MLE Sheet 4

May 2025

Exercise 1: Backpropagation for a Classification Task

Task 1

Softmax function:

$$\hat{y}_i = \frac{e^{\tilde{z}_i^{(L)}}}{\sum_{m=1}^{C} e^{\tilde{z}_m^{(L)}}} = \sigma(\tilde{\boldsymbol{z}}^{(L)})_i$$

Cross-entropy loss:

$$\mathcal{L}(\hat{\boldsymbol{y}}, \boldsymbol{y}) = -\sum_{i=1}^{C} y_i \log(\hat{y}_i)$$

Here, $\boldsymbol{y} \in \{0,1\}^C$ is a one-hot encoded vector of true class labels.
We want to compute:

$$\frac{\partial \mathcal{L}}{\partial \tilde{z}_j^{(L)}} = \sum_{i=1}^{C} \frac{\partial \mathcal{L}}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{\partial \tilde{z}_j^{(L)}}$$

We take derivative of the Loss w.r.t Softmax Output

$$\frac{\partial \mathcal{L}}{\partial \hat{y}_i} = -\frac{y_i}{\hat{y}_i}$$

We take derivative of Softmax w.r.t Preactivation

$$\frac{\partial \hat{y}_i}{\partial \tilde{z}_j^{(L)}} = \hat{y}_i(\delta_{ij} - \hat{y}_j)$$

where δ_{ij} is the Kronecker delta.
Using Chain Rule

$$\frac{\partial \mathcal{L}}{\partial \tilde{z}_j^{(L)}} = \sum_{i=1}^{C} \left(-\frac{y_i}{\hat{y}_i} \right) \cdot \hat{y}_i (\delta_{ij} - \hat{y}_j)$$
$$= -\sum_{i=1}^{C} y_i (\delta_{ij} - \hat{y}_j)$$

Since $\boldsymbol{y}$ is one-hot encoded, only the true class index k has $y_k = 1$, and all other $y_i = 0$. Therefore, the sum reduces to:

$$-(\delta_{kj} - \hat{y}_j) = \hat{y}_j - y_j$$

Therefore,

$$\delta^{(L)} := \nabla_{\tilde{\boldsymbol{z}}^{(L)}} \mathcal{L} = \hat{\boldsymbol{y}} - \boldsymbol{y}$$

This concludes the derivation of the initial step in the backpropagation recursion.

Task 2

From Task 1, we know that the gradient of the loss with respect to the preactivation of the output layer is:

$$\delta^{(L)} := \nabla_{\tilde{\boldsymbol{z}}^{(L)}} \mathcal{L} = \hat{\boldsymbol{y}} - \boldsymbol{y}$$

We now have to compute the gradients of the loss with respect to the parameters of the last hidden layer, i.e., with respect to $W^{(L-1)}$ and $\boldsymbol{b}^{(L-1)}$.

(a) Gradient with Respect to the Weights $W^{(L-1)}$

Using the backpropagation rule:

$$\nabla_{W^{(l)}} \mathcal{L} = \delta^{(l+1)} \cdot (\boldsymbol{z}^{(l)})^\top$$

for $l = L - 1$, we get:

$$\nabla_{W^{(L-1)}} \mathcal{L} = \delta^{(L)} \cdot (\boldsymbol{z}^{(L-1)})^\top$$

Dimensions

- $\delta^{(L)} \in \mathbb{R}^C$
- $\boldsymbol{z}^{(L-1)} \in \mathbb{R}^{d_{L-1}}$
- So, $\nabla_{W^{(L-1)}} \mathcal{L} \in \mathbb{R}^{C \times d_{L-1}}$

This matches the dimensions of the weight matrix $W^{(L-1)} \in \mathbb{R}^{C \times d_{L-1}}$.

(b) Gradient with Respect to the Biases $\boldsymbol{b}^{(L-1)}$

Using the backpropagation rule:

$$\nabla_{\boldsymbol{b}^{(l)}} \mathcal{L} = \delta^{(l+1)}$$

for $l = L-1$, we obtain:

$$\nabla_{\boldsymbol{b}^{(L-1)}} \mathcal{L} = \delta^{(L)}$$

Dimensions

- $\delta^{(L)} \in \mathbb{R}^C \Rightarrow \nabla_{\boldsymbol{b}^{(L-1)}} \mathcal{L} \in \mathbb{R}^C$

  This matches the dimensions of the bias vector $\boldsymbol{b}^{(L-1)} \in \mathbb{R}^C$.

Task 3

To compute the error signal for the last hidden layer (layer $L-1$), we use the backpropagation recursion formula:

$$\delta^{(L-1)} = \left(W^{(L-1)\top} \delta^{(L)}\right) \odot \phi' \left(\tilde{\boldsymbol{z}}^{(L-1)}\right)$$

From Task 1, we know:

$$\delta^{(L)} = \hat{\boldsymbol{y}} - \boldsymbol{y}$$

Substituting this into the formula:

$$\delta^{(L-1)} = \left(W^{(L-1)\top} (\hat{\boldsymbol{y}} - \boldsymbol{y})\right) \odot \phi' \left(\tilde{\boldsymbol{z}}^{(L-1)}\right)$$

ReLU Activation and Its Derivative

We now assume the activation function ϕ is the ReLU function:

$$\phi(x) = \max(0, x)$$

with derivative:

$$\phi'(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases}$$

Effect on Gradient Flow

Consider the j-th component $\delta_j^{(L-1)}$. If the preactivation $\tilde{z}_j^{(L-1)} < 0$, then:

$$\phi' \left(\tilde{z}_j^{(L-1)}\right) = 0 \quad \Rightarrow \quad \delta_j^{(L-1)} = 0$$

This means that the neuron j in layer $L-1$ does not contribute to the gradient update, effectively blocking the gradient from flowing backward through it.

Even at the boundary point $\tilde{z}_j^{(L-1)} = 0$, we adopt the common convention $\phi'(0) = 0$, so $\delta_j^{(L-1)} = 0$ holds there as well.

Conclusion

The use of the ReLU activation introduces sparsity in the backward pass: only those neurons that were *active* (i.e., had positive preactivations) during the forward pass can propagate error gradients backward. This has two important consequences:

- It can improve computational efficiency and reduce interference between gradients.
- However, it also risks the "dying ReLU" problem: if a neuron consistently receives negative inputs, it never activates, and its weights are never updated.

This insight explains why ReLU networks may require careful initialization and learning rate tuning in practice.

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

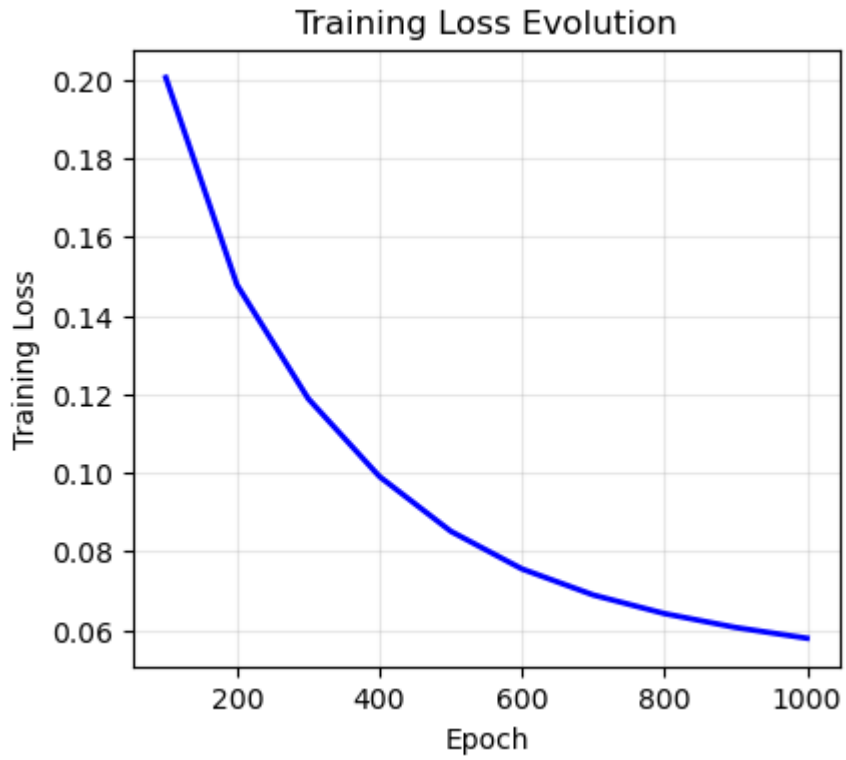
In [4]:
```
#Data loading and preprocessing (predefined)
X, y = make_moons(n_samples=500, noise=0.2, random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, ran


# 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
```

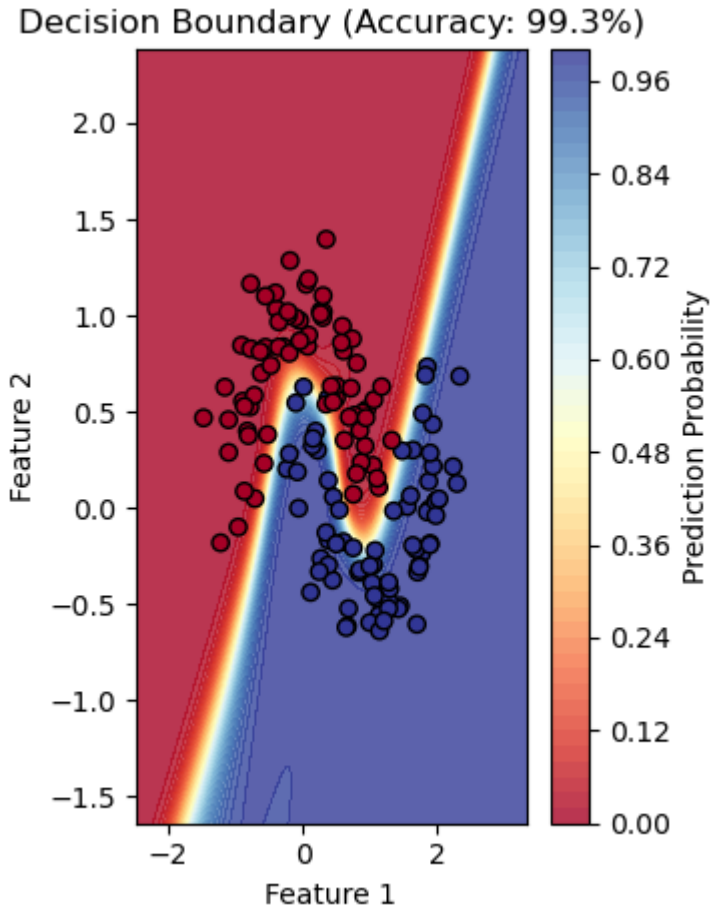


In [6]:

```
# 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%
```




```
============================================================
ANALYSIS:
============================================================
• The network successfully learned to classify the Two Moons dataset
• Final test accuracy: 99.33%
• The decision boundary successfully separates the two moon-shaped clusters
• The nonlinear activation functions (tanh in hidden layer) enable the netw
ork
  to learn the complex, nonlinear decision boundary required for this datas
et
• The smooth decision boundary shows the network has generalized well
============================================================
```

Exercise 3: Neural Playground

Task 1

Architecture:

- Hidden Layers: 3
- Neuron per layer: 8 neurons in each layer
- Activation Function: *tanh* for all layers
- Learning: 0.1
- Input features: $X1$ and $X2$
- Regularization: None

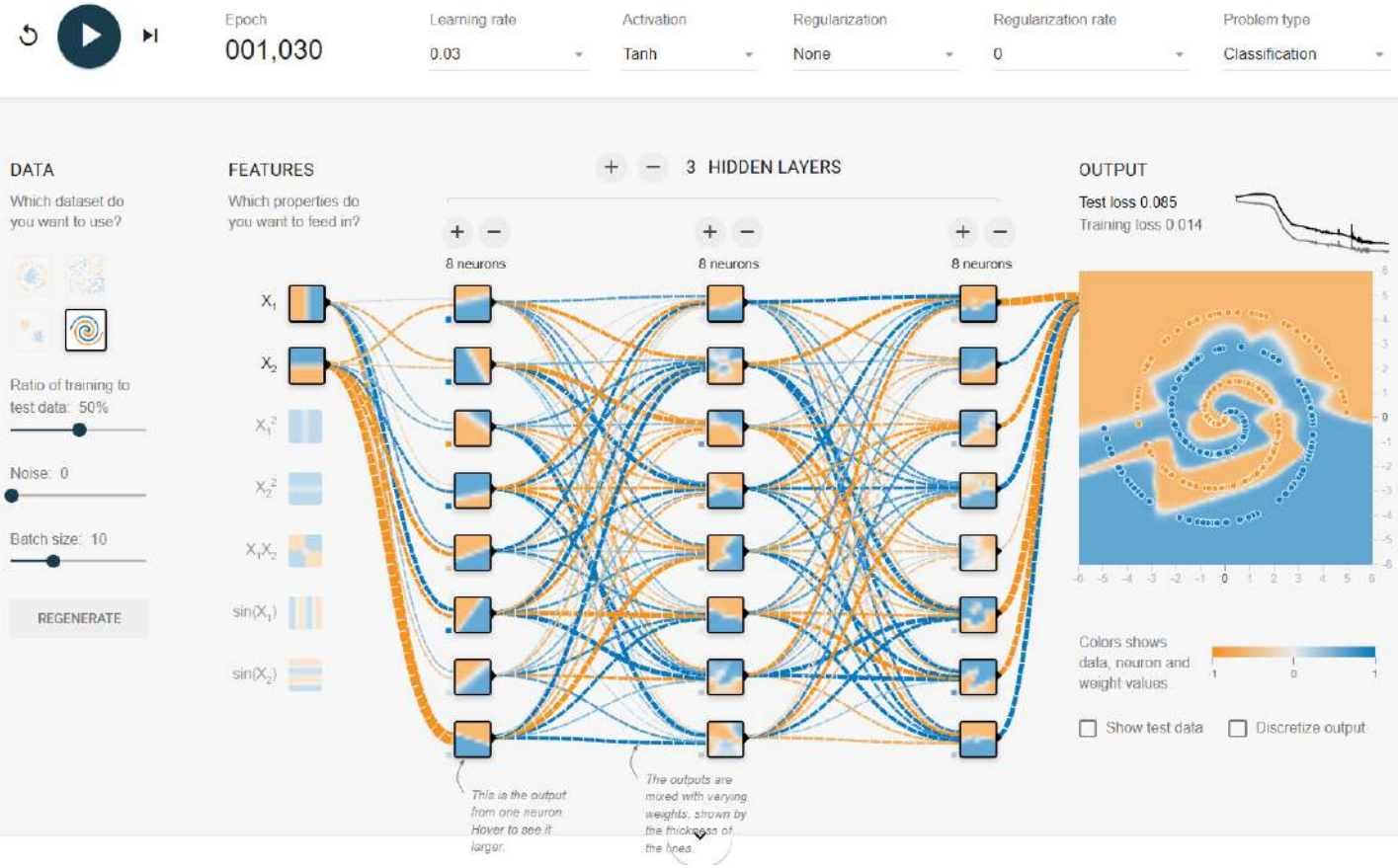
Why this architecture?

- The spiral dataset is highly nonlinear and to learn its twisting pattern might require multiple layers.
- I've tried with 2 layers, 4 and 5 layers which did not give a good loss that 3 layers did. I believe it finds a balance between underfitting and overfitting at layer 3.
- The *tanh* activation function worked better than ReLU or sigmoid. I believe because it can handle positive and negative input ranges which the spiral pattern requires.
- I tried with different learning rate but 0.1 gave me the fastest convergence without overshooting.

Outcome:

- Achieved a test loss <= 0.1 after 500 epochs and reached a constant 0.02 test loss after 800 epochs.

Tinker With a **Neural Network** Right Here in Your Browser.
Don't Worry, You Can't Break It. We Promise.



Task 2

Experimental Setup:

We used the Spiral dataset with all 7 available input features:

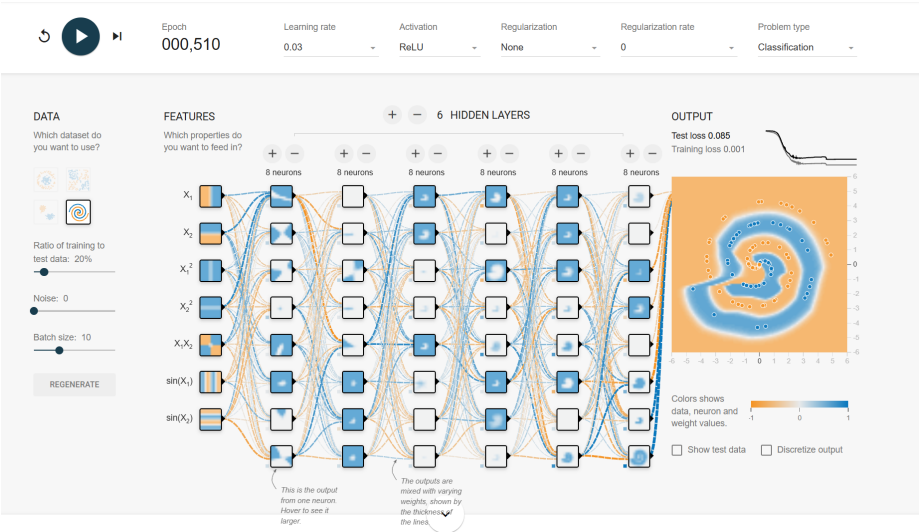
$$X_1,\ X_2,\ X_1^2,\ X_2^2,\ X_1X_2,\ \sin(X_1),\ \sin(X_2).$$

The network architecture consisted of 6 hidden layers with 8 neurons each, using the ReLU activation function. The learning rate was set to 0.03, and the training set size was restricted to 20% of the total data (80% test data). We conducted three experiments: without regularization, with L1 regularization, and with L2 regularization.

(a) No Regularization

Settings: Regularization disabled.

Observations: The model overfits quickly due to limited data availability. The training loss drops very close to zero, but the test loss remains relatively high.
(**Test loss: 0.085**).
The decision boundary follows the spiral quite well but showed signs of overfitting small fluctuations. Most neurons had strong activations (many thick connection lines).

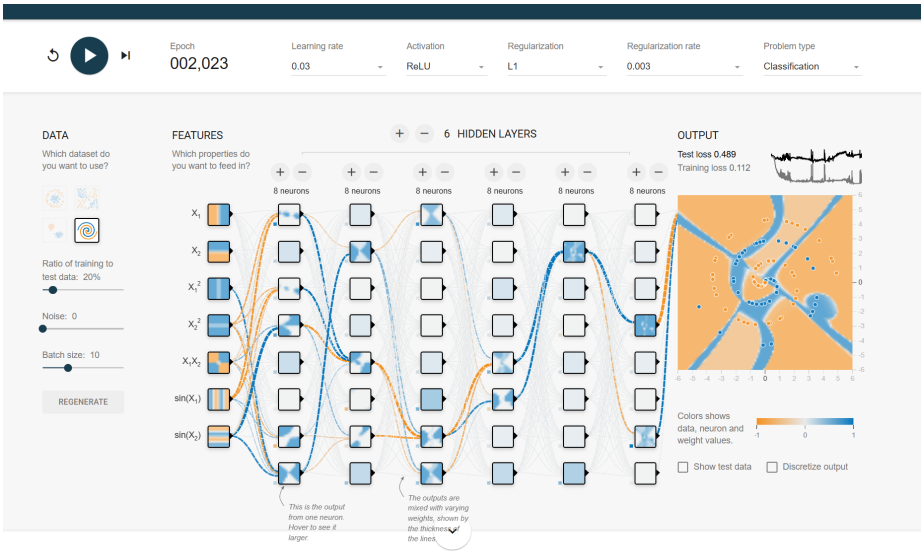


(b) L1 Regularization

Settings: L1 regularization enabled, regularization rate = 0.003.

Observations: L1 regularization results in many connections becoming inactive (thin or missing lines), which shows sparsity. The model simplifies the

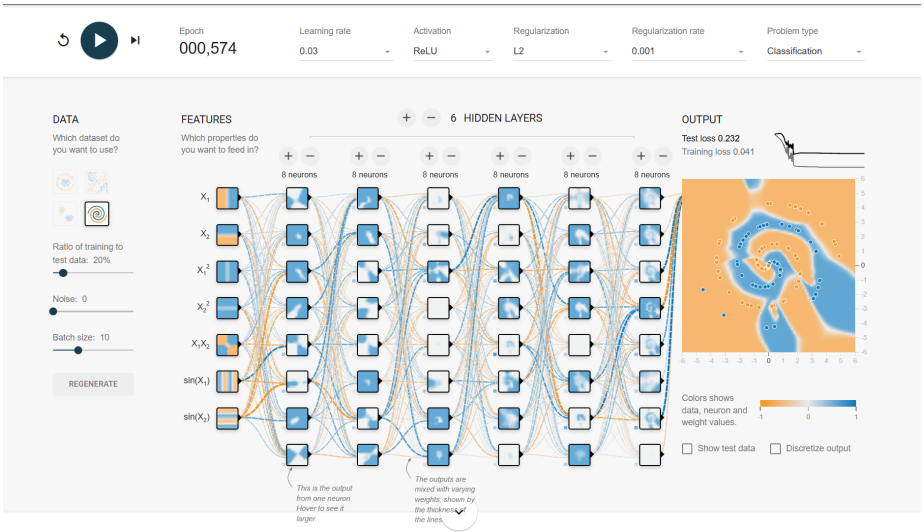
decision boundary considerably but lost its flexibility to fully model the spiral pattern, which has lead to its underfitting.
(**Test loss: 0.489**)
The network sacrifices model complexity to enforce sparse weights.



(c) L2 Regularization

Settings: L2 regularization enabled, regularization rate = 0.001.

Observations: L2 regularization seems to shrink weights more evenly across the network (visible as thinner lines, but no entirely disconnected neurons). The decision boundary still is the spiral but its in a smoother fashion compared to no regularization. Generalization has been improved, which has resulted in lower test loss compared to L1 regularization.
(**Test loss: 0.232**).



So In Summary:

- **No regularization:** Complex decision boundary, risk of overfitting with small training data.
- **L1 regularization:** Promoted sparsity, simplified network structure but underfits the highly nonlinear data.
- **L2 regularization:** Balanced complexity and generalization, which lead to the smooth decision boundary and best test performance in this setup.