \leftarrow \theta_{t-1}^i + \alpha \frac{m_t^i}{\sqrt{v_t^i + \epsilon}},$$

where α is the default learning rate, m_t is the momentum (exponential moving average of the gradient), and v_t is the adpative scaling (exponential moving average of the squared gradient).

$$m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t.$$

$$v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2.$$

Q2b. Why is it momentum helpful? Why is adaptive scaling helpful?

Answer:

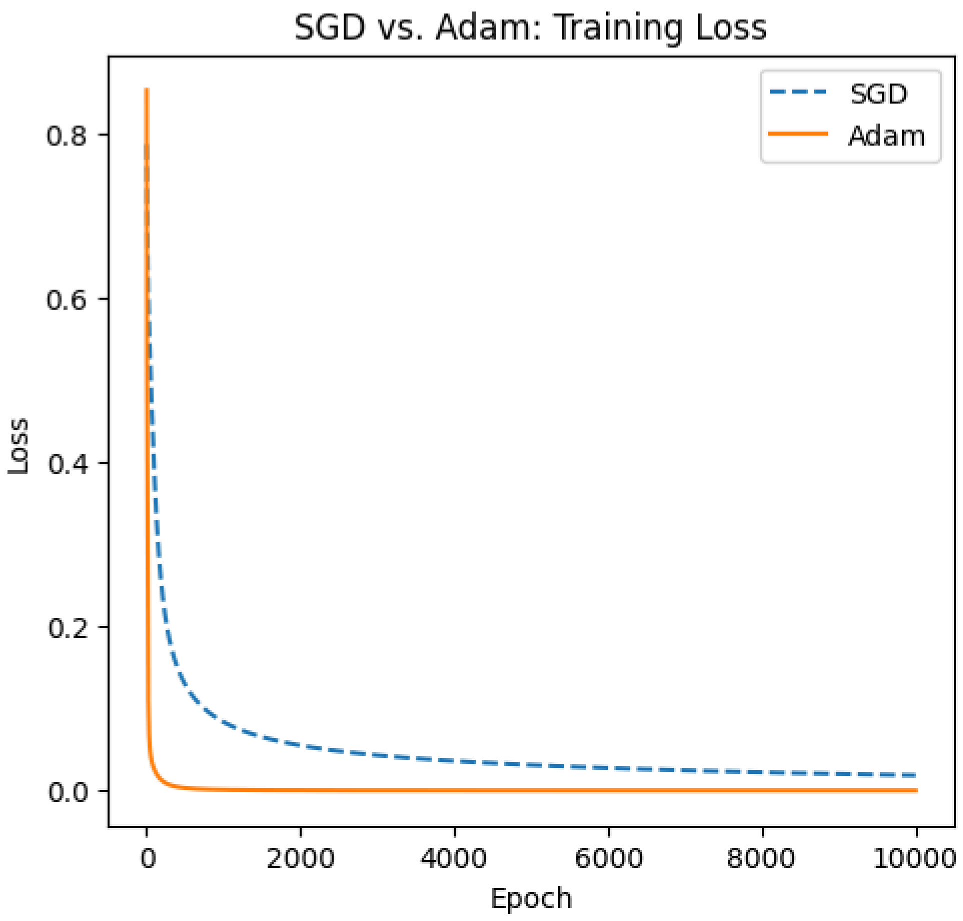
Q2c. Observe the loss curves of SGD and Adam. What do you see?

Answer:

```
In [ ]: import torch
        import torch.nn.functional as F

        W1.requires_grad = True
        W2.requires_grad = True
        b1.requires_grad = True
        b2.requires_grad = True
        # Hyperparameters
        epochs = 10000
        batch_size = 32
        learning_rate = 0.1 #1e-3

        # Initialize weights with Xavier (Glorot) initialization
        torch.manual_seed(RANDOM_SEED)  # For reproducibility
        torch.nn.init.xavier_uniform_(W1)
        torch.nn.init.xavier_uniform_(W2)
        b1.data.fill_(0)
        b2.data.fill_(0)

        # Define two optimizers: SGD and Adam
        optimizer_sgd = torch.optim.SGD([W1, b1, W2, b2], lr=learning_rate)
        optimizer_adam = torch.optim.Adam([W1, b1, W2, b2], lr=learning_rate)

        # Learning rate schedulers (optional)
        # scheduler_sgd = torch.optim.lr_scheduler.StepLR(optimizer_sgd, step_size=2
        # scheduler_adam = torch.optim.lr_scheduler.StepLR(optimizer_adam, step_size

        # Store loss & lr history
        loss_history_sgd, loss_history_adam = [], []
        lr_history_sgd, lr_history_adam = [], []

        # Training loop for both optimizers
        for optimizer_name, optimizer, loss_history, lr_history in [
            ("SGD", optimizer_sgd, loss_history_sgd, lr_history_sgd),
            ("Adam", optimizer_adam, loss_history_adam, lr_history_adam),
        ]:
            print(f"\nTraining with {optimizer_name}...\n")
```

```
    # Reset weights for fair comparison
    torch.nn.init.xavier_uniform_(W1)
    torch.nn.init.xavier_uniform_(W2)
    b1.data.fill_(0)
    b2.data.fill_(0)

    for epoch in range(epochs):
        # =================== Forward pass ===================
        z1 = X_train_tensor @ W1 + b1
        a1 = torch.relu(z1)
        z2 = a1 @ W2 + b2
        loss = F.cross_entropy(z2, y_train_tensor)

        # =================== Backward pass ===================
        optimizer.zero_grad()  # Reset gradients
        loss.backward()  # Compute gradients
        optimizer.step()  # Update weights

        # Save loss & learning rate
        loss_history.append(loss.item())

        lr_history.append(optimizer.param_groups[0]["lr"])  # Extract currer

        # Learning rate decay (if scheduler exists)
        # scheduler.step()

        # Print progress every 10 epochs
        if epoch % 10 == 0:
            print(
                f"{optimizer_name} - Epoch {epoch}: Loss = {loss.item():.4f}
            )
```

In [18]:
```
from util import plot_loss
plot_loss(loss_history_sgd, loss_history_adam)
```


SGD vs. Adam: Training Loss
SGD
Adam
Loss
0.0
0.2
0.4
0.6
0.8
Epoch
0
2000
4000
6000
8000
10000