Final Project of Multiclass Classification on Iris Dataset

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Github Repo: https://github.com/hyukahn16/data2060-final-project

This report is divided into two main sections.

1. Background Information: the first section provides an overview of the foundational concepts behind multiclass classification, including the One-vs-All and All-Pairs algorithms. It also explains the stochastic gradient descent algorithm and the underlying mathematical principles.

project

- 2. Code Implementation and Evaluation: the second section focuses on the code. It is further divided into three parts:
- The implementation of the model.
- Unit tests designed to validate the model.
- A comparison of the reproduced results on the Iris dataset with those obtained using Scikit-learn models.

1. Overviews

1.1 Overview of Multiclass Classification: One-vs-All and All-Pairs

One-vs-All

This algorithm creates a classifier for each class (3 classifiers if there exists 3 classes). For each classifier, it is responsible for predicting whether an input belongs to its corresponding class or not.

Each classifier is trained on the entire dataset with modifications corresponding to each classifier.

The modification changes the dataset such that when you're training a classifier for class 3, labels for all the other classes are modified to 0 and labels for the classifier's class are modified to 1. (More details will be provided in the Representation section)

All-Pairs

This algorithm creates a classifier for each pair of classes. For each classifier, it is responsible for predicting whether a given input belongs to one class or the other.

Each classifier is trained on a portion of the dataset with modifications corresponding to each classifier.

First, each classifier is assigned portion of the dataset that contains the classes the classifier is predicting for. Then, the assigned data's classes are changed so that one class is assigned the label of 1 and the other is assigned the label of 0.

<u>Advantages and Disadvantages of Multiclass Classification</u>

Multiclass classification algorithm is an algorithm that classifies an input that can belong to one of the multiple classes (more than two classes).

For this project, we will be implementing One-vs-All and All-Pairs algorithms for the multiclass classification of the UCI Iris dataset.

Compared to a multiclass classification algorithm that inherently encompasses multiclass classification (output of model predicts multiclass), the main advantages of One-vs-All and All-Pairs stems from the use of binary classifiers.

Because of the binary classifiers to represent multiclass classification, these two algorithms have implementation simplicity and easy interpretability of the predictions.

Unfortunately, the disadvantages also stem from the use of binary classifiers.

- The binary classifiers do not have any knowledge that it is used for multiclass classification and therefore, does not have inherent understanding of the multiclass classification problem.
- Due to training classifier for each class, each classifier is trained on a class imbalanced dataset and may result in overfitting.
- Training multiple classifiers can be computationally expensive.

1.2 Representation

Binary Logistic Regression

Given sample's feature values $x \in \mathbb{R}^d$ and a label $y \in \{0,1\}$, binary logistic regression classifier takes input x and calculates the logit of the input x through affine function:

$$y = \langle w, x \rangle$$

To predict the class of the input, the logit is passed through a sigmoid function to obtain a value between 0 and 1 (probability that input x belongs to class 1):

$$\sigma(y) = rac{1}{1 + e^{-y}}$$

If the value is less than or equal to 0.5, it belongs to class 0. If the value is greater than 0.5, it belongs to class 1.

Therefore, our hypothesis function defined on weights w is

$$h_w(x) = rac{1}{1 + e^{-\langle w, x
angle}}$$

Multiclass Logistic Regression

Now, using the binary logistic regression defined above, we will define one-vs-all and all-pairs multiclass logistic regression algorithms that can classify input x into multiple classes.

Algorithm Pseudocode for One-vs-All (Shalev-Shwartz and Ben-David, 2014)

For one-vs-all, the algorithm utilizes k binary classifiers (logistic regression in our case), where each classifier predicts whether the true class of x belongs in their corresponding class or not.

Given Inputs:

training set
$$S=(x_1,y_1),\ldots,(x_m,y_m)$$

class set C = (0, 1, ..., k), where k == number of classes
binary classifier - logistic regression L

for each $i \in C$:

Create dataset
$$S_i = (x_1, 1_{[y_1=i]}), \ldots, (x_m, 1_{[y_m=i]})$$

Train $h_i = L(S_i)$

Outputs:

$$h(x) \in argmax_{i \in Y} \ h_i(x)$$

Algorithm Pseudocode for All-Pairs (Shalev-Shwartz and Ben-David, 2014)

Given inputs:

training set $S=(x_1,y_1),\ldots,(x_m,y_m)$ class set C=(0,1,...,k), where k=number of classes binary classifier - logistic regression Lforeach $i,j\in C$ such that i< jInitialize empty dataset $S_{i,j}$ for $t=1,\ldots,m$ If $y_t=i$, then add $(x_t,1)$ to $S_{i,j}$ If $y_t=j$, then add $(x_t,0)$ to $S_{i,j}$ Train $h_{i,j}=L(S_{i,j})$

Outputs:

$$h(x) \in argmax_{i \in Y} \left(\Sigma_{j \in Y} \operatorname{sign}(j-i) h_{i,j}(x)
ight)$$

1.3 Loss: Logistic Loss

The loss function of a Logistic Regression classifier over k classes is the **log-loss**, also called **cross-entropy loss**. Since we will only use binary classifier, e.g. Binary Logistic Regression, in this project, only **Binary Log Loss** will be introduced in this section. To be noted, regularization is not used in our project.

The Binary Log Loss on a sample of m data points, also called the Binary Cross Entropy Loss, is:

$$L(h) = -rac{1}{m} \sum_{i=1}^m (y_i \log h(x_i) + (1-y_i) \log (1-h(x_i)))$$

(Scikit-learn. (2024) sklearn.metrics.log_loss)

1.4 Optimizer

One-vs-All and **All-Pairs** are algorithms used to solve muticlass classification problems through binary classifiers. To optimize the binary classifiers, we look to Stochastic Gradient Descent (Mini Batch) algorithm.

Given loss function L and learning rate α , the gradient descent equation for weight w_i update is

$$w_j = w_j - lpha \cdot rac{\partial L}{\partial w_j}$$

For each batch of size m, the gradient of the binary log loss L (given in the previous section) with respect to weight w_i is

$$rac{\partial L}{\partial w_j} = rac{1}{m} \sum_{i=1}^m (h(x_i) - y_i) \cdot x_{ij}$$

Therefore, our stochastic gradient update is

$$w_j = w_j - lpha \cdot \left(rac{1}{m} \sum_{i=1}^m (h(x_i) - y_i) \cdot x_{ij}
ight).$$

Pseudocode: Stochastic Gradient Descent for Logistic Regression (Shalev-Shwartz and Ben-David, 2014)

Given inputs:

Traning examples S, step size lpha, batch size b < |S|

initialize: $\mathbf{w} = 0$

for $t=1,2,\ldots,T$:

Randomly shuffle S

for i = 0 to |S|/b - 1:

S' = Extracted current batch using i

 $\mathbf{w} = \mathbf{w} - \alpha \cdot
abla L_{S'}(h_w)$ + regularization

return

2. Codes

2.1 Model

In [1]: import numpy as np
from sklearn.linear model import SGDClassifier

```
# Testing models using SGDClassifier from Scikit-learn (2024)
def sigmoid(x):
        Sigmoid function f(x) = 1/(1 + exp(-x))
        :param x: A scalar or Numpy array
        :return: Sigmoid function evaluated at x (applied element-wise if it is an array)
    return np.where(x > 0, 1 / (1 + np.exp(-x)), np.exp(x) / (np.exp(x) + np.exp(0)))
def get estimator(train epochs, lr):
        helper function to get SGDClassifier from Sklearn.
        Other parameters except for the number of max iterations and learning rate
        have already been set in SGDClassifier.
    0.00
        Since shuffling in SKlearn is different from that in our custom logistic regression
        model, here we turn the shuffling off.
        We also employ a log loss and constant learning rate in our SGDClassfier.
        The reason that we choose SGDClassifier instead of the logistic regression model in sklearn
        is that it employs SGD as its optimizor while the logistic regression model does not.
    0.00
    estimator = SGDClassifier(
        loss='log loss',
        tol=None,
        max iter=train epochs,
        shuffle=False.
        # shuffle=True.
        random state=0,
        learning rate='constant',
        eta0=lr,
        alpha=0)
    return estimator
```

2.1.1 Model: Representation - Logistic Regression

```
In [2]:
        import numpy as np
        #Modified Logistic regression taken from HW3 of data2060.
        class MyLogisticRegression:
            Binary Logistic Regression that learns weights using
            stochastic gradient descent.
            def __init__(self, batch_size=1, num_epochs=1, lr=0.0001):
                Initializes a LogisticRegression classifer.
                @attrs:
                    n features: the number of features in the classification problem
                    n classes: the number of classes in the classification problem
                    weights: The weights of the Logistic Regression model
                    alpha: The learning rate used in stochastic gradient descent
                1.1.1
                self.learning rate = lr
                self.num epochs = num epochs
                self.batch size = batch size
                self.weights = None
            def train(self, X, Y):
                Train the model, using batch stochastic gradient descent
                @params:
                    X: a 2D Numpy array where each row contains an example, padded by 1 column for the bias
                    Y: a 1D Numpy array containing the corresponding labels for each example
                @return:
                    None
                1.1.1
                num samples, num features = X.shape
                self.weights = np.zeros((1, num features))
                for epoch in range(self.num epochs):
                    shuffled X = X
                    shuffled Y = Y
                    """ if you want to turn on the shuffling, just uncomment codes below to replace the codes above
```

```
shuffled inds = np.random.permutation(num samples)
        shuffled X = X[shuffled inds]
        shuffled Y = Y[shuffled inds]
        for start in range(0, num samples, self.batch size):
            end = start + self.batch size
           X batch = shuffled X [start: min(end, num samples)]
            Y batch = shuffled Y [start: min(end, num samples)]
            predictions = sigmoid(np.dot(X batch, self.weights.T)) # num samples * 1 (num classes)
           Y batch = np.reshape(Y batch,(len(Y batch),1)) # num samples * 1, reshape Y to same dimension
            error = predictions - Y batch
           loss grad = np.dot(error.T, X batch)/len(X batch)
            self.weights -= self.learning rate * loss grad
def loss(self, X, Y):
    Computes the logistic loss (binary cross-entropy loss) for binary classification
   @params:
       X: 2D Numpy array where each row contains an example, padded by 1 column for the bias
       Y: 1D Numpy array containing the corresponding labels for each example
   @return:
       A float number which is the average loss of the model on the dataset
   # Clip predictions to prevent log(0)
   y pred = self.predict(X)
   y pred = np.clip(y pred, 1e-15, 1 - 1e-15)
   left half = Y.T @ np.log(y pred)
   right half = (1-Y).T @ np.log(1-y) pred
   # Calculate the logistic loss
   loss = -np.mean(left half + right half)
    return loss
def predict(self, X):
    Compute predictions based on the learned parameters and examples X
```

```
@params:
       X: a 2D Numpy array where each row contains an example, padded by 1 column for the bias
   @return:
       A 1D Numpy array with one element for each row in X containing the predicted class.
   # X.shape: (batch size, num features)
   # self.weights.shape: (1, num features)
   dot product = np.dot(self.weights, X.T) # n classes * n samples
   probs = sigmoid(dot product)
   probsall = np.vstack((1-probs, probs)) # probs are for class 2
   y predict = np.argmax(probsall, axis=0) #finding the index of the max value in a column
    return y predict
def accuracy(self, X, Y):
    Output the accuracy of the trained model on a given testing dataset X and labels Y.
   @params:
       X: a 2D Numpy array where each row contains an example, padded by 1 column for the bias
       Y: a 1D Numpy array containing the corresponding labels for each example
   @return:
        a float number indicating accuracy (between 0 and 1)
    predicted classes = self.predict(X)
   return np.mean(predicted classes == Y)
def predict proba(self, X):
    Compute probabilities for the input data X.
   @params:
   X: A 2D Numpy array where each row contains an example
   @return:
    Probabilities of each example being in class 1
   dot product = np.dot(self.weights, X.T) # n classes * n samples
   probs = sigmoid(dot product)
    return probs
```

2.1.2 Model: one-vs-all

```
In [3]: import numpy as np
        class OnevsAll:
            def init (self, n classes, batch size=1, epochs=1, lr=0.01):
                self.n classes = n classes
                self.lr = lr
                self.batch size = batch size
                self.epochs = epochs
                # self.conv threshold = conv threshold
            def train(self, X, Y):
                # Split data and train each representation
                self.S Y = np.array([np.array(Y) for in range(self.n classes)])
                self.h = np.array([
                    MyLogisticRegression(
                        batch size=self.batch size,
                        num epochs=self.epochs,
                        lr=self.lr
                        ) for in range(self.n classes)])
                self.conv epochs = [0] * self.n classes
                for cls in range(self.n classes):
                    # Create S i for each class i
                    S Y i = self.S Y[cls]
                    cls idx = S Y i == cls
                    S Y i[cls idx] = 1
                    non cls idx = np.logical_not(cls_idx)
                    S Y i[non cls idx] = 0
                    # Train h i for each class i on S i
                    h i = self.h[cls]
                    conv epoch = h i.train(X, S Y i)
                    self.conv epochs.append(conv epoch)
            Loss function is similar to accuracy function.
            As a result, we choose to only keep accuracy function.
            0.00
            # def loss(self, X, Y):
                  preds = self.predict(X)
                  # L1-loss
```

```
losses = np.abs(Y-preds)
     losses = np.sum(losses)
#
     return losses
def predict(self, X):
    \# h i in argmax h i(x)
    predictions = [0] * X.shape[0]
    for i, x in enumerate(X):
        preds = [0] * self.n classes
       # Get predictions from all hypotheses
       for c in range(self.n classes):
            preds[c] = self.h[c].predict proba(x)
       # Select max prediction
        predictions[i] = np.argmax(preds)
    return predictions
def accuracy(self, X, Y):
    predictions = self.predict(X)
    return np.mean(predictions == Y)
```

2.1.3 Model: all-pairs

```
In [4]: # You can only use python and numpy in this section.
import numpy as np

class AllPairs:
    def __init__(self, n_classes, batch_size, epochs, lr):
        self.n_classes = n_classes
        self.batch_size = batch_size
        self.epochs = epochs

        self.models = {}
        self.lr = lr

    def train(self, X, Y):
        if X.shape[0] == 0 or Y.shape[0] == 0:
            raise ValueError("No data provided")

    for i in range(self.n_classes):
```

```
for j in range(i + 1, self.n classes):
            selected indices = []
            for index, label in enumerate(Y):
                if label == i or label == j:
                    selected indices.append(index)
           X selected = X[selected indices]
           Y selected = Y[selected indices]
            for idx in range(len(Y selected)):
                if Y selected[idx] == i:
                    Y = ected[idx] = 0
                else:
                    Y \text{ selected[idx]} = 1
            model = MyLogisticRegression(batch size=self.batch size, num epochs=self.epochs, lr=self.l
            model.train(X selected, Y selected)
            key = i, j
            self.models[key] = model
def loss(self, X, Y):
   prediction = self.predict(X)
   losses = np.abs(Y - prediction)
    return np.sum(losses)
def predict(self, X):
   votes = np.zeros((X.shape[0], self.n classes))
   confidence scores = np.zeros((X.shape[0], self.n classes))
   for (i, j), model in self.models.items():
       probabilities = model.predict proba(X)
       predictions = (probabilities >= 0.5).astype(int).flatten()
       votes[:, i] += (1 - predictions)
       votes[:, j] += predictions
        confidence scores[:, i] += 1 - probabilities.flatten()
        confidence scores[:, j] += probabilities.flatten()
```

```
max_votes = np.max(votes, axis=1, keepdims=True)
candidates = (votes == max_votes).astype(int)
final_scores = confidence_scores * candidates
return np.argmax(final_scores, axis=1)

def accuracy(self, X, Y):
    predictions = self.predict(X)
    return np.mean(predictions == Y)
```

2.2 Unit Tests

We develop a series of unit tests to evaluate our models and provide helper functions for visualizing the results, which are compared against those of sklearn models. The unit tests are categorized based on their corresponding test models. For each model, we include the following components:

- A helper function for visualization.
- Unit tests on toy datasets to validate the model's internal functions.
- A unit test to compare the results with sklearn models on a linearly separable dataset.
- A unit test to compare the results with sklearn models on a more complex, non-linear dataset.

2.2.1 Check Logistic Regression

2.2.1.1 A helper function for visualization

```
# train my models
X \text{ bias} = \text{np.c} [X, \text{np.ones}(X.\text{shape}[0])]
my model = MyLogisticRegression(lr=lr, batch size=1, num epochs=num epochs)
my model.train(X bias, Y)
# train sklearn model
# SGDClassifier is always batch size == 1
sklearn model = get estimator(num epochs, lr)
sklearn model.fit(X, Y)
weights = my model.weights
assert isinstance(weights, np.ndarray)
assert weights.ndim==2 and weights.shape == (1,X.shape[1]+1)
# FIXME: relative tolerance might be not strict enough
print('my weight', weights[0])
print('sklearn weight', np.append(sklearn model.coef [0], sklearn model.intercept [0]))
assert weights[0][:-1] == pytest.approx(sklearn model.coef [0], 0.01)
assert weights[0][-1] == pytest.approx(sklearn model.intercept [0], 0.01)
# Create a meshgrid and predict on the grid points
x \min = \min(X[:, 0].\min(), X \operatorname{test}[:, 0].\min())
x max = max(X[:, 0].max(), X test[:, 0].max())
y \min = \min(X[:, 1].\min(), X test[:, 1].\min())
y \max = \max(X[:, 1].\max(), X \text{ test}[:, 1].\max())
x gap = x max - x min
y gap = y max - y min
xx, yy = np.meshgrid(np.linspace(x min -x gap/100, x max + x gap/100, 200), np.linspace(y min-y gap/100, x max + x gap/100, x 
bias = np.ones(xx.ravel().shape)
features with bias = np.c [xx.ravel(), yy.ravel(), bias]
my Z = my model.predict(features_with_bias)
my Z = my Z.reshape(xx.shape)
sklearn Z = sklearn model.predict(np.c [xx.ravel(), yy.ravel()])
sklearn Z = sklearn Z.reshape(xx.shape)
# check test data predictions
X test bias = np.c [X test, np.ones(X test.shape[0])]
my preds = my model.predict(X test bias)
sklearn preds = sklearn model.predict(X test)
```

```
assert (my preds == sklearn preds).all()
# Create subplots
fig, axes = plt.subplots(1, 2, figsize=(12, 6))
# Plot my model's results
axes[0].contourf(xx, yy, my Z, alpha=0.3, colors=['blue', 'red'], levels=[0, 0.5, 1])
train data label1 = X[np.where(Y == 1)]
train data label0 = X[np.where(Y == 0)]
test data label1 = X test[np.where(Y test == 1)]
test data label0 = X test[np.where(Y test == 0)]
axes[0].scatter(train data label1[:, 0], train data label1[:, 1], c='red', edgecolor='k', label='Train
axes[0].scatter(train data label0[:, 0], train data label0[:, 1], c='blue', edgecolor='k', label='Train
axes[0].scatter(test data label1[:, 0], test data label1[:, 1], c='red', edgecolor='k', label='Test Da
axes[0].scatter(test_data_label0[:, 0], test_data_label0[:, 1], c='blue', edgecolor='k', label='Test Data
axes[0].set title("Decision Boundary (My Model)")
axes[0].set xlabel("Feature 1")
axes[0].set ylabel("Feature 2")
axes[0].legend(loc='center left', bbox to anchor=(1, 0.5))
# Plot sklearn model's results
axes[1].contourf(xx, yy, sklearn Z, alpha=0.3, colors=['blue', 'red'], levels=[0, 0.5, 1])
axes[1].scatter(train data label1[:, 0], train data label1[:, 1], c='red', edgecolor='k', label='Train
axes[1].scatter(train data label0[:, 0], train data label0[:, 1], c='blue', edgecolor='k', label='Train
axes[1].scatter(test data label1[:, 0], test data label1[:, 1], c='red', edgecolor='k', label='Test Da
axes[1].scatter(test data label0[:, 0], test data label0[:, 1], c='blue', edgecolor='k', label='Test Data
axes[1].set title("Decision Boundary (Sklearn Model)")
axes[1].set xlabel("Feature 1")
axes[1].set ylabel("Feature 2")
axes[1].legend(loc='center left', bbox to anchor=(1, 0.5))
# Adjust layout and show the plot
plt.tight layout()
plt.show()
my acc = my model.accuracy(X=X test bias, Y=Y test)
sklearn acc = sklearn model.score(X=X test,y=Y test)
print('The test Accuracy of My Logistic Regression Model is ', my acc)
print('The test Accuracy of Sklearn SGD Classifier is ', sklearn acc)
```

2.2.1.2 2-Point Toy Dataset

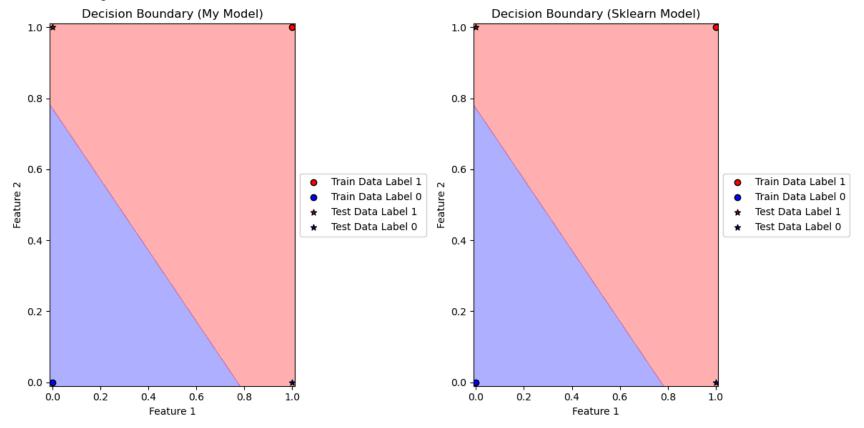
To evaluate the performance of different models when the test points are on the decision boundary.

```
In [6]: # Set random seed for testing purposes
    np.random.seed(0)

# Create Data
    X1_train = np.array([[0,0], [1,1]])
    Y1_train = np.array([0,1])

    X1_test = np.array([[0,1], [1,0]])
    Y1_test = np.array([1, 0])

CheckPlot_LR(X=X1_train, Y=Y1_train, X_test=X1_test, Y_test=Y1_test, lr=0.01, num_epochs=1000)
```



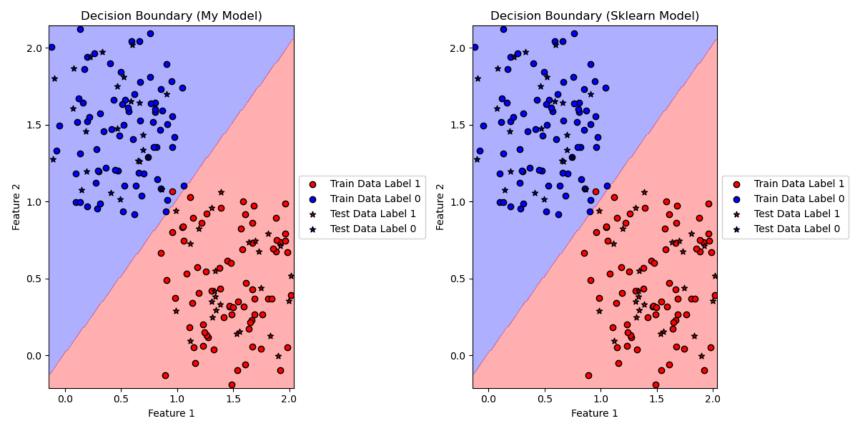
The test Accuracy of My Logistic Regression Model is 0.5 The test Accuracy of Sklearn SGD Classifier is 0.5

2.2.1.3 Linearly separated dataset

To evaluate performance of different models on linearly separated dataset

```
np.random.seed(0)
In [7]:
        # generate two linear seperated datasets
        class 0 = np.random.rand(100, 2) + [0, 1]
        class 1 = np.random.rand(100, 2) + [1, 0]
         # add noises
        noise 0 = np.random.normal(0, 0.1, class 0.shape)
        noise 1 = np.random.normal(0, 0.1, class 1.shape)
         class 0 += noise 0
        class 1 += noise 1
        X2 = np.vstack((class 0, class 1))
        Y2 = np.hstack((np.zeros(100), np.ones(100)))
         # Split train and test datasets
         indices = np.arange(X2.shape[0])
        shuffled inds = np.random.permutation(indices)
        X2 = X2[shuffled inds]
        Y2 = Y2[shuffled inds]
        X2 train = X2[indices[:150]]
        Y2 train = Y2[indices[:150]]
        X2 \text{ test} = X2[\text{indices}[-51:-1]]
        Y2 \text{ test} = Y2[\text{indices}[-51:-1]]
         # check
        CheckPlot LR(X=X2 train, Y=Y2 train, X test=X2 test, Y test=Y2 test,
                      lr=0.01, num epochs=1000)
```

my weight [8.62864918 -8.61004358 0.14766954] sklearn weight [8.62864918 -8.61004358 0.14766954]

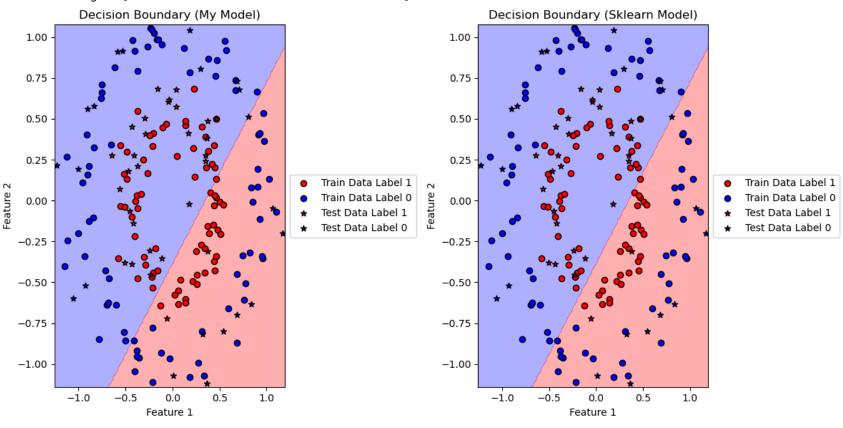


The test Accuracy of My Logistic Regression Model is 1.0 The test Accuracy of Sklearn SGD Classifier is 1.0

2.2.1.4 Non-Linearly separated datasets

To evaluate the models' performance on a more non-trivial case -- on non-linearly separated dataset

my weight [0.24860853 -0.22378149 -0.08607428] sklearn weight [0.24860853 -0.22378149 -0.08607428]



The test Accuracy of My Logistic Regression Model is 0.3 The test Accuracy of Sklearn SGD Classifier is 0.3

2.2.2 Check Model: one-vs-all

2.2.2.1 A helper function for visualization

```
In [9]: import numpy as np
                    import matplotlib.pyplot as plt
                    from sklearn.multiclass import OneVsRestClassifier
                    # Testing models using OneVsRestClassifier from Scikit-learn (2024)
                    def CheckPlot OnevsAll(X train, Y train, X test, Y test, lr, num epochs):
                              helper function for visualizing the differences of our OnevsAll model
                              and OneVsRestClassifier from sklearn.
                              X train bias = np.c [X train, np.ones(X train.shape[0])]
                             X test bias = np.c [X test, np.ones(X test.shape[0])]
                              # initialize model
                              n classes = len(np.unique(Y train))
                              my model = OnevsAll(n classes, epochs=num epochs, lr=lr)
                              estimator = get estimator(num epochs, lr)
                              sklearn model = OneVsRestClassifier(estimator)
                              my model.train(X train bias, Y train)
                              sklearn model.fit(X train, Y train)
                              # generate meshgrids and predict on it
                              x \min = \min(X \text{ train}[:, 0].\min(), X \text{ test}[:, 0].\min())
                              x max = max(X train[:, 0].max(), X test[:, 0].max())
                              y min = min(X train[:, 1].min(), X test[:, 1].min())
                              y max = max(X train[:, 1].max(), X test[:, 1].max())
                              x gap = x max - x min
                              y gap = y max - y min
                              xx, yy = np.meshgrid(np.linspace(x min -x gap/100, x max + x gap/100, 200), np.linspace(y min-y gap/100, x max + x gap/100, x 
                              bias = np.ones(xx.ravel().shape)
                              features with bias = np.c [xx.ravel(), yy.ravel(), bias]
                              my Z = np.array(my model.predict(features with bias))
                              my Z = my Z.reshape(xx.shape)
                              sklearn Z = sklearn model.predict(np.c [xx.ravel(), yy.ravel()])
```

```
sklearn Z = sklearn Z.reshape(xx.shape)
# check test data predictions
my preds = my model.predict(X test bias)
sklearn preds = sklearn model.predict(X test)
assert (my preds == sklearn preds).all()
# Step 6: Visualize the decision boundaries
fig, axes = plt.subplots(1, 2, figsize=(14, 6))
# Custom OvA model
axes[0].contourf(xx, yy, my Z.reshape(xx.shape), alpha=0.3, cmap="coolwarm")
axes[0].scatter(X train[:, 0], X train[:, 1],
                c=Y train, edgecolor="k", cmap="coolwarm", label='Train Data')
axes[0].scatter(X test[:, 0], X test[:, 1],
                c=Y test, edgecolor="k", cmap="coolwarm", marker='*', label='Test Data')
axes[0].set title("My One-vs-All Model")
axes[0].set xlabel("Feature 1")
axes[0].set ylabel("Feature 2")
axes[0].legend()
# Sklearn OvA model
axes[1].contourf(xx, yy, sklearn Z.reshape(xx.shape), alpha=0.3, cmap="coolwarm")
axes[1].scatter(X train[:, 0], X train[:, 1],
                c=Y train, edgecolor="k", cmap="coolwarm", label='Train Data')
axes[1].scatter(X test[:, 0], X test[:, 1],
                c=Y test, edgecolor="k", cmap="coolwarm", marker='*', label='Test Data')
axes[1].set title("Sklearn One-vs-Rest Model")
axes[1].set xlabel("Feature 1")
axes[1].set ylabel("Feature 2")
axes[1].legend()
plt.tight layout()
plt.show()
my acc = my model.accuracy(X=X test bias, Y=Y test)
sk acc = sklearn model.score(X test, y=Y test)
print('The test accuracy of my One-vs-All model is', my acc)
print('The test accuracy of sklearn One-vs-All model is', sk acc)
```

2.2.2.2 10-Point Toy Model

A toy dataset to train on to compare the weights of Binary classifiers for different classes.

```
In [10]: import numpy as np
         import pytest
         from sklearn.multiclass import OneVsRestClassifier
         from sklearn.linear model import SGDClassifier
         # Testing models using OneVsRestClassifier from Scikit-learn (2024)
         # Testing models using SGDClassifier from Scikit-learn (2024)
         np.random.seed(0)
         X = \text{np.array}([[0,4], [0,3], [5,0], [4,1], [0,5], [1,0], [2,1], [3,2], [4,3], [5,4]])
         X \text{ bias} = \text{np.array}([[0,4,1], [0,3,1], [5,0,1], [4,1,1], [0,5,1], [1,0,1], [2,1,1], [3,2,1], [4,3,1], [5,4,1])
         Y = np.array([0,0,0,1,1,1,1,2,2,2])
         n classes = len(np.unique(Y))
         # Initialize models:
         train epochs = 100
         lr = 0.01
         my model = OnevsAll(n classes, epochs=train epochs, lr=lr)
         estimator = get estimator(train epochs, lr)
         sklearn model = OneVsRestClassifier(estimator)
         my model.train(X bias, Y)
         sklearn model.fit(X, Y)
         # Check that S is populated correctly
         assert my model.S Y.shape[0] == n classes
         assert my model.S Y.shape[1] == Y.shape[0]
         # Check h (individual classifiers)
         assert len(my model.h) == n classes
         assert len(sklearn model.estimators ) == n classes
         for h in my model.h:
             assert isinstance(h, MyLogisticRegression)
         for i in range(n classes):
             my weights = my model.h[i].weights[0][:-1]
```

```
my bias = my model.h[i].weights[0][-1]
     sklearn weights = sklearn model.estimators [i].coef [0]
     sklearn bias = sklearn model.estimators [i].intercept [0]
     print(" === ", i)
     print(my weights)
     print(sklearn weights)
     print(my bias)
     print(sklearn bias)
     # assert my weights == pytest.approx(sklearn weights, 0.01)
     # assert my bias == pytest.approx(sklearn bias, 0.01)
 # Check predictions
 predictions = my model.predict(X bias)
 print("My Predictions:", np.array(predictions))
 sklearn predictions = sklearn model.predict(X)
 print("sklearn Predictions:", sklearn predictions)
 print('num samples', X.shape[0])
 print('Differences', np.sum(np.abs(np.array(predictions)-sklearn predictions)))
 === 0
[-0.31197662 -0.10912839]
[-0.31197662 -0.10912839]
-0.026783970677386276
-0.02678397067738624
 === 1
[-0.25499991 -0.25585737]
[-0.25499991 -0.25585737]
0.533835614573224
0.533835614573224
 === 2
[0.29462046 0.07319256]
[0.29462046 0.07319256]
-1.1883256927760357
-1.1883256927760357
My Predictions: [0 1 2 2 0 1 1 2 2 2]
sklearn Predictions: [0 1 2 2 0 1 1 2 2 2]
num samples 10
Differences 0
```

2.2.2.3 4-Point Toy Dataset

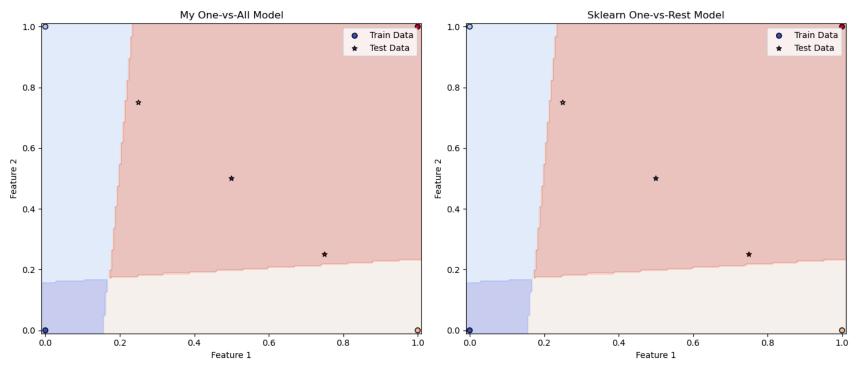
To evaluate the performance of models when test points are on decision boundary.

```
In [11]: import numpy as np

np.random.seed(0)

X7_train = np.array([[0,0],[0,1],[1,0],[1,1]])
Y7_train = np.array([[0,1,2,3])
X7_test = np.array([[0.5,0.5],[0.75,0.25],[0.25,0.75]])
Y7_test = np.array([[0,2,1])

#check
CheckPlot_OnevsAll(X7_train, Y7_train, X7_test, Y7_test, lr=0.01, num_epochs=100)
```

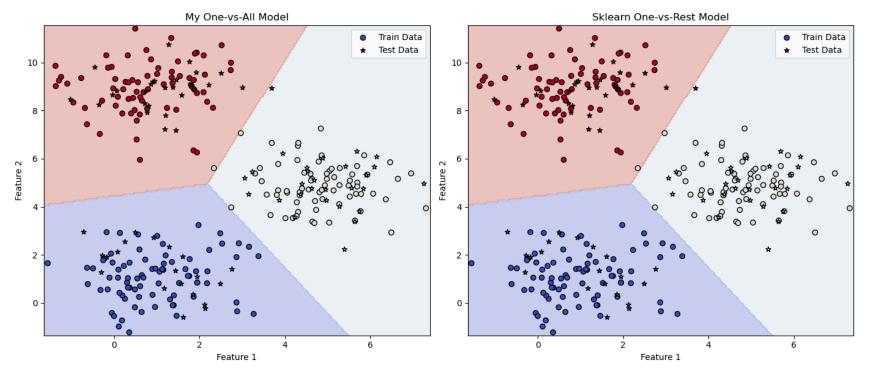


The test accuracy of my One-vs-All model is 0.0 The test accuracy of sklearn One-vs-All model is 0.0

2.2.2.4 Linearly-separated Datasets

To evaluate performance of different models on linearly separated dataset

```
In [12]:
         import numpy as np
         np.random.seed(0)
         # Generate 100 samples for each class
         n \text{ samples} = 100
         # class 0 centered on [1,1]
         class 1 = np.random.randn(n samples, 2) + [1, 1]
         # class 1 centered on [6,6]
         class 2 = np.random.randn(n samples, 2) + [5, 5]
         # class 2 centered on [3,4]
         class 3 = np.random.randn(n samples, 2) + [1, 9]
         X5 = np.vstack([class 1, class 2, class 3])
         Y5 = np.hstack([np.zeros(n samples), np.ones(n samples), np.full(n samples, 2)])
         indices = np.arange(X5.shape[0])
         shuffled inds = np.random.permutation(indices)
         X5 = X5[shuffled inds]
         Y5 = Y5[shuffled inds]
         X5 train = X5[indices[:225]]
         Y5 train = Y5[indices[:225]]
         X5 \text{ test} = X5[\text{indices}[-76:-1]]
         Y5 test = Y5[indices[-76:-1]]
         #check
         CheckPlot OnevsAll(X5 train, Y5 train, X5 test, Y5 test, lr=0.01, num epochs=1000)
```

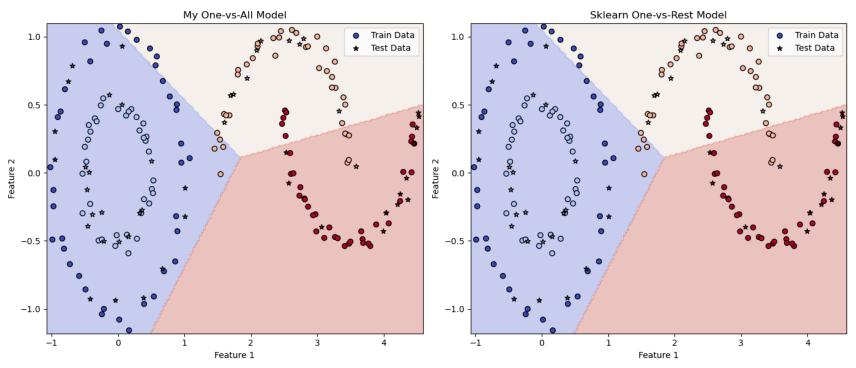


The test accuracy of my One-vs-All model is 0.986666666666667 The test accuracy of sklearn One-vs-All model is 0.986666666666667

2.2.2.5 Non-linearly Separated Data

To evaluate the models' performance on a more non-trivial case -- on non-linearly separated dataset

```
shuffled_inds = np.random.permutation(indices)
X6 = X6[shuffled_inds]
Y6 = Y6[shuffled_inds]
X6_train = X6[indices[:150]]
Y6_train = Y6[indices[:150]]
X6_test = X6[indices[-51:-1]]
Y6_test = Y6[indices[-51:-1]]
#check
CheckPlot_OnevsAll(X6_train, Y6_train, X6_test, Y6_test, lr=0.01, num_epochs=1000)
```



The test accuracy of my One-vs-All model is 0.7 The test accuracy of sklearn One-vs-All model is 0.7

2.2.3 Check Model: all-pairs

2.2.3.1 A helper function for visualization

```
In [14]: import numpy as np
                     import matplotlib.pyplot as plt
                     from sklearn.datasets import make classification
                     from sklearn.multiclass import OneVsOneClassifier
                     # Testing models using OneVsOneClassifier from Scikit-learn (2024)
                     def CheckPlot AllPairs(X train, Y train, X test, Y test, lr, num epochs):
                               a helper function for visualizing the differences of our AllPairs model
                               and the OneVsOneClassifier from sklearn.
                              X_train_bias = np.c_[X_train, np.ones(X train.shape[0])]
                              X test bias = np.c [X test, np.ones(X test.shape[0])]
                              # initialize model
                               n classes = len(np.unique(Y train))
                              my model = AllPairs(n classes=n classes, batch size=1, epochs=num epochs, lr=lr)
                               estimator = get estimator(num epochs, lr)
                               sklearn model = OneVsOneClassifier(estimator)
                               my model.train(X train bias, Y train)
                               sklearn model.fit(X train, Y train)
                               # generate meshgrids and predict on it
                              x min = min(X train[:, 0].min(), X test[:, 0].min())
                              x max = max(X train[:, 0].max(), X test[:, 0].max())
                              y min = min(X train[:, 1].min(), X test[:, 1].min())
                              y max = max(X train[:, 1].max(), X test[:, 1].max())
                              x gap = x max - x min
                              y gap = y max - y min
                               xx, yy = np.meshgrid(np.linspace(x min -x gap/100, x max + x gap/100, 200), np.linspace(y min-y gap/100, x max + x gap/100, x 
                               bias = np.ones(xx.ravel().shape)
                               features with bias = np.c [xx.ravel(), yy.ravel(), bias]
                              my Z = np.array(my model.predict(features with bias))
                              my Z = my Z.reshape(xx.shape)
                               sklearn Z = sklearn model.predict(np.c [xx.ravel(), yy.ravel()])
                               sklearn Z = sklearn Z.reshape(xx.shape)
```

```
# check test data predictions
my preds = my model.predict(X test bias)
sklearn preds = sklearn model.predict(X test)
assert (my preds == sklearn preds).all()
# Step 6: Visualize the decision boundaries
fig, axes = plt.subplots(1, 2, figsize=(14, 6))
# Custom OvA model
axes[0].contourf(xx, yy, my Z.reshape(xx.shape), alpha=0.3, cmap="coolwarm")
axes[0].scatter(X train[:, 0], X train[:, 1],
                c=Y train, edgecolor="k", cmap="coolwarm", label='Train Data')
axes[0].scatter(X test[:, 0], X test[:, 1],
                c=Y test, edgecolor="k", cmap="coolwarm", marker='*', label='Test Data')
axes[0].set title("My AllPair Model")
axes[0].set xlabel("Feature 1")
axes[0].set ylabel("Feature 2")
axes[0].legend()
# Sklearn OvA model
axes[1].contourf(xx, yy, sklearn_Z.reshape(xx.shape), alpha=0.3, cmap="coolwarm")
axes[1].scatter(X train[:, 0], X train[:, 1],
                c=Y train, edgecolor="k", cmap="coolwarm", label='Train Data')
axes[1].scatter(X test[:, 0], X test[:, 1],
                c=Y test, edgecolor="k", cmap="coolwarm", marker='*', label='Test Data')
axes[1].set title("Sklearn Allpair Model")
axes[1].set xlabel("Feature 1")
axes[1].set ylabel("Feature 2")
axes[1].legend()
plt.tight layout()
plt.show()
my acc = my model.accuracy(X=X test bias, Y=Y test)
sk acc = sklearn model.score(X test, y=Y test)
print('The test accuracy of my One-vs-All model is', my acc)
print('The test accuracy of sklearn One-vs-All model is', sk acc)
```

2.2.3.2 10-Point Toy Model

A toy dataset to train on to compare the weights of Binary Classifiers for different pairs.

```
In [15]: #Does not work when shuffle is enabled
         import numpy as np
         import pytest
         from sklearn.multiclass import OneVsOneClassifier
         from sklearn.linear model import SGDClassifier
         # Testing models using OneVsOneClassifier from Scikit-learn (2024)
         # Testing models using SGDClassifier from Scikit-learn (2024)
         X = np.array([[0,4], [0,3], [5,0], [4,1], [0,5], [1,0], [2,1], [3,2], [4,3], [5,4]])
         X \text{ bias} = \text{np.array}([[0,4,1], [0,3,1], [5,0,1], [4,1,1], [0,5,1], [1,0,1], [2,1,1], [3,2,1], [4,3,1], [5,4,1])
         Y = np.array([0,0,0,1,1,1,1,2,2,2])
         n classes = len(np.unique(Y))
         train epochs = 100
         lr = 0.01
         my model = AllPairs(n classes, batch size=1, epochs=train epochs, lr=lr)
         my model.train(X bias, Y)
         estimator = get estimator(train epochs, lr)
         sklearn model = OneVsOneClassifier(estimator)
         sklearn model.fit(X, Y)
         def test train basic():
             Test if the model trains the correct number of binary classifiers
             my model = AllPairs(n classes, batch size=1, epochs=train epochs, lr=lr)
             my model.train(X bias, Y)
             assert len(my model.models) == (n classes * (n classes - 1)) // 2, "Incorrect number of models trained
         def test train weights():
             0.00
             Compare weights and biases of trained models against Scikit-learn's OneVsOneClassifier.
             my model = AllPairs(n classes, batch size=1, epochs=train epochs, lr=lr)
             my model.train(X bias, Y)
```

```
for i in range(n classes):
       for j in range(i + 1, n_classes):
            key = (i, j)
           model = my model.models[key]
           my weights = model.weights[0][:-1]
           my bias = model.weights[0][-1]
           model index = int(i * n classes - i * (i + 1) / 2 + j - i - 1)
            sklearn weights = sklearn model.estimators [model index].coef [0]
            sklearn bias = sklearn model.estimators [model index].intercept [0]
           np.testing.assert allclose(my weights, sklearn weights, atol=1e-1, err msg=f"Weights mismatch
           np.testing.assert allclose(my bias, sklearn bias, atol=1e-1, err msg=f"Bias mismatch for class
def test predict basic():
    Compare final prediction result with Scikit-learn's OneVsOneClassifier.
    my model = AllPairs(n classes, batch size=1, epochs=train epochs, lr=lr)
   my model.train(X bias, Y)
   predictions = my model.predict(X bias)
   sklearn predictions = sklearn model.predict(X)
   assert len(predictions) == len(sklearn predictions), "Prediction length mismatch."
   np.testing.assert array equal(predictions, sklearn predictions, "Predictions do not match Scikit-learn
def test edge cases():
   Testing for
    - Empty dataset
   - Single class dataset
    - Dataset with unbalanced classes
   my model = AllPairs(n classes, batch size=1, epochs=train epochs, lr=lr)
   X = mpty = np.empty((0, X bias.shape[1]))
   Y = np.empty((0, ))
   with pytest.raises(ValueError, match="No data provided"):
```

```
my model.train(X empty, Y empty)
    X single class = X bias[:3]
   Y single class = np.zeros((3,))
    my model.train(X single class, Y single class)
    predictions = my model.predict(X single class)
    assert all(predictions == 0), "All predictions should match the single class."
    X unbalanced = np.vstack([X_bias[:8], X_bias[:2]])
    Y unbalanced = np.hstack([Y[:8], Y[:2]])
    my model.train(X unbalanced, Y unbalanced)
    predictions = my model.predict(X unbalanced)
    assert len(predictions) == len(Y unbalanced), "Prediction length mismatch for unbalanced dataset."
def test accuracy():
    Compare accuracy with Scikit-learn's OneVsOneClassifier.
    my model = AllPairs(n classes, batch size=1, epochs=train epochs, lr=lr)
    my model.train(X bias, Y)
    my accuracy = my model.accuracy(X bias, Y)
    sklearn accuracy = sklearn model.score(X, Y)
    assert np.isclose(my accuracy, sklearn accuracy, atol=1e-2), "Accuracy mismatch between models."
print("Running test train basic...")
test train basic()
print("test train basic passed.")
print("Running test train weights...")
test train weights()
print("test train weights passed.")
print("Running test predict basic...")
test predict basic()
print("test predict basic passed.")
print("Running test edge cases...")
```

```
test_edge_cases()
print("test_edge_cases passed.")

print("Running test_accuracy...")
test_accuracy()
print("test_accuracy passed.")

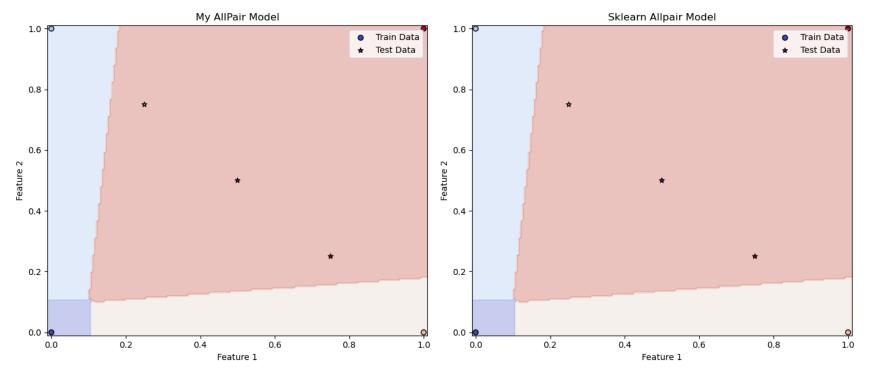
print("All tests passed successfully!")
```

```
Running test_train_basic...
test_train_basic passed.
Running test_train_weights...
test_train_weights passed.
Running test_predict_basic...
test_predict_basic passed.
Running test_edge_cases...
test_edge_cases passed.
Running test_accuracy...
test_accuracy passed.
All tests passed successfully!
```

2.2.3.3 4-Point Toy Dataset

To evaluate the performance of models when test points are on decision boundary.

```
In [16]: np.random.seed(0)
#check
CheckPlot_AllPairs(X7_train, Y7_train, X7_test, Y7_test, 0.01, 100)
```

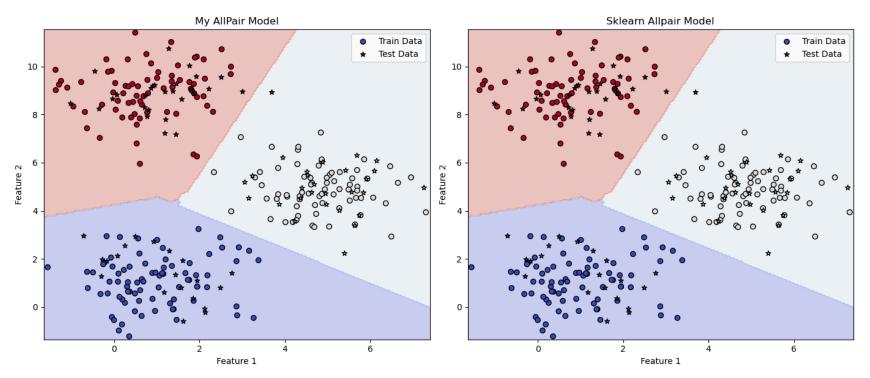


The test accuracy of my One-vs-All model is 0.0 The test accuracy of sklearn One-vs-All model is 0.0

2.2.3.4 Linearly Separated Datasets

To evaluate performance of different models on linearly separated dataset

```
In [17]: np.random.seed(0)
   CheckPlot_AllPairs(X5_train, Y5_train, X5_test, Y5_test, 0.01, 1000)
```

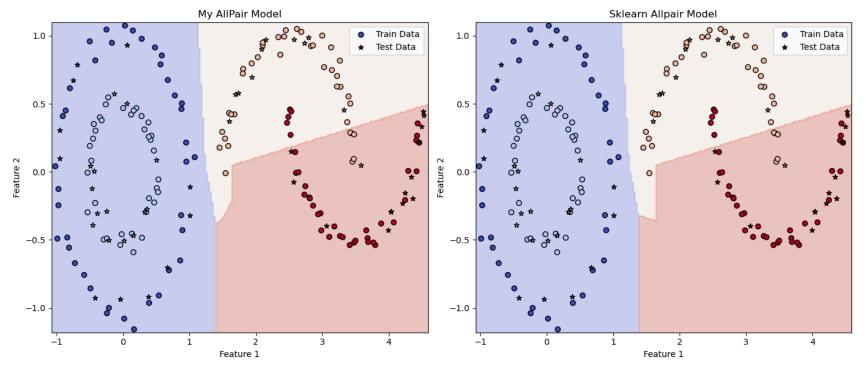


The test accuracy of my One-vs-All model is 0.986666666666667
The test accuracy of sklearn One-vs-All model is 0.986666666666667

2.2.3.5 Non-linearly Separated Datasets

To evaluate the models' performance on a more non-trivial case -- on non-linearly separated dataset

```
In [18]: np.random.seed(0)
CheckPlot_AllPairs(X6_train, Y6_train, X6_test, Y6_test, 0.01, 1000)
```



The test accuracy of my One-vs-All model is 0.7 The test accuracy of sklearn One-vs-All model is 0.7

2.3 Performance on Iris Dataset

```
In [19]: from sklearn.datasets import load_iris
#Iris dataset for testing, Fisher (1936), accessed via Scikit-learn's load_iris
"""

This block is to split training and testing datasets from Iris dataset
"""

data = load_iris()

X_iris = data.data
Y_iris = data.target
n_classes = len(np.unique(Y_iris))

# split datasets
indices = np.arange(X_iris.shape[0])
```

```
shuffled_inds = np.random.permutation(indices)
X_iris = X_iris[shuffled_inds]
Y_iris = Y_iris[shuffled_inds]

X_iris_train = X_iris[indices[:125]]
X_iris_train_biased = np.hstack((X_iris_train, np.ones((X_iris_train.shape[0], 1))))
Y_iris_train = Y_iris[indices[:125]]

X_iris_test = X_iris[indices[-26:-1]]
X_iris_test_biased = np.hstack((X_iris_test, np.ones((X_iris_test.shape[0], 1))))
Y_iris_test = Y_iris[indices[-26:-1]]
```

2.3.1 One-vs-all Model

To compare the results of our custom One-vs-All model and results of One-vs-Rest Classifier from Sklearn

```
In [20]: import numpy as np
         from sklearn.multiclass import OneVsRestClassifier
         # Testing models using OneVsRestClassifier from Scikit-learn (2024)
         np.random.seed(0)
         # Initialize models:
         np.random.seed(0)
         train epochs = 1000
         lr = 0.01
         batch size = 1
         my model = OnevsAll(n classes, epochs=train epochs, lr=lr)
         my model.train(X iris train biased, Y iris train)
         estimator = get estimator(train epochs, lr)
         sklearn model = OneVsRestClassifier(estimator)
         sklearn model.fit(X iris train, Y iris train)
         my preds = my model.predict(X iris test biased)
         sklearn preds = sklearn model.predict(X iris test)
         my acc = my model.accuracy(X iris test biased, Y iris test)
         sk acc = sklearn model.score(X iris test, Y iris test)
```

```
print("Predictions of our One-vs-All model:", np.array(my_preds))
print("Predictions of sklearn OneVsRest Classifier:", sklearn_preds)

print('num_samples of training dataset', X_iris_train.shape[0])
print('num_samples of testing dataset', X_iris_test.shape[0])
print('Differences', np.sum(np.abs(np.array(my_preds)-sklearn_preds)))

print("Accuracy of our One-vs-All model:", my_acc)
print("Accuracy of sklearn OneVsRest Classifier:", sk_acc)

Predictions of our One-vs-All model: [2 0 2 1 1 1 2 2 2 2 0 1 2 2 0 1 1 2 1 0 0 0 2 1 2]
Predictions of sklearn OneVsRest Classifier: [2 0 2 1 1 1 2 2 2 2 0 1 2 2 0 1 1 2 1 0 0 0 2 1 2]
num_samples of training dataset 125
num_samples of testing dataset 25
Differences 0
Accuracy of our One-vs-All model: 0.88
Accuracy of sklearn OneVsRest Classifier: 0.88
```

2.3.2 All-Pairs Model

To compare results of our All-Pairs model and results of One-vs-One Classifier from sklearn.

```
In [21]: import numpy as np
         from sklearn.multiclass import OneVsOneClassifier
         # Testing models using OneVsOneClassifier from Scikit-learn (2024)
         np.random.seed(0)
         lr = 0.01
         train epochs = 1000
         batch size = 1
         model = AllPairs(n classes=n classes, batch size=1, epochs=train epochs, lr=lr)
         model.train(X iris train biased, Y iris train)
         predictions = model.predict(X iris test biased)
         my acc = model.accuracy(X iris test biased, Y iris test)
         estimator = get estimator(train epochs, lr)
         sklearn model ap = OneVsOneClassifier(estimator)
         sklearn model ap.fit(X iris train, Y iris train)
         sklearn predictions = sklearn model ap.predict(X iris test)
         sk acc = sklearn model ap.score(X iris test, Y iris test)
```

```
print("Predictions of our All-Pairs Model:", np.array(predictions))
print("Predictions of sklearn OneVsOne Classifier:", sklearn_predictions)
print('num_samples of training dataset', X_iris_train.shape[0])
print('num_samples of testing dataset', X_iris_test.shape[0])
print('Differences', np.sum(np.abs(np.array(predictions)-sklearn_predictions)))
print("Accuracy of our All-Pairs model:", my_acc)
print("Accuracy of sklearn OneVsOne Classifier:", sk_acc)
```

```
Predictions of our All-Pairs Model: [2 0 2 1 1 1 2 2 2 1 0 1 2 2 0 1 1 2 1 0 0 0 2 1 2]

Predictions of sklearn OneVsOne Classifier: [2 0 2 1 1 1 2 2 2 1 0 1 2 2 0 1 1 2 1 0 0 0 2 1 2]

num_samples of training dataset 125

num_samples of testing dataset 25

Differences 0

Accuracy of our All-Pairs model: 0.92

Accuracy of sklearn OneVsOne Classifier: 0.92
```

References

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