Machine Learning Essentials SS25 - Exercise Sheet 4

Instructions

- `TODO`'s indicate where you need to complete the implementations.
- You may use external resources, but **write your own solutions**.
- Provide concise, but comprehensible comments to explain what your code does.
- Code that's unnecessarily extensive and/or not well commented will not be scored.

Exercise 2

Task 1

(a) derive d/dx tanh(x) =

- d/dx tan (x) = d/dx (sin(x) / cos(x))
- = (cos(x) * cos(x) - sin(x) * sin(x)) / cos^2(x)
- = 1 / cos^2(x) , because cos^2 x - sin^2x = 1
- = sec ^2(x)
- = 1 - tan^2(x)
- (b) Gradient of BCE loss w.r.t. output layer's preactivation: δ(2) = ŷ - y

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import make_moons
from sklearn.model_selection import train_test_split
from matplotlib.colors import ListedColormap
```

Task 2

In [2]:
```
# TODO: Define the needed helper functions
def tanh_prime(x_activated):
    return 1 - x_activated ** 2

def sigmoid(x):
    return 1 / (1 + np.exp(-x))

def binary_cross_entropy(y_hat, y):
    """
    Computes the BCE loss over samples.
    """
    # Hint: Add a small epsilon to y_hat to prevent numerical issues w/ log(
    epsilon = 1e-15
```

```
    y_hat = np.clip(y_hat, epsilon, 1 - epsilon)  # no log 0
    return -np.mean(y * np.log(y_hat) + (1 - y) * np.log(1 - y_hat))
```

In [3]:

```
# MLP Class
class MLP:
    def __init__(self, layer_dims, initialization_scale=1):
        """
        Initializes the multi-layer perceptron.
        Args:
            layer_dims (list of int): List containing the number of neurons
                                      [d0, d1, d2] = [2, 10, 1] for the exer
                                      d0: input dimension
                                      d1: hidden layer dimension
                                      d2: output dimension
            initialization_scale (float): Scaling factor for weight initiali
        """
        self.parameters = {}
        self.num_layers = len(layer_dims)

        # Weights are initialized by drawing from a standard normal distribu
        # For more complex networks, one usually uses techniques like Xavier
        # Layer 0 -> Layer 1
        self.parameters['W0'] = np.random.randn(layer_dims[1], layer_dims[0]
        self.parameters['b0'] = np.zeros((layer_dims[1], 1))
        # Layer 1 -> Layer 2
        self.parameters['W1'] = np.random.randn(layer_dims[2], layer_dims[1]
        self.parameters['b1'] = np.zeros((layer_dims[2], 1))

        self.cache = {} # For storing intermediate values (needed for backpr

    def forward(self, X_batch):
        """
        Forward pass through the network. Store intermediate values in self.
        """
        # TODO: Implement the forward pass & store the needed values in self
        z0 = X_batch

        # Hidden layer (layer 1)
        z1_tilde = self.parameters['W0'] @ z0 + self.parameters['b0']  # Pre
        z1 = np.tanh(z1_tilde)  # Activation

        # Output layer (layer 2)
        z2_tilde = self.parameters['W1'] @ z1 + self.parameters['b1']  # Pre
        y_hat = sigmoid(z2_tilde)  # Sigmoid activation for binary classific

        # Store values needed for backpropagation
        self.cache = {
            'z0': z0,           # Input
            'z1_tilde': z1_tilde,  # Hidden preactivation
            'z1': z1,           # Hidden activation
            'z2_tilde': z2_tilde,  # Output preactivation
            'y_hat': y_hat      # Final output
        }

        return y_hat

    def backward(self, Y_batch):
        """
        Performs the backward pass (= backpropagation) to compute gradients
        Gradients are stored in the grads dictionary (see update_params meth
        """
```

```
        # TODO: Implement the backward pass
        # Get cached values
        z0 = self.cache['z0']
        z1_tilde = self.cache['z1_tilde']
        z1 = self.cache['z1']
        y_hat = self.cache['y_hat']

        m = Y_batch.shape[1]  # Number of samples in batch

        # Step 1: Compute δ(2) = ŷ - y (gradient w.r.t. output preactivation
        delta2 = y_hat - Y_batch

        # Step 2: Compute gradients for output layer parameters
        dW1 = (1/m) * (delta2 @ z1.T)  # Average over batch
        db1 = (1/m) * np.sum(delta2, axis=1, keepdims=True)

        # Step 3: Compute δ(1) using backpropagation recursion
        delta1 = (self.parameters['W1'].T @ delta2) * tanh_prime(z1)

        # Step 4: Compute gradients for hidden layer parameters
        dW0 = (1/m) * (delta1 @ z0.T)  # Average over batch
        db0 = (1/m) * np.sum(delta1, axis=1, keepdims=True)

        # Store gradients in dictionary
        grads = {
            'dW0': dW0,
            'db0': db0,
            'dW1': dW1,
            'db1': db1
        }

        return grads

    def update_params(self, grads, learning_rate):
        """
        Updates the parameters using gradient descent.
        Args:
            grads (dict): Dictionary of gradients.
            learning_rate (float): The learning rate.
        """
        self.parameters['W0'] -= learning_rate * grads['dW0']
        self.parameters['b0'] -= learning_rate * grads['db0']
        self.parameters['W1'] -= learning_rate * grads['dW1']
        self.parameters['b1'] -= learning_rate * grads['db1']
```

Task 3

TODO: Explain why using vectorized operations is generally preferred in ML.

Vectorized operations are preferred in ML because:

1. **Performance**: Vectorized operations use optimized linear algebra libraries (BLAS, LAPACK) that are implemented in C/Fortran and can leverage hardware acceleration (SIMD instructions, multi-threading, GPU parallelization).

2. **Memory efficiency**: Vectorized operations minimize memory allocations and improve cache locality by processing data in contiguous memory blocks.

3. **Readability**: Matrix/vector notation is more concise and closer to mathematical formulation, making code easier to understand and debug.

4. **Numerical stability**: Optimized libraries often include better handling of edge cases and numerical precision issues.

For example, computing gradients with explicit loops over neurons/features would be much slower than using matrix multiplication, especially for large networks and datasets.

Task 4

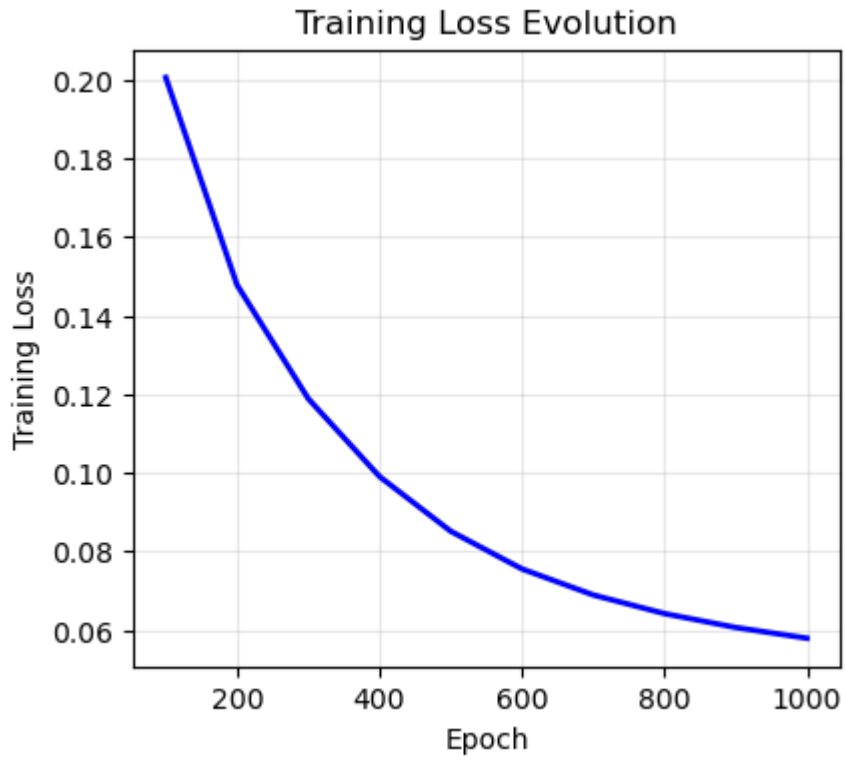
In [4]:
```
#Data loading and preprocessing (predefined)
X, y = make_moons(n_samples=500, noise=0.2, random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, ran


# NOTE: Different libraries/languages use different conventions for the shap
#   - In ML textbooks/mathematical notation, X is often (n_features, n_sampl
#   - This is consistent with some languages (e.g. Julia, Matlab), which sto
#   - However, most ML code (e.g. NumPy, sklearn, Pytorch) is optimized for
#     (The reason for that is that most of these libraries run C/C++/CUDA co
# --> Juggling the shapes of arrays to be correctly aligned with the used mo

X_train = X_train.T  # Shape: (2, 350)
X_test = X_test.T    # Shape: (2, 150)
y_train = y_train.reshape(1, -1)  # Shape: (1, 350)
y_test = y_test.reshape(1, -1)    # Shape: (1, 150)


# TODO: The MLP class you're using expects its inputs in a specific shape, m
print(f"Shape of X_train: {X_train.shape}")
print(f"Shape of y_train: {y_train.shape}")
print(f"Shape of X_test: {X_test.shape}")
print(f"Shape of y_test: {y_test.shape}")
```

```
Shape of X_train: (2, 350)
Shape of y_train: (1, 350)
Shape of X_test: (2, 150)
Shape of y_test: (1, 150)
```

In [5]:
```
# Training
layer_dimensions = [X_train.shape[0], 10, 1] # d0, d1, d2 as given in the ex
mlp = MLP(layer_dimensions) # Initialize the MLP

# Hyperparameters
learning_rate = 0.5   # Good balance between speed and stability
num_epochs = 1000     # Sufficient for convergence
print_loss = 100      # Print every 100 epochs
train_losses = []


for epoch in range(1,num_epochs+1):
    # Forward pass
    y_hat_train = mlp.forward(X_train)
    # Compute loss
    train_loss = binary_cross_entropy(y_hat_train, y_train)
    # Backward pass = backprop
    grads = mlp.backward(y_train)
   # Update parameters by gradient descent
```

```
    mlp.update_params(grads, learning_rate)

    if epoch % print_loss == 0 or epoch == num_epochs:
        train_losses.append(train_loss)
        print(f"Epoch {epoch}/{num_epochs} - Training Loss: {train_loss:.4f}"

# Plotting the training loss
plt.figure(figsize=(10, 4))

plt.subplot(1, 2, 1)
plt.plot(range(print_loss, num_epochs + 1, print_loss), train_losses, 'b-',
plt.xlabel('Epoch')
plt.ylabel('Training Loss')
plt.title('Training Loss Evolution')
plt.grid(True, alpha=0.3)
```

```
Epoch 100/1000 - Training Loss: 0.2006
Epoch 200/1000 - Training Loss: 0.1478
Epoch 300/1000 - Training Loss: 0.1188
Epoch 400/1000 - Training Loss: 0.0990
Epoch 500/1000 - Training Loss: 0.0851
Epoch 600/1000 - Training Loss: 0.0755
Epoch 700/1000 - Training Loss: 0.0689
Epoch 800/1000 - Training Loss: 0.0641
Epoch 900/1000 - Training Loss: 0.0606
Epoch 1000/1000 - Training Loss: 0.0579
```

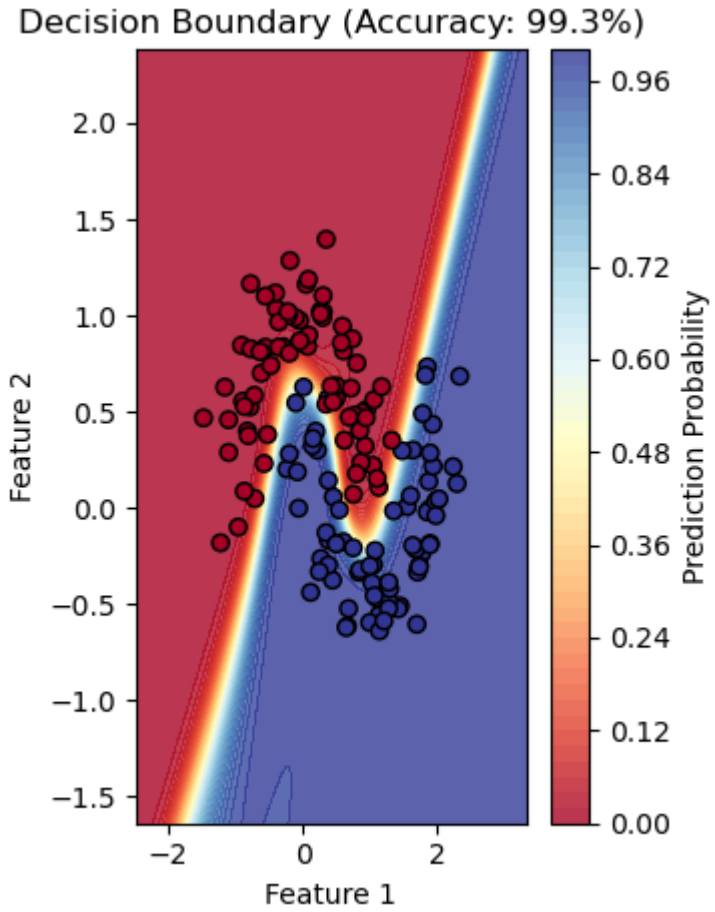


In [6]:

```
# Evaluation
# TODO: Compute the accuracy on the test set and plot the decision boundary

y_hat_test = mlp.forward(X_test)
test_loss = binary_cross_entropy(y_hat_test, y_test)

# Compute accuracy
predictions = (y_hat_test > 0.5).astype(int)
accuracy = np.mean(predictions == y_test) * 100

print(f"\nTest Loss: {test_loss:.4f}")
```

```
print(f"Test Accuracy: {accuracy:.2f}%")

# Plot decision boundary
def plot_decision_boundary(mlp, X, y, title="Decision Boundary"):
    """Plot the decision boundary of the trained MLP"""
    # Create a mesh of points
    h = 0.02
    x_min, x_max = X[0, :].min() - 1, X[0, :].max() + 1
    y_min, y_max = X[1, :].min() - 1, X[1, :].max() + 1
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                         np.arange(y_min, y_max, h))

    # Make predictions on the mesh
    mesh_points = np.c_[xx.ravel(), yy.ravel()].T
    Z = mlp.forward(mesh_points)
    Z = Z.reshape(xx.shape)

    # Create the plot
    plt.contourf(xx, yy, Z, levels=50, alpha=0.8, cmap=plt.cm.RdYlBu)
    plt.colorbar(label='Prediction Probability')

    # Plot the data points
    scatter = plt.scatter(X[0, :], X[1, :], c=y.ravel(), cmap=plt.cm.RdYlBu,
    plt.xlabel('Feature 1')
    plt.ylabel('Feature 2')
    plt.title(title)

plt.subplot(1, 2, 2)
plot_decision_boundary(mlp, X_test, y_test, f"Decision Boundary (Accuracy: {

plt.tight_layout()
plt.show()

print("\n" + "="*60)
print("ANALYSIS:")
print("="*60)
print(f"• The network successfully learned to classify the Two Moons dataset
print(f"• Final test accuracy: {accuracy:.2f}%")
print(f"• The decision boundary successfully separates the two moon-shaped c
print(f"• The nonlinear activation functions (tanh in hidden layer) enable t
print(f"  to learn the complex, nonlinear decision boundary required for thi
print(f"• The smooth decision boundary shows the network has generalized wel
print("="*60)
```

```
Test Loss: 0.0598
Test Accuracy: 99.33%
```




```
============================================================
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============================================================
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• Final test accuracy: 99.33%
• The decision boundary successfully separates the two moon-shaped clusters
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============================================================
```