in3050_in4050_2023_assignment_2

March 27, 2023

0.1 IN3050/IN4050 Mandatory Assignment 2, 2023: Supervised Learning

0.1.1 Initialization

[4]:
```
import numpy as np
import matplotlib.pyplot as plt
import sklearn #for datasets
```

0.2 Datasets

We start by making a synthetic dataset of 2000 datapoints and five classes, with 400 individuals in each class. (See https://scikit-learn.org/stable/modules/generated/sklearn.datasets.make_blobs.html regarding how the data are generated.) We choose to use a synthetic dataset—and not a set of natural occuring data—because we are mostly interested in properties of the various learning algorithms, in particular the differences between linear classifiers and multi-layer neural networks together with the difference between binary and multi-class data.

When we are doing experiments in supervised learning, and the data are not already split into training and test sets, we should start by splitting the data. Sometimes there are natural ways to split the data, say training on data from one year and testing on data from a later year, but if that is not the case, we should shuffle the data randomly before splitting. (OK, that is not necessary with this particular synthetic data set, since it is already shuffled by default by scikit, but that will not be the case with real-world data.) We should split the data so that we keep the alignment between X and t, which may be achieved by shuffling the indices. We split into 50% for training, 25% for validation, and 25% for final testing. The set for final testing *must not be used* till the end of the assignment in part 3.

We fix the seed both for data set generation and for shuffling, so that we work on the same datasets when we rerun the experiments. This is done by the `random_state` argument and the `rng = np.random.RandomState(2022)`.

[5]:
```
from sklearn.datasets import make_blobs
X, t_multi = make_blobs(n_samples=[400,400,400, 400, 400],
                        centers=[[0,1],[4,2],[8,1],[2,0],[6,0]],
                        cluster_std=[1.0, 2.0, 1.0, 0.5, 0.5],
                        n_features=2, random_state=2022)
```

[6]:
```
indices = np.arange(X.shape[0])
rng = np.random.RandomState(2022)
```

```
rng.shuffle(indices)
indices[:10]
```

[6]:
```
array([1018, 1295,  643, 1842, 1669,   86,  164, 1653, 1174,  747])
```

[529]:
```
X_train = X[indices[:1000],:]
X_val = X[indices[1000:1500],:]
X_test = X[indices[1500:],:]
t_multi_train = t_multi[indices[:1000]]
t_multi_val = t_multi[indices[1000:1500]]
t_multi_test = t_multi[indices[1500:]]
```

Next, we will make a second dataset by merging classes in (X,t) into two classes and call the new set (X, t2). This will be a binary set. We now have two datasets:

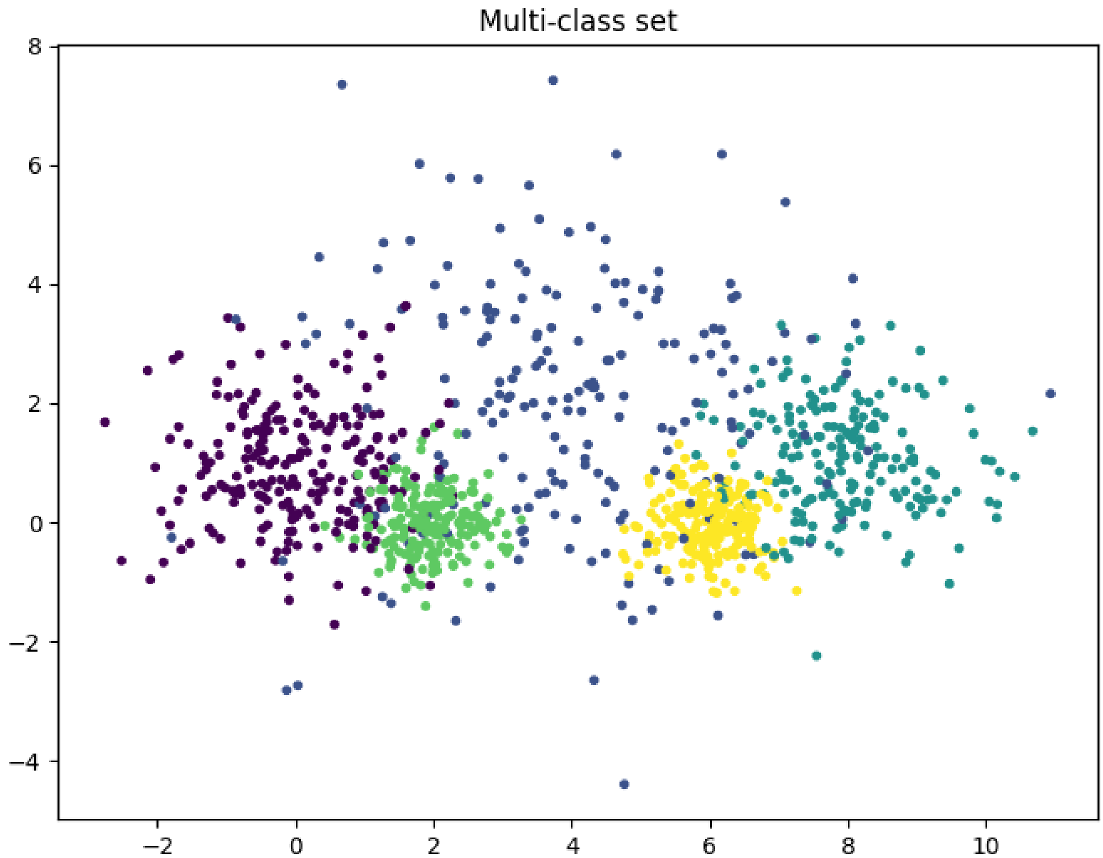
- Binary set: `(X, t2)`
- Multi-class set: `(X, t_multi)`

[530]:
```
t2_train = t_multi_train >= 3
t2_train = t2_train.astype('int')
t2_val = (t_multi_val >= 3).astype('int')
t2_test = (t_multi_test >= 3).astype('int')
```

We can plot the two traning sets.

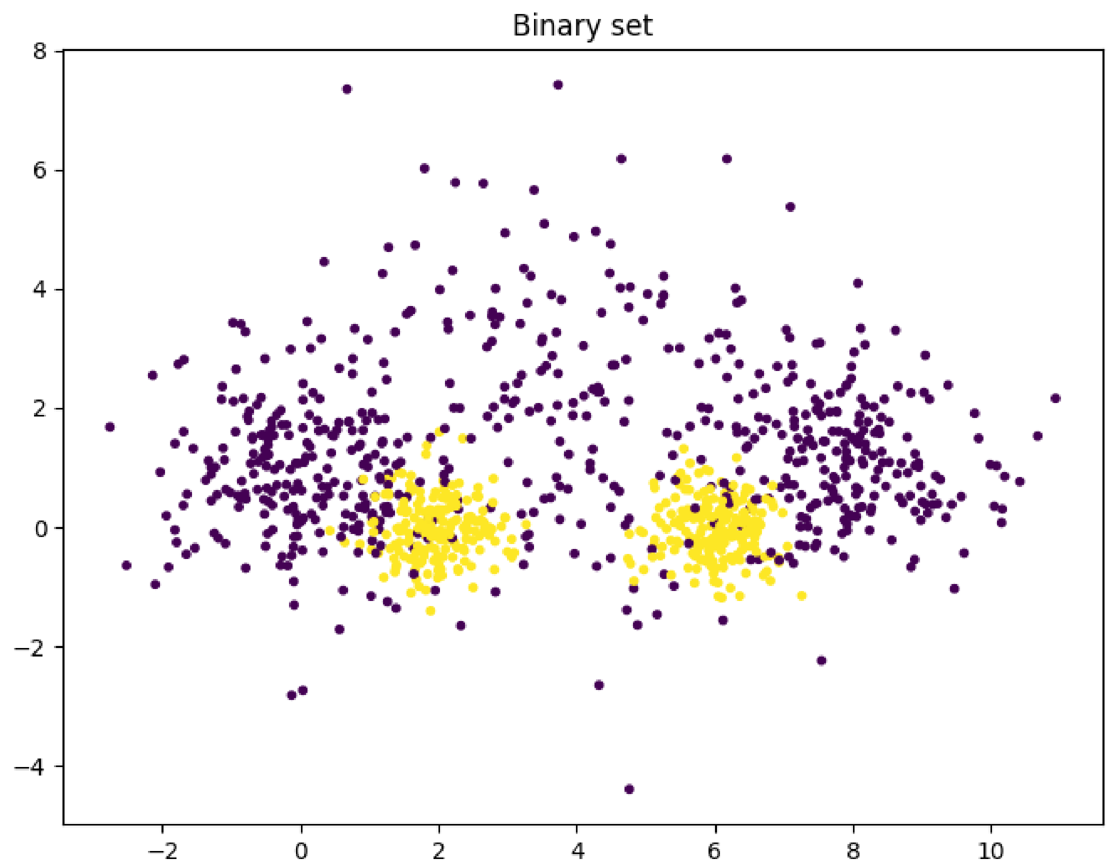
[217]:
```
plt.figure(figsize=(8,6)) # You may adjust the size
plt.scatter(X_train[:, 0], X_train[:, 1], c=t_multi_train, s=10.0)
plt.title('Multi-class set')
```

[217]:
```
Text(0.5, 1.0, 'Multi-class set')
```



[218]:
```
plt.figure(figsize=(8,6))
plt.scatter(X_train[:, 0], X_train[:, 1], c=t2_train, s=10.0)
plt.title('Binary set')
```

[218]: `Text(0.5, 1.0, 'Binary set')`



1 Part I: Linear classifiers

1.1 Linear regression

We see that that set (X, t2) is far from linearly separable, and we will explore how various classifiers are able to handle this. We start with linear regression. You may make your own implementation from scratch or start with the solution to the weekly exercise set 7. We include it here with a little added flexibility.

[323]:
```
def add_bias(X, bias):
    """X is a Nxm matrix: N datapoints, m features
    bias is a bias term, -1 or 1. Use 0 for no bias
    Return a Nx(m+1) matrix with added bias in position zero
    """
    N = X.shape[0]
    biases = np.ones((N, 1))*bias # Make a N*1 matrix of bias-s
    # Concatenate the column of biases in front of the columns of X.
    return np.concatenate((biases, X), axis  = 1)
```

[324]:
```python
class NumpyClassifier():
    """Common methods to all numpy classifiers --- if any"""
```

[341]:
```python
class NumpyLinRegClass(NumpyClassifier):

    def __init__(self, bias=-1):
        self.bias=bias

    def fit(self, X_train, t_train, eta = 0.1, epochs=10, clip=None):
        """X_train is a Nxm matrix, N data points, m features
        t_train is avector of length N,
        the targets values for the training data"""

        if self.bias:
            X_train = add_bias(X_train, self.bias)

        (N, m) = X_train.shape

        self.weights = weights = np.zeros(m)

        for e in range(epochs):
            gradient = X_train.T @ (X_train @ weights - t_train)
            if clip: gradient = np.clip(gradient, -clip, clip)
            weights -= eta / N * gradient

    def predict(self, X, threshold=0.5):
        """X is a Kxm matrix for some K>=1
        predict the value for each point in X"""
        if self.bias:
            X = add_bias(X, self.bias)
        ys = X @ self.weights
        return ys > threshold
```

We can train and test a first classifier.

[326]:
```python
def accuracy(predicted, gold):
    return np.mean(predicted == gold)
```

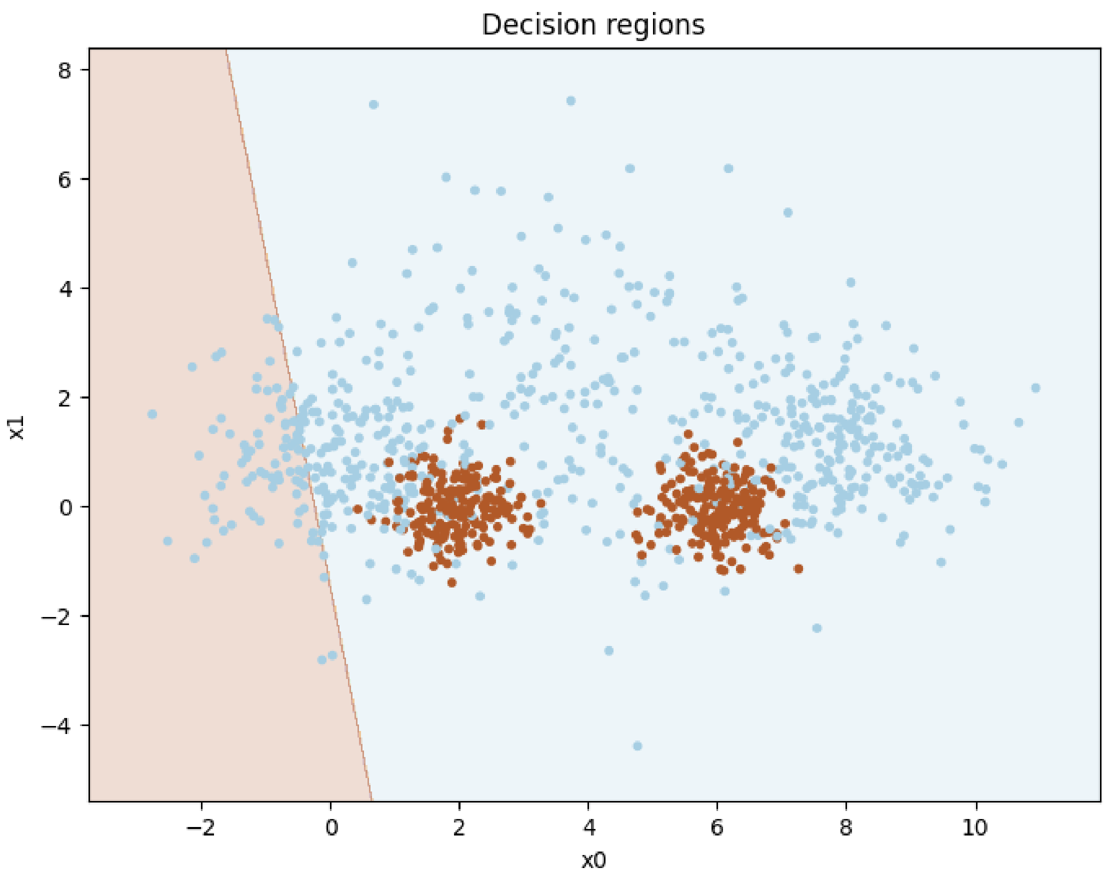
[327]:
```python
cl = NumpyLinRegClass()
cl.fit(X_train, t2_train)
accuracy(cl.predict(X_val), t2_val)
```

[327]: 0.522

The following is a small procedure which plots the data set together with the decision boundaries. You may modify the colors and the rest of the graphics as you like. The procedure will also work for multi-class classifiers

[328]:
```python
def plot_decision_regions(X, t, clf=[], size=(8,6)):
    """Plot the data set (X,t) together with the decision boundary of the␣
 ↪classifier clf"""
    # The region of the plane to consider determined by X
    x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
    y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1

    # Make a make of the whole region
    h = 0.02  # step size in the mesh
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
    Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
    # Classify each meshpoint.
    Z = Z.reshape(xx.shape)

    plt.figure(figsize=size) # You may adjust this

    # Put the result into a color plot
    plt.contourf(xx, yy, Z, alpha=0.2, cmap = 'Paired')

    plt.scatter(X[:,0], X[:,1], c=t, s=10.0, cmap='Paired')

    plt.xlim(xx.min(), xx.max())
    plt.ylim(yy.min(), yy.max())
    plt.title("Decision regions")
    plt.xlabel("x0")
    plt.ylabel("x1")

#    plt.show()
```

[329]:
```python
plot_decision_regions(X_train, t2_train, cl)
```



1.1.1 Task: Tuning

The result is far from impressive. Remember that a classifier which always chooses the majority class will have an accuracy of 0.6 on this data set.

Your task is to try various settings for the two training hyper-parameters, *eta* and *epochs*, to get the best accuracy on the validation set.

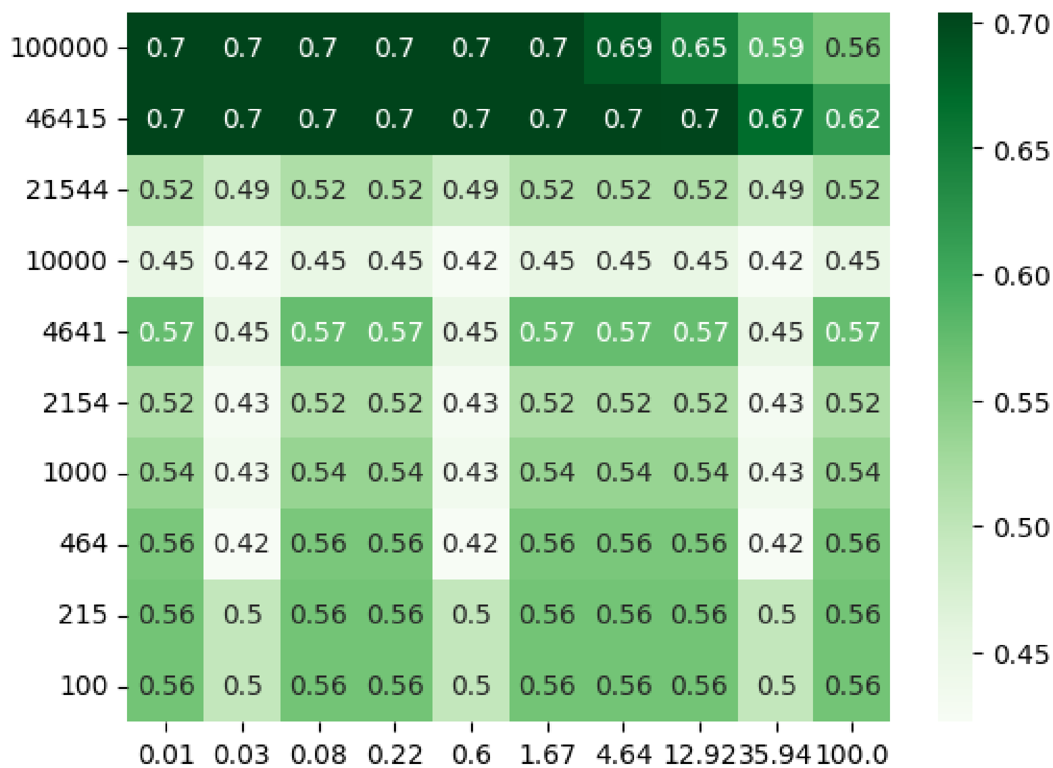
Report how the accuracy vary with the hyper-parameter settings. It it not sufficient to give the final hyperparemters. You must also show how you found them and results for alternative values you tried out.

When you are satisfied with the result, you may plot the decision boundaries, as above.

[330]:
```
import seaborn as sns

etas = [round(e, 2) for e in np.logspace(-2, 2, num=10)]
epochs = [int(e) for e in np.logspace(5, 2, num=10)]

accuracy_matrix = np.zeros((len(etas), len(epochs)))
```

```
for i, eta in enumerate(etas):
    for j, epoch in enumerate(epochs):
        cl = NumpyLinRegClass()
        cl.fit(X_train, t2_train, eta=eta, epochs=epoch, clip=100000)
        predicted = cl.predict(X_val)
        acc = accuracy(predicted, t2_val)
        accuracy_matrix[i, j] = acc

sns.heatmap(accuracy_matrix, cmap='Greens', annot=True, xticklabels=etas,
 ↪yticklabels=epochs)
```

```
[330]: <AxesSubplot: >
```

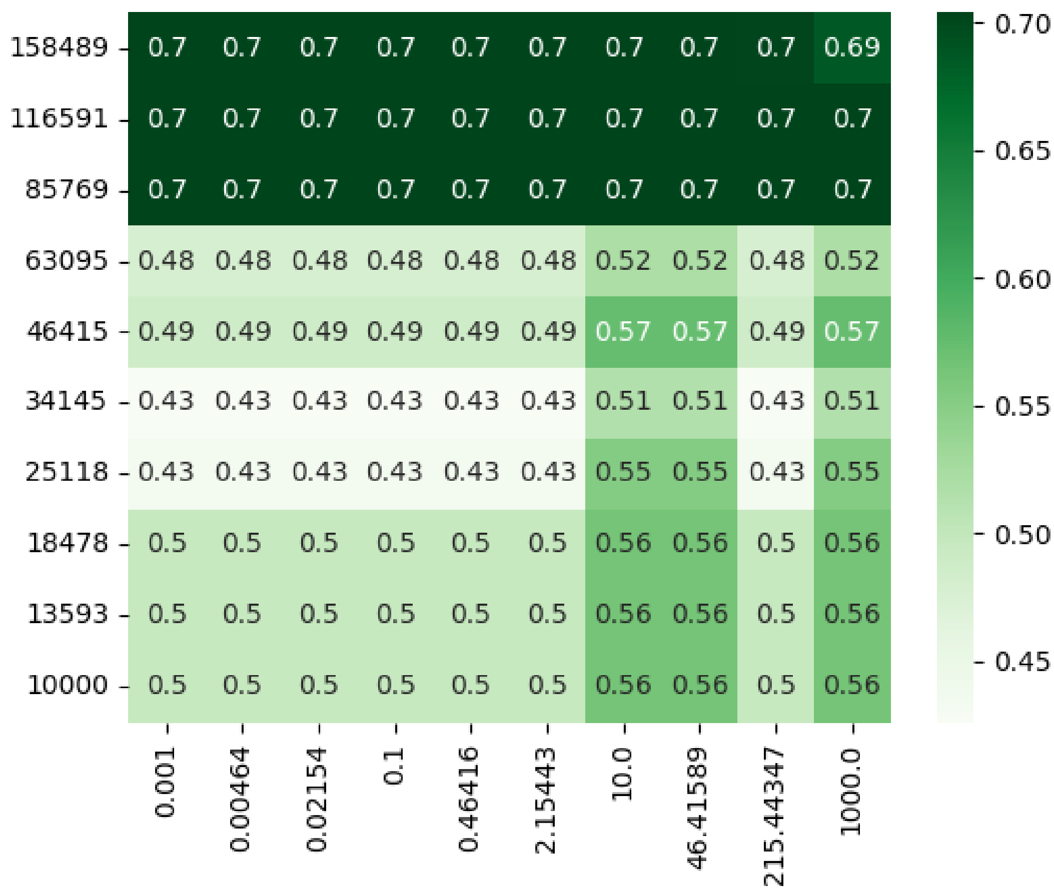


ANSWER: After introducing clipping to the fit function, we can explore different combinations of etas and epochs. Without clipping we were overflowing during the matrix multiplication.

Over the x-axis, we see different step values, and vertically we can see the number of epochs used. A greedy approach will mean taking large steps, but without overshooting, allowing us to reduce the number of epochs. Trying different epoch values between 100 and 1M, we notice major improvements after going above 20k epochs. We also see best results at etas close to 10, Which we can inspect further. Currently, the best accuracy is of 0.7.

[342]:
```python
import seaborn as sns

etas = [round(e, 5) for e in np.logspace(-3, 3, num=10)]
epochs = [int(e) for e in np.logspace(5.2, 4, num=10)]
clip = 100*1000

accuracy_matrix = np.zeros((len(etas), len(epochs)))

for i, eta in enumerate(etas):
    for j, epoch in enumerate(epochs):
        cl = NumpyLinRegClass()
        cl.fit(X_train, t2_train, eta=eta, epochs=epoch, clip=clip)
        predicted = cl.predict(X_val)
        acc = accuracy(predicted, t2_val)
        accuracy_matrix[i, j] = acc

sns.heatmap(accuracy_matrix, cmap='Greens', annot=True, xticklabels=etas, yticklabels=epochs)
```

[342]: <AxesSubplot: >

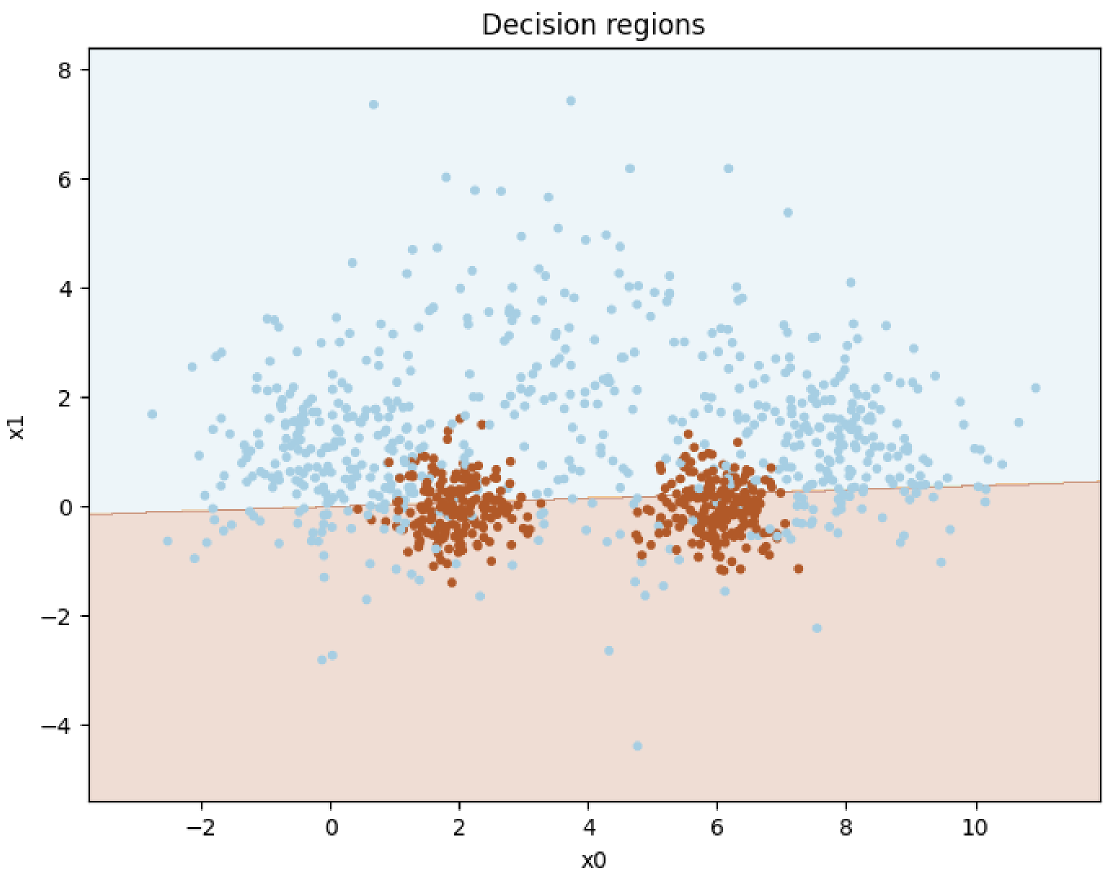


ANSWER: After closer inspection, it seems the best fit values are at 20 eta, and at around 90000 epochs. We can move this into a function, so we don't need to look at the seamap manually:

[343]:
```
def find_best_hyperparams(X_train, t_train, X_val, t_val, eta_range,␣
↪epochs_range, clip=None):
    best_eta = None
    best_epochs = None
    best_accuracy = 0.0

    for eta in eta_range:
        for epochs in epochs_range:
            cl = NumpyLinRegClass()
            cl.fit(X_train, t_train, eta=eta, epochs=epochs, clip=clip)
            predicted = cl.predict(X_val)
            val_accuracy = accuracy(predicted, t_val)

            if val_accuracy > best_accuracy:
                best_eta = eta
                best_epochs = epochs
                best_accuracy = val_accuracy

    return best_eta, best_epochs, best_accuracy
```

[344]:
```
cl = NumpyLinRegClass()

etas = [round(e, 5) for e in np.logspace(-3, 3, num=10)]
epochs = [int(e) for e in np.logspace(5.2, 4, num=10)]
clip = 1000*1000*1000

best_eta, best_epochs, best_accuracy = find_best_hyperparams(X_train, t2_train,␣
↪X_val, t2_val, eta_range, epochs_range, clip=clip)
print(f"{best_eta=}, {best_epochs=} at {best_accuracy=}")

cl.fit(X_train, t2_train, eta=best_eta, epochs=best_epochs, clip=clip)
plot_decision_regions(X_train, t2_train, cl)
```

```
best_eta=0.029836472402833405, best_epochs=470 at best_accuracy=0.704
```



ANSWER: Looks pretty good to me :)

I'm going to keep best_eta=0.0298, best_epochs=470 for the next tasks.

[355]:
```
def get_cached_hyperparameters():
    best_eta = 0.0298
    best_epochs = 470
    clip = 1000**3
    return best_eta, best_epochs, clip
```

1.1.2 Task: Loss

The linear regression classifier is trained with mean squared error loss. So far, we have not calculated the loss explicitly in the code. Extend the code to calculate the loss on the training set for each epoch and to store the losses such that the losses can be inspected after training.

Also extend the classifier to calculate the accuracy on the training data after each epoch.

Train a classifier with your best settings from last point. After training, plot the loss as a function of the number of epochs. Then plot the accuracy as a function of the number of epochs.

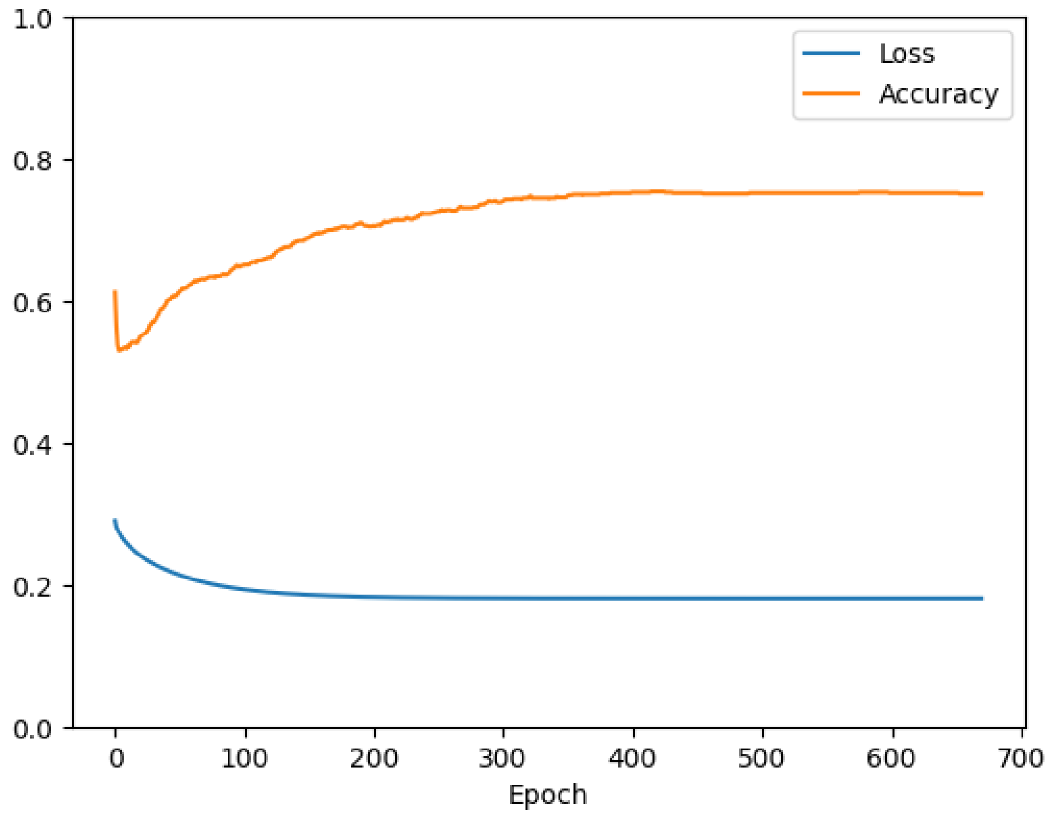
Comment on what you see: Are the function monotone? Is this as expected?

[553]:
```python
class NumpyLinRegClass(NumpyClassifier):

    def __init__(self, bias=-1):
        self.bias=bias

    def fit(self, X_train, t_train, eta = 0.1, epochs=10, clip=None):
        """X_train is a Nxm matrix, N data points, m features
        t_train is avector of length N,
        the targets values for the training data"""

        if self.bias:
            X_train = add_bias(X_train, self.bias)

        (N, m) = X_train.shape

        self.weights = weights = np.zeros(m)
        self.losses = []
        self.accuracies = []

        for e in range(epochs):
            gradient = X_train.T @ (X_train @ weights - t_train)
            if clip: gradient = np.clip(gradient, -clip, clip)
            weights -= eta / N * gradient

            # Calculate mean squared error loss on training data
            t_pred = X_train @ weights
            loss = np.mean((t_pred - t_train) ** 2)
            self.losses.append(loss)

            # Calculate accuracy on training data
            t_pred_binary = t_pred > 0.5
            accuracy = np.mean(t_pred_binary == t_train)
            self.accuracies.append(accuracy)

    def predict(self, X, threshold=0.5):
        """X is a Kxm matrix for some K>=1
        predict the value for each point in X"""
        if self.bias:
            X = add_bias(X, self.bias)
        ys = X @ self.weights
        return ys > threshold
```

[552]:
```python
cl = NumpyLinRegClass()
eta, epochs, clip = get_cached_hyperparameters()

epochs += 200  # just for the visualization
```

```python
for e in range(epochs):
    cl.fit(X_train, t2_train, eta=eta, epochs=epochs, clip=clip)
    cl.predict(X_train)

print(f"Final accuracy: {cl.accuracies[-1]}")
print(f"Final loss: {cl.losses[-1]}")
plt.plot(cl.losses, label="Loss")
plt.plot(cl.accuracies, label="Accuracy")
plt.xlabel("Epoch")
plt.ylim((0, 1.0))
plt.legend()
plt.show()
```

```
Final accuracy: 0.751
Final loss: 0.18085948490339826
```



ANSWER: We can see the loss going down at a stable but slow rate over time, which is expected. The accuracy grows at a steady rate after an initial drop during the early epochs, which can probably be explained by the weights being initialized to random values, and noise affecting it quite a bit. Once it gets past the noise, and can work on imporiving the underlying patterns, it starts growing as we expect. Aditionally

it seems to flatten out towards the end of our epochs. The functions are monotone, except the early dip.

1.1.3 Task: Scaling

we have seen in the lectures that scaling the data may improve training speed.

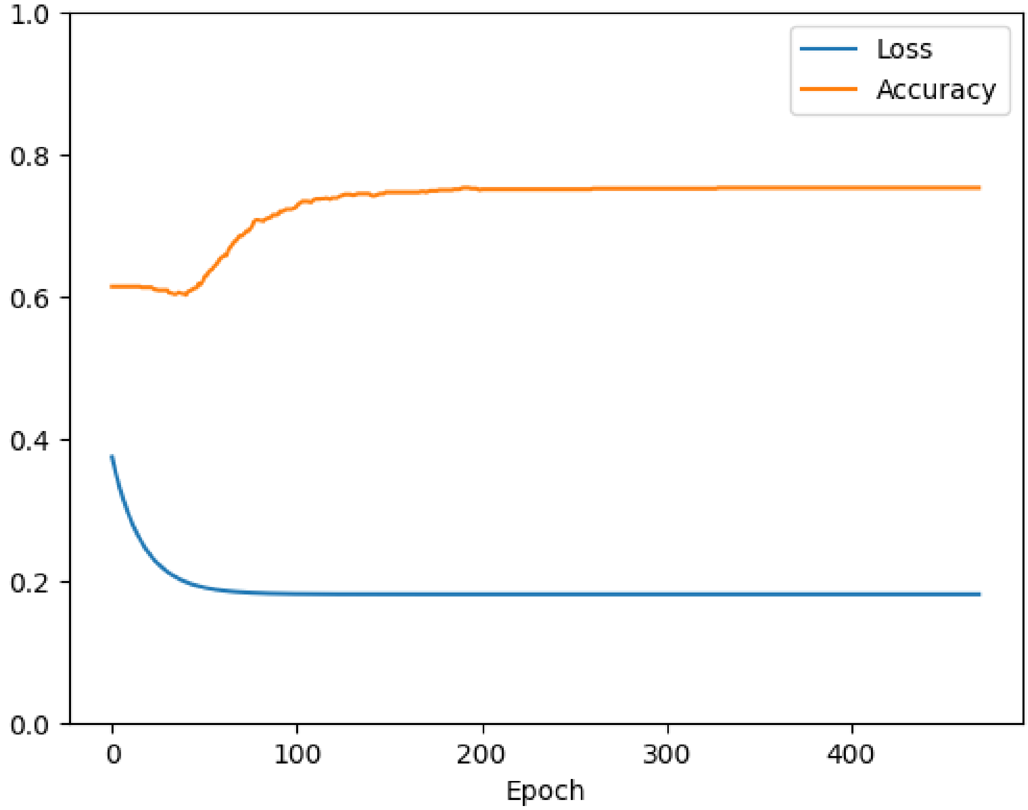
- Implement a scaler, either standard scaler (normalizer) or max-min scaler
- Scale the data
- Train the model on the scaled data
- Experiment with hyper-parameter settings and see whether you can speed up the training.
- Report final hyper-meter settings and show how you found them.
- Plot the loss curve and the accuracy curve for the classifier trained on scaled data with the best settings you found.

[390]:
```python
class StandardScaler:
    def __init__(self):
        self.mean = None
        self.std = None

    def tune(self, X):
        self.mean = np.mean(X, axis=0)
        self.std = np.std(X, axis=0)

    def transform(self, X):
        return (X - self.mean) / self.std
```

[397]:
```python
scaler = StandardScaler()
scaler.tune(X_train)



X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)

cl = NumpyLinRegClass()
eta, epochs, clip = get_cached_hyperparameters()

for epoch in range(epochs):
    cl.fit(X_train_scaled, t2_train, eta=eta, epochs=epochs, clip=clip)
    cl.predict(X_train_scaled)

print(f"Final accuracy: {cl.accuracies[-1]}")
print(f"Final loss: {cl.losses[-1]}")
plt.plot(cl.losses, label="Loss")
plt.plot(cl.accuracies, label="Accuracy")
plt.xlabel("Epoch")
plt.ylim((0, 1.0))
plt.legend()
```

```
plt.show()
```

```
Final accuracy: 0.753
Final loss: 0.18085927539474342
```



ANSWER: After using a scaler, we see a much faster drop in the loss, and the accuracy hits its max value after only 100 epochs. That's much faster! We needed around 400 epochs previously. The drop in accuracy at the beginning is mostly gone now, too.

1.2 Logistic regression

a) You should now implement a logistic regression classifier similarly to the classifier based on linear regression. You may use code from the solution to weekly exercise set week07.

b) In addition to the method `predict` which predicts a class for the data, include a method `predict_probability` which predicts the probability of the data belonging to the positive class.

c) As with the classifier based on linear regression, we want to calculate loss and accuracy after each epoch. The prefered loss for logistic regression is binary cross-entropy. You could have used mean squared error. The most important is that your implementation of the loss corresponds to your implementation of the gradient descent.

d) In addition, extend the fit-method with optional arguments for a validation set (X_val, t_val). If a validation set is included in the call to fit, calculate the loss and the accuracy for the validation set after each epoch.

e) The training runs for a number of epochs. We cannot know beforehand for how many epochs it is reasonable to run the training. One possibility is to run the training until the learning does not improve much. Extend the fit-method with two keyword arguments, `tol` and `n_epochs_no_update` and stop training when the loss has not improved with more than `tol` after running `n_epochs_no_update` epochs. A possible default value for `n_epochs_no_update` is 5. Also, add an attribute to the classifier which tells us after fitting how many epochs were ran.

f) Train classifiers with various learning rates, and with varying values for `tol` for finding optimal values. Also consider the effect of scaling the data.

g) After a succesful training, plot both training loss and validation loss as functions of the number of epochs in one figure, and both accuracies as functions of the number of epochs in another figure. Comment on what you see.

[ ]:
```
class LogisticRegression:
    def fit(self, X_train, t_train, eta = 0.1, epochs=10, X_val=None,␣
↪t_val=None, tolerance=0.01, patience=10, bias=-1):
        # from week 7
        self.bias = bias
        self.train_loss = []
        self.val_loss = []
        (N, m) = X_train.shape

        X_train = add_bias(X_train, bias)
        self.weights = weights = np.zeros(m+1)

        ttl = patience
        while ttl >= patience:

            weights -= (eta / N) * (X_train.T @ (self.forward(X_train) -␣
↪t_train))

            loss = self.binary_cross_entropy_loss(X_train, t_train)
            self.train_loss.append(loss)

            if X_val is not None and t_val is not None:
                loss_val = self.binary_cross_entropy_loss(X_val, t_val)
                self.val_loss.append(loss_val)

            for e in range(epochs):
                weights -= eta / N *  X_train.T @ (self.forward(X_train) -␣
↪t_train)

            # should we continue
```

```
            if abs(loss) < tolerance:
                ttl -= 1
            else:
                ttl = patience
            epochs -= 1
            if epochs == 0:
                break

    def logistic(self, x):
        return 1 / (1 + np.exp(-x))

    def forward(self, X):
        return self.logistic(X @ self.weights)

    def predict(self, X, threshold=0.5):
        X_biased = add_bias(X, self.bias)
        return (self.forward(X_biased) > threshold).astype('int')

    def predict_probability(self, X):
        X_biased = add_bias(X, self.bias)
        return self.forward(X_biased)

    def binary_cross_entropy_loss(self, X, t, clip=1e-15):
        predicted = np.clip(self.forward(X), clip, 1-clip)
        return -(t * np.log(predicted) + (1 - t) * np.log(1 - predicted)).mean()

    def get_boundaries(self, index1, index2):
        xmin, xmax = X[:, index1].min() - 0.5, X[:, index1].max() + 0.5
        ymin, ymax = X[:, index2].min() - 0.5, X[:, index2].max() + 0.5
        xx, yy = np.meshgrid(np.arange(xmin, xmax, 0.01), np.arange(ymin, ymax,␣
↪0.01))
```

[ ]:
```
import matplotlib.pyplot as plt
import numpy as np

eta, epochs = 20, 20000
cl = LogisticRegression()

cl.fit(X, t_multi, eta=eta, epochs=epochs, tolerance=50, patience=50)

# Create a grid of points to plot the decision boundary
xmin, xmax = X[:, 0].min() - 0.5, X[:, 0].max() + 0.5
ymin, ymax = X[:, 1].min() - 0.5, X[:, 1].max() + 0.5
xx, yy = np.meshgrid(np.arange(xmin, xmax, 0.01), np.arange(ymin, ymax, 0.01))
grid = np.c_[xx.ravel(), yy.ravel()]
```

```python
# Predict the class of each point in the grid
Z = cl.predict(grid)

# Reshape the predictions to match the shape of the plot
Z = Z.reshape(xx.shape)

# Plot the decision boundary and the data points
plt.contourf(xx, yy, Z, cmap=plt.cm.Paired)
plt.scatter(X[:, 0], X[:, 1], c=t_multi, cmap=plt.cm.Paired, edgecolors='k')
plt.show()
```

1.3 Multi-class classifiers

We turn to the task of classifying when there are more than two classes, and the task is to ascribe one class to each input. We will now use the set (X, t_multi).

1.3.1 "One-vs-rest" with logistic regression

We saw in the lecture how a logistic regression classifier can be turned into a multi-class classifier using the one-vs-rest approach. We train one logistic regression classifier for each class. To predict the class of an item, we run all the binary classifiers and collect the probability score from each of them. We assign the class which ascribes the highest probability.

Build such a classifier. Train the resulting classifier on (X_train, t_multi_train), test it on (X_val, t_multi_val), tune the hyper-parameters and report the accuracy.

Also plot the decision boundaries for your best classifier similarly to the plots for the binary case.

[547]:
```python
class OneVsRestLogRegression:
    def __init__(self, n_classifiers, eta=0.1, epochs=10, tolerance=0.01,␣
↪patience=10):
        self.classifiers = [LogisticRegression() for _ in range(n_classifiers)]
        self.tolerance = tolerance
        self.patience = patience

    def fit(self, X_train, t_train, eta=0.1, epochs=10, X_val=None, t_val=None):
        self.train_loss = []
        self.val_loss = []

        for i, cl in enumerate(self.classifiers):
            t_train_class = (t_train == i+1).astype(int)
            cl.fit(X_train, t_train_class, eta=eta, epochs=epochs, X_val=X_val,␣
↪t_val=t_val, tolerance=self.tolerance, patience=self.patience)

        return self

    def predict(self, X):
        probs = np.zeros((X.shape[0], len(self.classifiers)))
```

```
        for i, cl in enumerate(self.classifiers):
            probs[:, i] = cl.predict_probability(X)

        return np.argmax(probs, axis=1)

    def accuracy(self, X, t):
        return np.mean(self.predict(X) == t)

    def get_boundaries(self, i):
        return self.classifiers[i].get_boundaries(i, i+1)
```

[ ]:
```
import matplotlib.pyplot as plt
import numpy as np

eta, epochs = 10, 10000

ovr_cl = OneVsRestLogRegression(n_classifiers=5, eta=eta, epochs=epochs,␣
 ↪tolerance=0.01, patience=10)
ovr_cl.fit(X_train, t_multi_train, X_val=X_val, t_val=t_multi_val)

# Evaluate the accuracy of the classifier on the validation data
accuracy = ovr.accuracy(X_val, t_multi_val)
print(f"Accuracy on validation data: {accuracy:.4f}")

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, 0.1), np.arange(y_min, y_max, 0.1))
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, alpha=0.4)

# Plot the training points
plt.scatter(X_train[:, 0], X_train[:, 1], c=t_multi_train, cmap=plt.cm.Set1,␣
 ↪edgecolor='k')
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.title('Decision boundaries for multi-class classification')
plt.show()
```

2 Part II Multi-layer neural networks

2.1 A first non-linear classifier

The following code it a simple implementation of a multi-layer perceptron. It is quite restricted. There is only one hidden layer. It can only handle binary classification. In addition, it uses a simple final layer similar to the linear regression classifier above. One way to look at it is what happens when we add a hidden layer to the linear regression classifier.

It can be used to make a non-linear classifier for the set (X, t2). Experiment with settings for learning rate and epochs and see how good results you can get. Report results for variouse settings. Be prepared to train for a looooong time. Plot the training set together with the decision regions as in part I.

[544]:
```python
class MLPBinaryLinRegClass(NumpyClassifier):
    """A multi-layer neural network with one hidden layer"""

    def __init__(self, bias=-1, dim_hidden = 6):
        """Intialize the hyperparameters"""
        self.bias = bias
        self.dim_hidden = dim_hidden

        def logistic(x):
                return 1/(1+np.exp(-x))
        self.activ = logistic

        def logistic_diff(y):
            return y * (1 - y)
        self.activ_diff = logistic_diff

    def fit(self, X_train, t_train, eta=0.001, epochs = 100):
        """Intialize the weights. Train *epochs* many epochs.

        X_train is a Nxm matrix, N data points, m features
        t_train is a vector of length N of targets values for the training␣
 ↪data,
        where the values are 0 or 1.
        """
        self.eta = eta

        T_train = t_train.reshape(-1,1)

        dim_in = X_train.shape[1]
        dim_out = T_train.shape[1]

        # Itilaize the wights
        self.weights1 = (np.random.rand(
            dim_in + 1,
            self.dim_hidden) * 2 - 1)/np.sqrt(dim_in)
        self.weights2 = (np.random.rand(
            self.dim_hidden+1,
            dim_out) * 2 - 1)/np.sqrt(self.dim_hidden)
        X_train_bias = add_bias(X_train, self.bias)

        for e in range(epochs):
```

```
            # One epoch
            hidden_outs, outputs = self.forward(X_train_bias)
            # The forward step
            out_deltas = (outputs - T_train)
            # The delta term on the output node
            hiddenout_diffs = out_deltas @ self.weights2.T
            # The delta terms at the output of the jidden layer
            hiddenact_deltas = (hiddenout_diffs[:, 1:] *
                                self.activ_diff(hidden_outs[:, 1:]))
            # The deltas at the input to the hidden layer
            self.weights2 -= self.eta * hidden_outs.T @ out_deltas
            self.weights1 -= self.eta * X_train_bias.T @ hiddenact_deltas
            # Update the weights

    def forward(self, X):
        """Perform one forward step.
        Return a pair consisting of the outputs of the hidden_layer
        and the outputs on the final layer"""
        hidden_activations = self.activ(X @ self.weights1)
        hidden_outs = add_bias(hidden_activations, self.bias)
        outputs = hidden_outs @ self.weights2
        return hidden_outs, outputs

    def predict(self, X):
        """Predict the class for the mebers of X"""
        Z = add_bias(X, self.bias)
        forw = self.forward(Z)[1]
        score= forw[:, 0]
        return (score > 0.5)
```

2.2 Improving the classifier

You should now make changes to the classifier similarly to what you did with the logistic regression classifier in part 1.

a) In addition to the method predict, which predicts a class for the data, include a method predict_probability which predict the probability of the data belonging to the positive class. The training should be based on this value as with logistic regression.

b) Calculate the loss and the accuracy after each epoch and store them for inspection after training.

c) In addition, extend the fit-method with optional arguments for a validation set (X_val, t_val). If a validation set is included in the call to fit, calculate the loss and the accuracy for the validation set after each epoch.

d) The training runs for a number of epochs. We cannot know beforehand for how many epochs it is reasonable to run the training. One possibility is to run the training until the learning does not improve much. Extend the fit method with two keyword arguments, `tol` and `n_epochs_no_update` and stop training when the loss has not improved with more than tol after `n_epochs_no_update`. A possible default value for `n_epochs_no_update` is 5. Also, add an attribute to the classifier which tells us after fitting how many epochs were ran.

e) Tune the hyper-parameters:`eta`, `tol`and `dim-hidden`. Also consider the effect of scaling the data.

f) After a succesful training with a best setting for the hyper-parameters, plot both training loss and validation loss as functions of the number of epochs in one figure, and both accuracies as functions of the number of epochs in another figure. Comment on what you see.

g) The algorithm contains an element of non-determinism. Hence, train the classifier 10 times with the optimal hyper-parameters and report the mean and standard deviation of the accuracies over the 10 runs.

[554]:
```
class MLPBinaryLinRegClass(NumpyClassifier):
    """A multi-layer neural network with one hidden layer"""

    def __init__(self, bias=-1, dim_hidden = 6):
        """Intialize the hyperparameters"""
        self.bias = bias
        self.dim_hidden = dim_hidden

        def logistic(x):
            return 1/(1+np.exp(-x))
        self.activ = logistic

        def logistic_diff(y):
            return y * (1 - y)
        self.activ_diff = logistic_diff

    def fit(self, X_train, t_train, eta=0.001, epochs=100, patience=10,␣
 ↪tolerance=0.005,
            X_val=None, t_val=None):
        """Intialize the weights. Train *epochs* many epochs.

        X_train is a Nxm matrix, N data points, m features
        t_train is a vector of length N of targets values for the training data,
        where the values are 0 or 1.

        X_val is a matrix containing the validation input data
        t_val is a vector of targets for the validation data
        """
        self.eta = eta

        T_train = t_train.reshape(-1, 1)

        dim_in = X_train.shape[1]
        dim_out = T_train.shape[1]
```

```
        # Initialize the weights
        self.weights1 = (np.random.rand(dim_in + 1, self.dim_hidden) * 2 - 1) /
np.sqrt(dim_in)
        self.weights2 = (np.random.rand(self.dim_hidden + 1, dim_out) * 2 - 1) /
 np.sqrt(self.dim_hidden)
        X_train_bias = add_bias(X_train, self.bias)

        # Store the loss and accuracy after each epoch for training and
validation data
        self.train_losses = []
        self.train_accuracies = []
        self.val_losses = []
        self.val_accuracies = []

        for e in range(epochs):
            # One epoch
            hidden_outs, outputs = self.forward(X_train_bias)
            # The forward step
            out_deltas = (outputs - T_train)
            # The delta term on the output node
            hiddenout_diffs = out_deltas @ self.weights2.T
            # The delta terms at the output of the hidden layer
            hiddenact_deltas = (hiddenout_diffs[:, 1:] * self.
activ_diff(hidden_outs[:, 1:]))

            # The deltas at the input to the hidden layer
            self.weights2 -= self.eta * hidden_outs.T @ out_deltas
            self.weights1 -= self.eta * X_train_bias.T @ hiddenact_deltas
            # Update the weights

            # Calculate the loss and accuracy after the epoch for training data
            y_proba_train = self.predict_probability(X_train)
            y_pred_train = self.predict(X_train)
            train_loss = self.binary_cross_entropy_loss(T_train, y_proba_train)
            train_accuracy = accuracy_score(t_train, y_pred_train)

            # Calculate the loss and accuracy after the epoch for validation
data
            if X_val is not None and t_val is not None:
                y_proba_val = self.predict_probability(X_val)
                y_pred_val = self.predict(X_val)
                val_loss = self.binary_cross_entropy_loss(t_val, y_proba_val)
                val_accuracy = accuracy_score(t_val, y_pred_val)
                self.val_losses.append(val_loss)
                self.val_accuracies.append(val_accuracy)

            # Store the loss and accuracy for training data
```

```
            self.train_losses.append(train_loss)
            self.train_accuracies.append(train_accuracy)

            if train_accuracy < tolerance:
                ttl -= 1
            else:
                ttl = patience

            if ttl <= 0:
                break


    def forward(self, X):
        """Perform one forward step.
        Return a pair consisting of the outputs of the hidden_layer
        and the outputs on the final layer"""
        hidden_activations = self.activ(X @ self.weights1)
        hidden_outs = add_bias(hidden_activations, self.bias)
        outputs = hidden_outs @ self.weights2
        return hidden_outs, outputs

    def predict(self, X):
        """Predict the class for the mebers of X"""
        Z = add_bias(X, self.bias)
        forw = self.forward(Z)[1]
        score= forw[:, 0]
        return (score > 0.5)

    def predict_probability(self, X):
        """Predict the probability of the positive class for the members of X"""
        Z = add_bias(X, self.bias)
        forw = self.forward(Z)[1]

    def binary_cross_entropy_loss(self, X, t):
        predicted = self.forward(X)
        return -(t * np.log(predicted) + (1 - t) * np.log(1 - predicted)).mean()
```

[555]:

```
import matplotlib.pyplot as plt

cl = MLPBinaryLinRegClass()

# Train the model with validation set
cl.fit(X_train, t_multi_train, X_val=X_val, t_val=t_multi_val, epochs=100)

# Plot the loss and accuracy for both training and validation sets
plt.plot(model.losses, label='Training Loss')
```

```
plt.plot(model.val_losses, label='Validation Loss')
plt.plot(model.accuracies, label='Training Accuracy')
plt.plot(model.val_accuracies, label='Validation Accuracy')
plt.legend()
plt.show()
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
Cell In[555], line 6
      3 cl = MLPBinaryLinRegClass()
      5 # Train the model with validation set
----> 6 cl.fit(X_train, t_multi_train, X_val=X_val, t_val=t_multi_val,␣
 ↪epochs=100)
      8 # Plot the loss and accuracy for both training and validation sets
      9 plt.plot(model.losses, label='Training Loss')

Cell In[554], line 64, in MLPBinaryLinRegClass.fit(self, X_train, t_train, eta,␣
 ↪epochs, patience, tolerance, X_val, t_val)
     62 y_proba_train = self.predict_probability(X_train)
     63 y_pred_train = self.predict(X_train)
---> 64 train_loss = self.binary_cross_entropy_loss(T_train, y_proba_train)
     65 train_accuracy = accuracy_score(t_train, y_pred_train)
     67 # Calculate the loss and accuracy after the epoch for validation data

Cell In[554], line 111, in MLPBinaryLinRegClass.binary_cross_entropy_loss(self,␣
 ↪X, t)
    110 def binary_cross_entropy_loss(self, X, t):
--> 111     predicted = self.forward(X)
    112     return -(t * np.log(predicted) + (1 - t) * np.log(1 - predicted)).
 ↪mean()

Cell In[554], line 93, in MLPBinaryLinRegClass.forward(self, X)
     89 def forward(self, X):
     90     """Perform one forward step.
     91     Return a pair consisting of the outputs of the hidden_layer
     92     and the outputs on the final layer"""
---> 93     hidden_activations = self.activ(X @ self.weights1)
     94     hidden_outs = add_bias(hidden_activations, self.bias)
     95     outputs = hidden_outs @ self.weights2

ValueError: matmul: Input operand 1 has a mismatch in its core dimension 0, wit␣
 ↪gufunc signature (n?,k),(k,m?)->(n?,m?) (size 3 is different from 1)
```

3 Part III: Final testing

We can now perform a final testing on the held-out test set.

3.1 Binary task (X, t2)

Consider the linear regression classifier, the logistic regression classifier and the multi-layer network with the best settings you found. Train each of them on the training set and calculate accuracy on the held-out test set, but also on the validation set and the training set. Report in a 3 by 3 table.

Comment on what you see. How do the three different algorithms compare? Also, compare the results between the different data sets. In cases like these, one might expect slightly inferior results on the held-out test data compared to the validation data. Is that the case here?

Also report precision and recall for class 1.

ANSWER: Without actually having completed the logistic regression classifier, nor the multilayer network; it's hard to actually compare them, but in general the logistic and multi-layered networks will gain better accuracy because they can capture non-linear regressions. Furthermore, we can expect the test data to perform slightly worse than our validation set, as the models are never trained on the test data at all.