

# Ans 1.

## Optimization problems

When dealing with Support Vector Machines we come across the concept of unconstrained optimization and constrained optimization. Unconstrained optimization deals with minimizing or maximizing a function without any given constraints. But in SVMs we mainly deal with constrained optimization problems where we want to optimize (minimize/ maximize) a function given a constraint. Below is an example of a constraint optimization problem:

$$\text{Minimize } f(w) \text{ such that } h(w) = 0$$

Here  $f(w)$  is the objective function and  $h(w)$  is the equality constraint, here we just have one constraint however the model is valid for multiple equality constraint.

## Solution to constrained optimization

Lagrange Multipliers

We can solve this problem of constrained optimization using Lagrange multipliers.

$$L(w, B) = f(w) + B \cdot h(w)$$

$B$  - Lagrange multiplier

## Theorem

- if  $w$  is a minima then  $dL/dw = 0$  and  $dL/dB = 0$
- if  $f(w)$  is convex then  $dL/dw = 0$  and  $dL/dB = 0$

implies that  $w$  is a minima

## Optimality Conditions : Primal Function

For a constrained optimization problem:

$$\text{min } f(x) \text{ such that } h_i(x) = 0$$

$$x \in \mathbb{R}^m$$

$$i = 1, 2, \dots, N$$

Construct the Lagrangian:

$$L(x, B) = f(x) + \sum_{i=1}^N B_i \cdot h_i(x)$$

then  $x$  is a local minima if there exists a unique  $B$  such that:

- $\nabla_x L(x, B) = 0$

- $\nabla_x L(x, B) = 0$
- $y^T (\nabla^2_{xx} L(x, B)) \succeq 0$

such that  $\nabla_x h(x^*) = 0$

## Lagrangian Dual Function

Need of a dual function?

- This approach may lead to a simpler optimization problem.
- For cases where the number of primal variables (dimensions of  $x$ ) is greater than the number of constraints.
- The relationship between the primal and dual variables can provide useful insights about the optimal primal solution.

$$\max_{\lambda, \mu} q(\lambda, \mu) \text{ such that } \lambda \succeq 0$$

where,

$$q(\lambda, \mu) = \min_x [ f(x) + \lambda^T \cdot g(x) + \mu^T \cdot h(x) ]$$

## Types of Duality

- The dual is always concave, even if the primal is not.
- Weak Duality:  $f(x) \geq q(\lambda, \mu)$  for feasible values of  $\lambda, \mu, x$
- Strong Duality: exists if the optimal values of primal = optimal values of dual i.e,  $f(x) = q(\lambda, \mu)$
- Strong duality exists only if the primal objective function and the constraints satisfy the following conditions:

1.  $f(x)$  and  $g(x)$  are convex and  $h(x)$  is affine
2. there exists some  $x$  such that  $g(x) \leq 0$  (slater's condition)
3. there exists primal solution  $x$  and dual solution  $(\lambda, \mu)$  such that  $f(x) = q(\lambda, \mu^*)$
4.  $x, \lambda, \mu^*$  satisfy the KKT conditions

## KKT Conditions

1.  $\nabla_x L(x, \lambda, \mu^*) = 0$
2.  $\nabla_{\mu} L(x, \lambda, \mu^*) = 0$
3.  $\lambda^* \succeq 0$  [ Dual Feasibility ]
4.  $g(x^*) \leq 0$  [ Primal Feasibility ]
5.  $\lambda^T g(x) = 0$  [ Complimentary Slackness ]

## Complimentary Slackness

If  $g(x) < 0$  then  $\lambda = 0$ ,

similarly if  $\lambda > 0$  then  $g(x) = 0$

## Code Explanation of complimentary slackness

Import libraries

In [2]:

```
import warnings
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm
from sklearn import svm
from sklearn.svm import SVC
from sklearn.model_selection import train_test_split, ShuffleSplit
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import accuracy_score
warnings.filterwarnings("ignore")
```

Create 40 linearly separable data points

In [3]:

```
np.random.seed(40)
X = np.r_[np.random.randn(20, 2) - [2, 2], np.random.randn(20, 2) + [2, 2]]
y = [0] * 20 + [1] * 20
```

## Hard Margin SVM

$\min w, b \left( \frac{1}{2} \cdot \|w\|^2 \right)$

such that  $1 - y_i (w^T \cdot x_i + b) \leq 0$

- the objective is convex
- the constraints are affine
- since the data is separable we know there exists at least one hyperplane ( $w$ ) that is feasible

## Formulating the Dual

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^N (\alpha_i [y_i (w^T \cdot x_i + b) - 1])$$

$$\text{such that } q(\alpha) = \min_{w, b} L(w, b, \alpha)$$

- minimize the Lagrangian wrt  $w$  and  $b$
- calculate the partial derivatives wrt  $w$  and  $b$
- substitute back in the Lagrangian to obtain the dual

Hence

$$dL(w, b, \alpha) / db = d/db \left[ - \sum_{i=1}^N (\alpha_i y_i b) \right] = 0$$

$$\sum_{i=1}^N (\alpha_i \cdot y_i) = 0$$

## The Dual

$$\max_{\alpha} \theta(\alpha) = \left( \sum_{i=1}^N \alpha_i \right) - \left( \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j x_i^T x_j \right)$$

such that

- $\alpha_i \geq 0$
- $\sum_{i=1}^N (\alpha_i * y_i) = 0$

In [4]:

```
clf = svm.SVC(kernel="linear", C=1)
clf.fit(X, y)

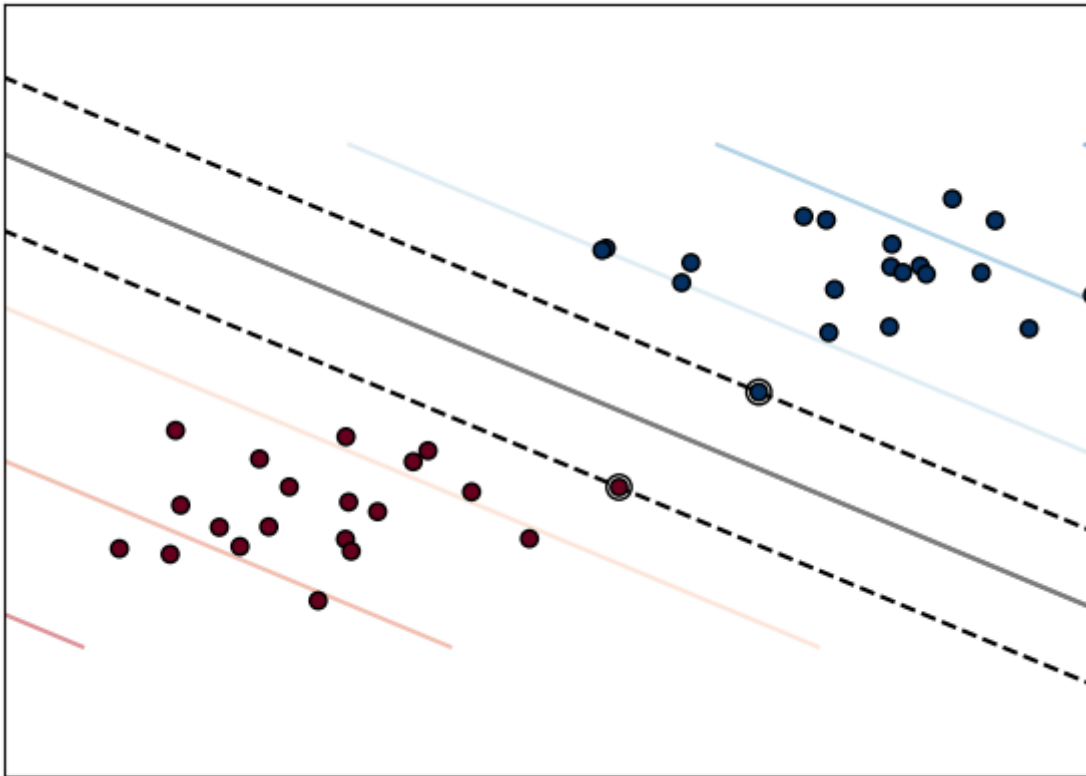
w = clf.coef_[0]
a = -w[0] / w[1]
xx = np.linspace(-5, 5)
yy = a * xx - (clf.intercept_[0] / w[1])

margin = 1 / np.sqrt(np.sum(clf.coef_**2))
yy_down = yy - np.sqrt(1 + a**2) * margin
yy_up = yy + np.sqrt(1 + a**2) * margin
```

In [5]:

```
plt.figure(figsize=(7, 5))
plt.clf()
plt.plot(xx, yy, "k-")
plt.plot(xx, yy_down, "k--")
plt.plot(xx, yy_up, "k--")
plt.scatter(clf.support_vectors[:, 0], clf.support_vectors[:, 1], s=80, facecolor='white', edgecolor='k', zorder=10)
plt.scatter(X[:, 0], X[:, 1], c=y, zorder=10, cmap=cm.get_cmap("RdBu"), edgecolor='k')
plt.axis("tight")
x_min = -4.8
x_max = 4.2
y_min = -6
y_max = 6

YY, XX = np.meshgrid(yy, xx)
xy = np.vstack([XX.ravel(), YY.ravel()]).T
Z = clf.decision_function(xy).reshape(XX.shape)
plt.contour(XX, YY, Z, cmap=cm.get_cmap("RdBu"), alpha=0.5, linestyles=["-"])
plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)
plt.xticks(())
plt.yticks(())
plt.show()
```



Given the dual optimization solution  $\alpha^*$

- from the complimentary slackness we can say that  $\alpha^* > 0$  which means the corresponding constraint  $g_i(w, b) = 0$
- Hence, the corresponding training instance has a margin = 1 known as the support vectors.

Optimal solution for the weight vector:

- $w = \sum_{i=1}^N (\alpha_i y_i x_i)$
- training instances will have  $\alpha_i = 0$
- prediction for new instances depend on their inner product with support vectors

$$w^T x' + b = \left[ \sum_{i=1}^N \alpha_i y_i x_i \right]^T$$

$$= \sum_{i=1}^N \alpha_i y_i \langle x_i, x' \rangle + b$$

The points through which the margin passes in the above example has their  $\alpha_i > 0$  (support vectors) while the farther points have their  $\alpha_i = 0$ .

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## Soft Margin SVM

$$\min_{w, b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^N \xi_i$$

$$\text{subject to: } y_i (w^T x_i + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

We use the slack variable  $\xi_i$  that transforms the constraints to soft constraints allowing soft constraints allowing instances to have a margin less than 1.

However, for violating constraints we pay a linear penalty ( $C * \xi_i$ )

## Formulating the Dual

$$L = 1/2 ||w||^2 + C \cdot \sum_{i=1}^N (\xi_i) - \sum_{i=1}^N (\alpha_i [y_i (w^T \cdot x_i + b) - 1 + \xi_i]) - \sum_{i=1}^N (n_i \cdot \xi_i)$$

where  $\theta(\alpha) = \min w, b, \xi L$

- minimize the Lagrangian wrt primal variables
- calculate partial derivatives wrt  $w, b$  and slack variable
- substitute back in Lagrangian to obtain the dual

## The Dual

$$\max_{\alpha} \theta(\alpha) = \sum_{i=1}^N (\alpha_i) - 1/2 \sum_{i=1}^N \sum_{j=1}^N (y_i \cdot y_j \cdot \alpha_i \cdot \alpha_j \cdot x_i^T \cdot x_j)$$

subject to :  $0 \leq \alpha_j \leq C$

$$\sum_{i=1}^N (\alpha_i \cdot y_i) = 0$$

In [6]:

```
clf = svm.SVC(kernel="linear", C=0.02)
clf.fit(X, y)

w = clf.coef_[0]
a = -w[0] / w[1]
xx = np.linspace(-5, 5)
yy = a * xx - (clf.intercept_[0] / w[1])

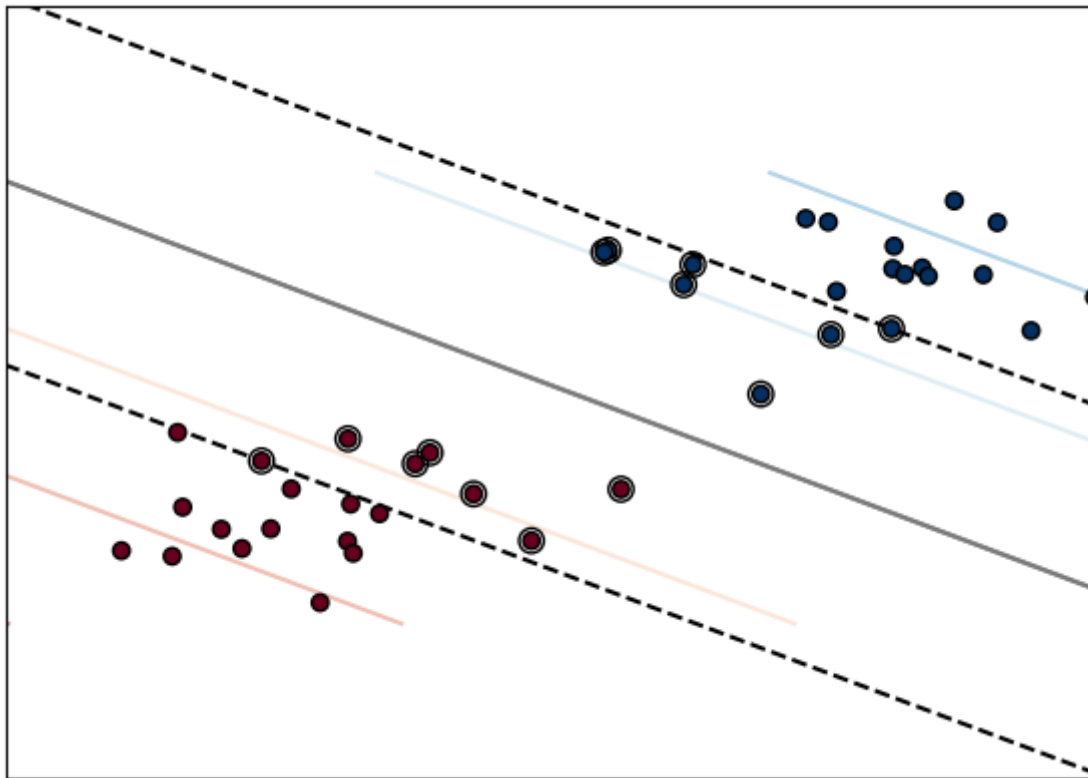
margin = 1 / np.sqrt(np.sum(clf.coef_**2))
yy_down = yy - np.sqrt(1 + a**2) * margin
yy_up = yy + np.sqrt(1 + a**2) * margin
```

In [7]:

```
plt.figure(figsize=(7, 5))
plt.clf()
plt.plot(xx, yy, "k-")
plt.plot(xx, yy_down, "k--")
plt.plot(xx, yy_up, "k--")
plt.scatter(clf.support_vectors_[0], clf.support_vectors_[1], s=80, facecolor='white', edgecolor='black')
plt.scatter(X[:, 0], X[:, 1], c=y, zorder=10, cmap=cm.get_cmap("RdBu"), edgecolor='black')
plt.axis("tight")
x_min = -4.8
x_max = 4.2
y_min = -6
y_max = 6

YY, XX = np.meshgrid(yy, xx)
xy = np.vstack([XX.ravel(), YY.ravel()]).T
Z = clf.decision_function(xy).reshape(XX.shape)
plt.contour(XX, YY, Z, cmap=cm.get_cmap("RdBu"), alpha=0.5, linestyles=["-"])
plt.xlim(x_min, x_max)
```

```
plt.ylim(y_min, y_max)
plt.xticks(())
plt.yticks(())
plt.show()
```



Given the dual solution  $\alpha^*$

- from the complementary slackness we know that  $\alpha_i = 0$  implies that the corresponding constraint is inactive  $g_i(w, b) < 0$  that is margin  $> 1$
- $\alpha_i = C$  implies that the corresponding constraint is violated  $g_i(w, b) > 0$  that is margin  $< 1$
- $0 < \alpha_i < C$  implies that the corresponding constraint is active  $g_i(w, b) = 0$  that is margin = 0

Optimal solution for the weight vector:

$$w^* = \sum_{i=1}^N (\alpha_i \cdot y_i \cdot x_i)$$

- depends on only support vectors other training instances will have  $\alpha_i = 0$
- prediction for new instances only depend on their inner product with support vectors

$$w^{*T} \cdot x' + b = \left[ \sum_{i=1}^N (\alpha_i \cdot y_i \cdot x_i) \right]^T + b$$

$$= \sum_{i=1}^N (\alpha_i \cdot y_i \cdot x_i^T + b)$$

## Ans 2.

Importing libraries

```
In [8]: import numpy as np
import pandas as pd
from sklearn.datasets import make_moons, make_circles
import seaborn as sns
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.svm import SVC
from sklearn.model_selection import cross_val_score
from sklearn.inspection import DecisionBoundaryDisplay
```

## Half-Circles dataset

Plotting the data points

```
In [9]: feature_names = ["Feature #0", "Features #1"]
target_name = "class"

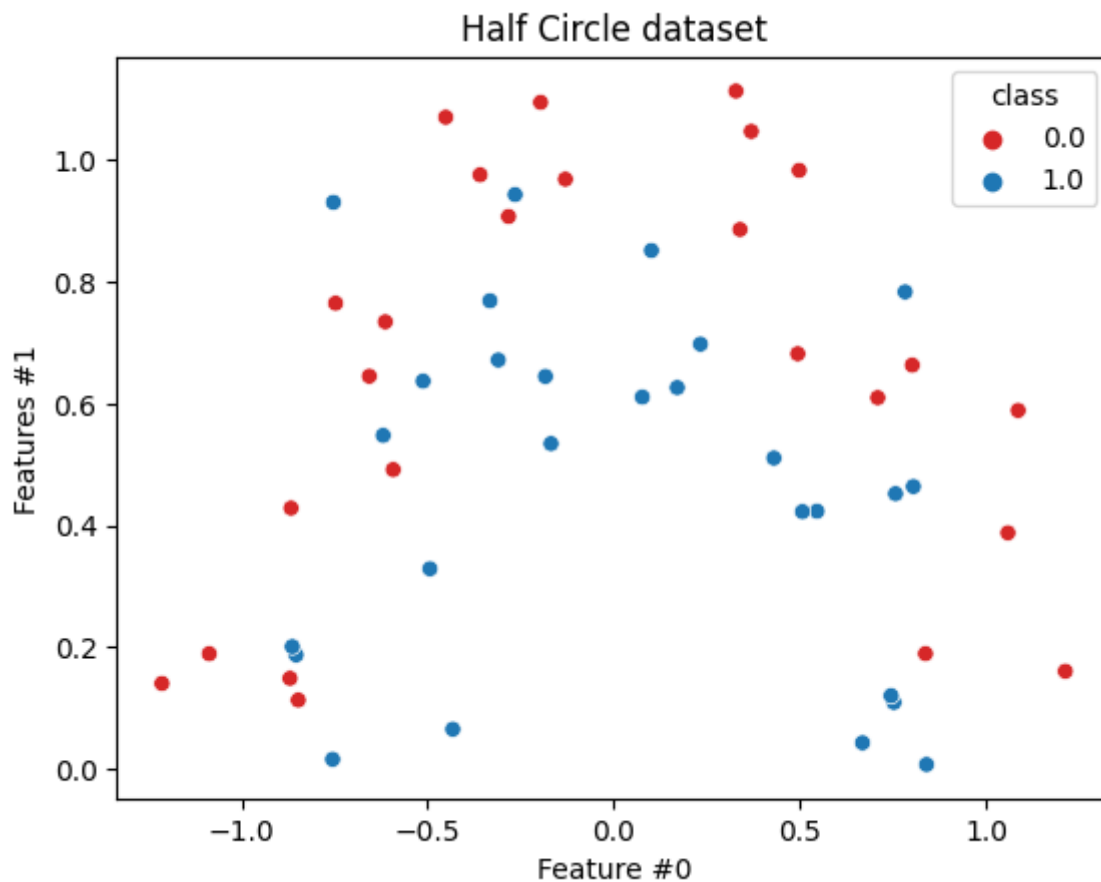
X, y = make_circles(n_samples=100, noise=0.13, random_state=42)
```

```
In [10]: # We store both the data and target in a dataframe to ease plotting
circles = pd.DataFrame(np.concatenate([X, y[:, np.newaxis]], axis=1), columns=fe
circles = circles[circles['Features #1'] >= 0]
#moons = moons[moons['Feature #0'] >= 0]
data_circles, target_circles = circles[feature_names], circles[target_name]
```

```
In [11]: sns.scatterplot(data = circles, x=feature_names[0], y=feature_names[1], hue=targ
plt.title("Half Circle dataset")
```

```
Out[11]: Text(0.5, 1.0, 'Half Circle dataset')
```





## Linear Kernel Decision Boundary

```
In [12]: linear_model = make_pipeline(StandardScaler(), SVC(kernel="linear", C=1, gamma=1))
```

Train validation split

```
In [13]: train_set, validation_set = train_test_split(circles, test_size=0.2, random_state=42)
```

```
In [14]: X_train = train_set.iloc[:,0:-1].values
y_train = train_set.iloc[:, -1].values
X_val = validation_set.iloc[:, 0:-1].values
y_val = validation_set.iloc[:, -1].values
```

K-Fold cross validation on train data

```
In [15]: accuracies=cross_val_score(estimator=linear_model,X=X_train,y=y_train,cv=10)
accuracies
```

```
Out[15]: array([0.8 , 0.75, 0.25, 0.25, 0.5 , 0.5 , 0.75, 0.75, 0.75, 0.75])
```

```
In [16]: print("average accuracy :",np.mean(accuracies))
print("average std :",np.std(accuracies))
```

average accuracy : 0.605  
average std : 0.20426698215815497

Fitting the model and checking accuracy on validation data

In [17]:

```
linear_model.fit(X_train,y_train)
print("test accuracy :",linear_model.score(X_val,y_val))
```

test accuracy : 0.5454545454545454

Grid Search for hyperparameter tuning, changing hyperparameters in the kernel as given by the  
Grid Search for best results

In [18]:

```
param_grid = {'C': [0.1,1, 10, 100], 'gamma': [1,0.1,0.01,0.001], 'kernel': ['rbf',
grid = GridSearchCV(SVC(),param_grid,refit=True,verbose=2)
grid.fit(X_train,y_train)
```

Fitting 5 folds for each of 48 candidates, totalling 240 fits

```
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
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[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
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[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
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[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=sigmoid; total time= 0.0s
```

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12/40

13/40

```
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
```

Out[18]:

```

  ▸ GridSearchCV
    ▸ estimator: SVC
      ▸ SVC

```

In [19]:

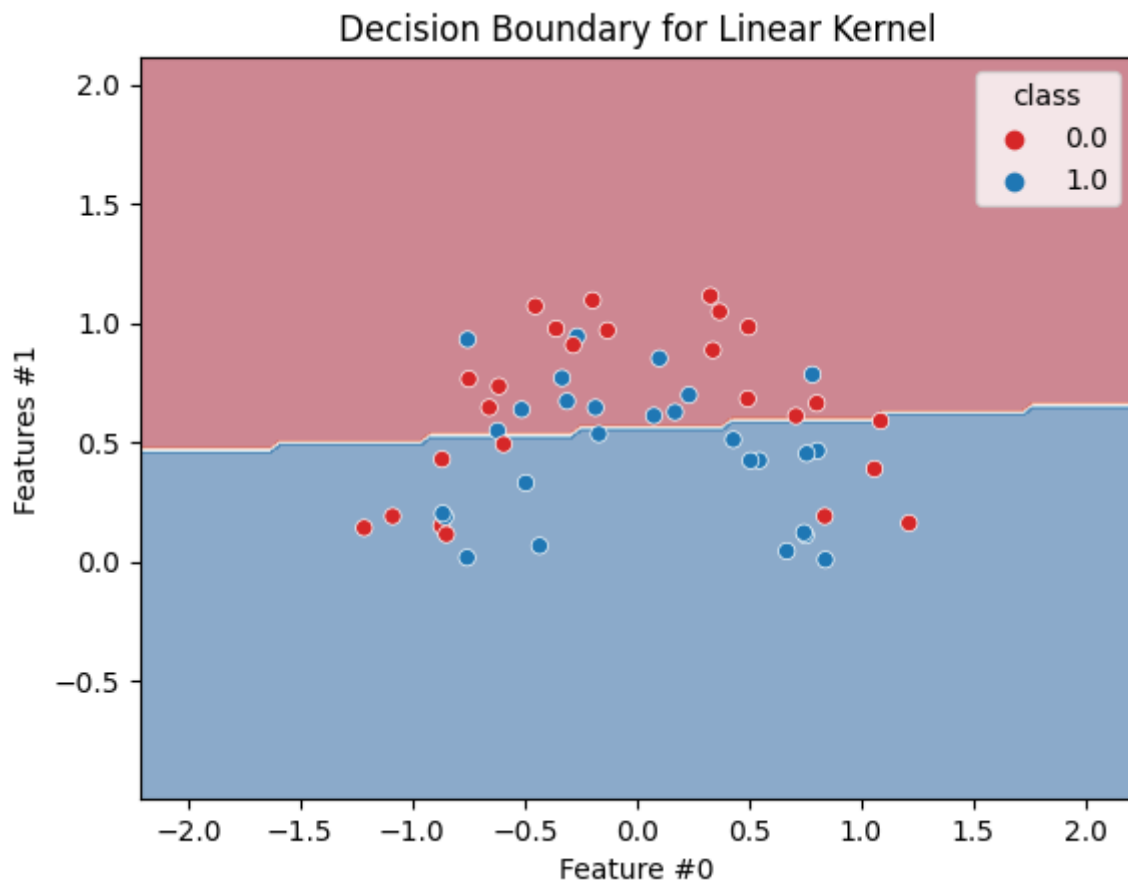
```
print(grid.best_estimator_)
```

SVC(C=100, gamma=1)

In [20]:

```
linear_model.fit(data_circles, target_circles)
DecisionBoundaryDisplay.from_estimator(linear_model, data_circles, response_meth
sns.scatterplot(data=circles, x=feature_names[0], y = feature_names[1], hue = ta
plt.title("Decision Boundary for Linear Kernel")
```

Out[20]: Text(0.5, 1.0, 'Decision Boundary for Linear Kernel')



The linear kernel decision boundary does not classify the two classes very accurately and performs poorly, hence we try a non-linear kernel as the data points are not linearly separable. We need to plot the data in a higher dimension where we might get a decision boundary. Hence we try the non-linear RBF kernel.

## RBF Kernel Decision Boundary

```
In [21]: kernel_model = make_pipeline(StandardScaler(), SVC(kernel='rbf', C=100, gamma=1))
```

Train Validation data split

```
In [22]: train_set, validation_set = train_test_split(circles, test_size=0.2, random_stat
```

```
In [23]: X_train = train_set.iloc[:,0:-1].values
y_train = train_set.iloc[:, -1].values
X_val = validation_set.iloc[:, 0:-1].values
y_val = validation_set.iloc[:, -1].values
```

K fold Cross Validation

```
In [24]: accuracies=cross_val_score(estimator=kernel_model,X=X_train,y=y_train,cv=10)
accuracies
```

```
Out[24]: array([1. , 1. , 0.75, 1. , 0.75, 1. , 1. , 1. , 0.75, 0.75])
```

In [25]:

```
print("average accuracy :",np.mean(accuracies))
print("average std :",np.std(accuracies))
```

```
average accuracy : 0.9
average std : 0.12247448713915891
```

Fitting the model and checking the accuracy on validation data

In [26]:

```
kernel_model.fit(X_train,y_train)
print("test accuracy :",kernel_model.score(X_val,y_val))
```

```
test accuracy : 0.5454545454545454
```

Grid Search for hyperparameter tuning, changing hyperparameters in the kernel as given by the Grid Search for best results

In [27]:

```
param_grid = {'C': [0.1,1, 10, 100], 'gamma': [1,0.1,0.01,0.001], 'kernel': ['rbf',
grid = GridSearchCV(SVC(),param_grid,refit=True,verbose=2)
grid.fit(X_train,y_train)
```

Fitting 5 folds for each of 48 candidates, totalling 240 fits

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[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
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[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
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[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
```



[illegible]

[illegible]

[illegible]

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[CV] END .....C=100, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=poly; total time= 0.0s
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[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
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[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
```

Out[27]:

```
▸ GridSearchCV
  ▸ estimator: SVC
    ▸ SVC
```

In [28]:

```
print(grid.best_estimator_)
```

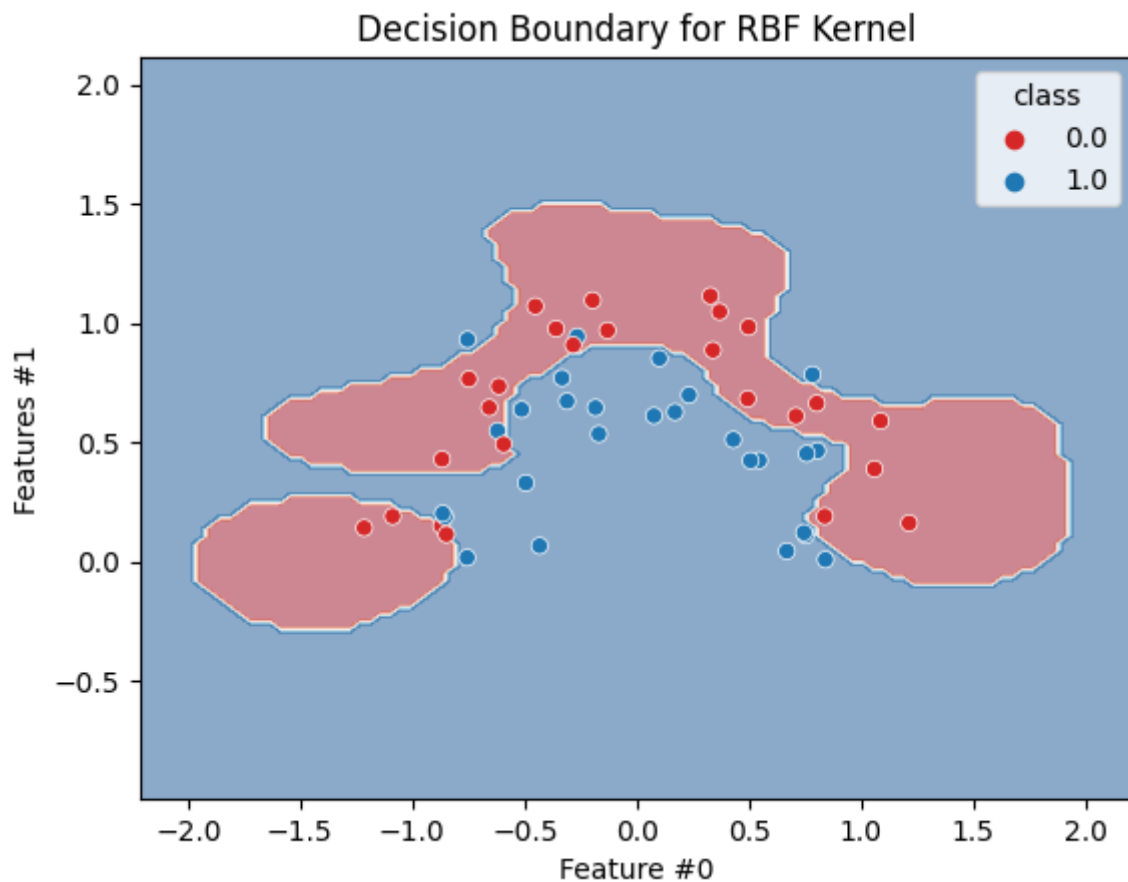
```
SVC(C=100, gamma=1)
```

In [29]:

```
kernel_model.fit(data_circles, target_circles)
DecisionBoundaryDisplay.from_estimator(kernel_model, data_circles, response_method=
sns.scatterplot(data=circles, x = feature_names[0], y = feature_names[1], hue =
plt.title("Decision Boundary for RBF Kernel")
```

Out[29]:

```
Text(0.5, 1.0, 'Decision Boundary for RBF Kernel')
```



The RBF kernel performs well in making a non-linear decision boundary ( sort of like a semi-circle boundary ) around the blue data points separating them from the red ones.

## Moons dataset

Plotting the data points

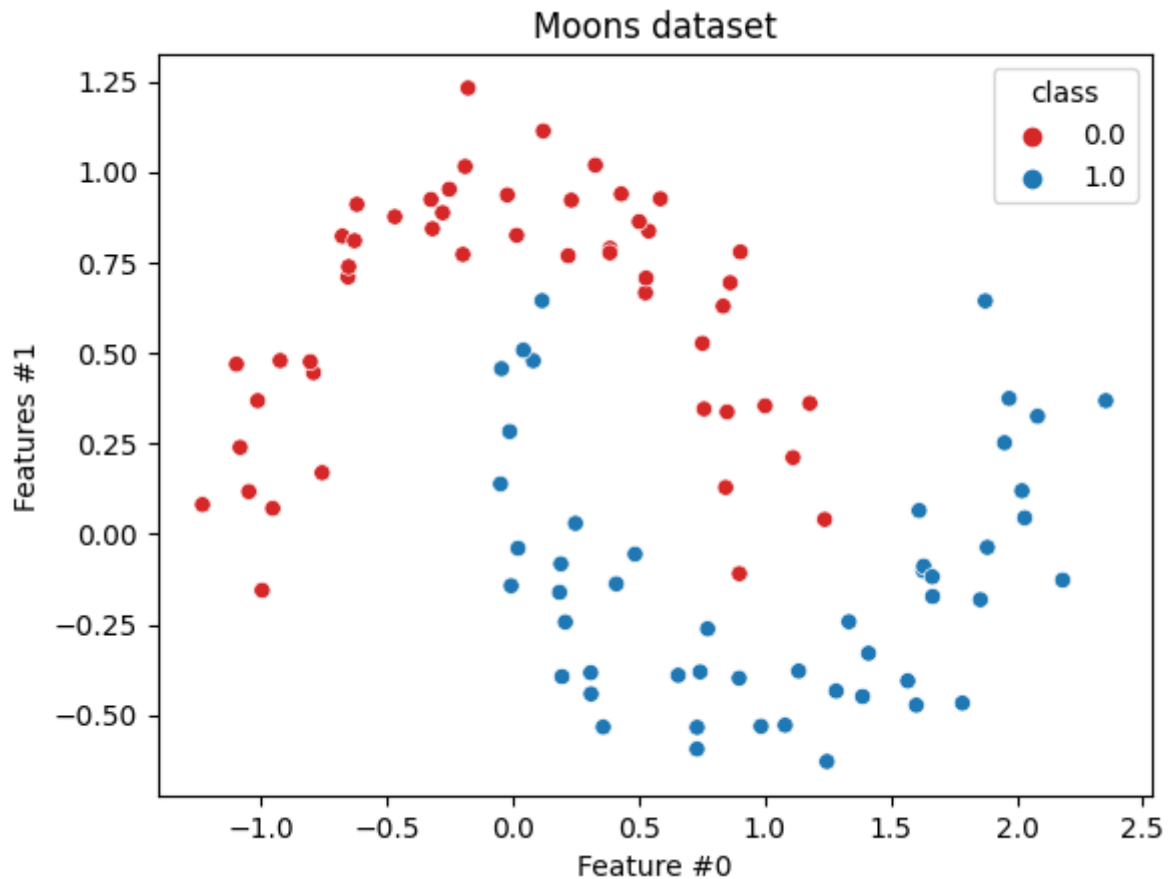
```
In [30]: feature_names = ["Feature #0", "Features #1"]
         target_name = "class"

         X, y = make_moons(n_samples=100, noise=0.13, random_state=42)

         # We store both the data and target in a dataframe to ease plotting
         moons = pd.DataFrame(np.concatenate([X, y[:, np.newaxis]], axis=1), columns=feature_names, target_moons = moons[target_name])
```

```
In [31]: sns.scatterplot(data = moons, x=feature_names[0], y=feature_names[1], hue=target_name)
         plt.title("Moons dataset")
```

```
Out[31]: Text(0.5, 1.0, 'Moons dataset')
```



## Linear Kernel Decision Boundary

```
In [32]: linear_model = make_pipeline(StandardScaler(), SVC(kernel="linear", C=10, gamma=
```

Train validation data split

```
In [33]: train_set, validation_set = train_test_split(moons, test_size=0.2, random_state=
```

```
In [34]: X_train = train_set.iloc[:,0:-1].values
y_train = train_set.iloc[:, -1].values
X_val = validation_set.iloc[:, 0:-1].values
y_val = validation_set.iloc[:, -1].values
```

K fold cross validation on train data set

```
In [35]: accuracies=cross_val_score(estimator=linear_model,X=X_train,y=y_train,cv=10)
accuracies
```

```
Out[35]: array([0.875, 0.625, 0.875, 0.75 , 0.875, 0.875, 0.875, 0.875, 0.75 ,
0.875])
```

```
In [36]: print("average accuracy :",np.mean(accuracies))
print("average std :",np.std(accuracies))
```

average accuracy : 0.825  
average std : 0.08291561975888499

In [37]:

```
linear_model.fit(X_train,y_train)
print("test accuracy :",linear_model.score(X_val,y_val))
```

test accuracy : 1.0

Grid Search for hyperparameter tuning, changing hyperparameters in the kernel as given by the  
Grid Search for best results

In [38]:

```
param_grid = {'C': [0.1,1, 10, 100], 'gamma': [1,0.1,0.01,0.001],'kernel': ['rbf',
grid = GridSearchCV(SVC(),param_grid,refit=True,verbose=2)
grid.fit(X_train,y_train)
```

Fitting 5 folds for each of 48 candidates, totalling 240 fits

```
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
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[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
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[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
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[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
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[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=sigmoid; total time= 0.0s
```

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[illegible]

[illegible]

```
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
```

Out[38]:

```

  ▸ GridSearchCV
  ▸ estimator: SVC
    ▸ SVC

```

In [39]:

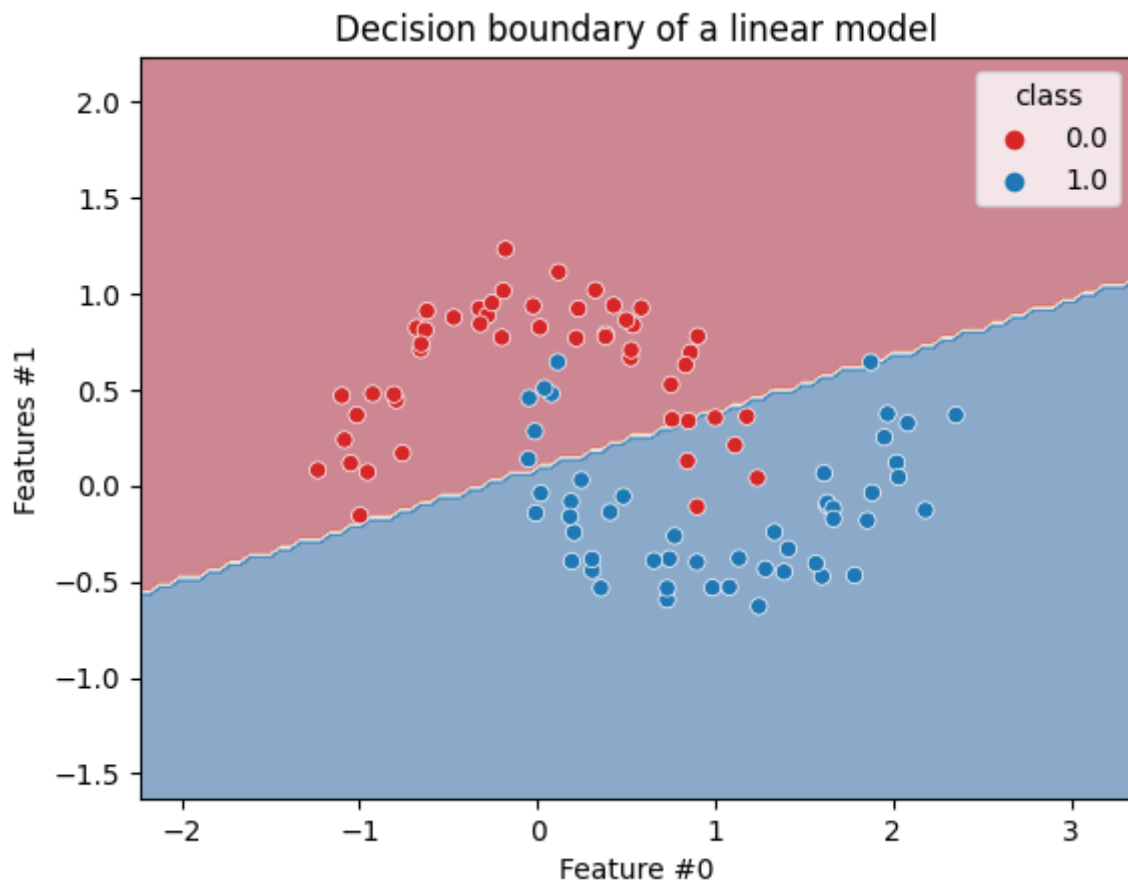
```
print(grid.best_estimator_)
```

SVC(C=10, gamma=1)

In [40]:

```
linear_model.fit(data_moons, target_moons)
DecisionBoundaryDisplay.from_estimator(linear_model, data_moons, response_method
sns.scatterplot(data=moons, x=feature_names[0], y=feature_names[1], hue=target_m
plt.title("Decision boundary of a linear model")
```

Out[40]: Text(0.5, 1.0, 'Decision boundary of a linear model')



The linear kernel decision boundary does not classify the two classes very accurately and performs poorly, hence we try a non-linear kernel as the data points are not linearly separable. We need to plot the data in a higher dimension where we might get a decision boundary. Hence we try the non-linear RBF kernel.

## RBF Kernel Decision Boundary

```
In [41]: kernel_model = make_pipeline(StandardScaler(), SVC(kernel="rbf", C = 100, gamma=
```

Train validation data split

```
In [42]: train_set, validation_set = train_test_split(moons, test_size=0.2, random_state=
```

```
In [43]: X_train = train_set.iloc[:,0:-1].values
y_train = train_set.iloc[:, -1].values
X_val = validation_set.iloc[:, 0:-1].values
y_val = validation_set.iloc[:, -1].values
```

K fold cross validation on train data set

```
In [44]: accuracies=cross_val_score(estimator=kernel_model,X=X_train,y=y_train,cv=10)
accuracies
```

```
Out[44]: array([1.    , 0.875, 0.875, 1.    , 1.    , 1.    , 1.    , 1.    , 1.    ,
1.    ])
```

In [45]:

```
print("average accuracy :",np.mean(accuracies))
print("average std :",np.std(accuracies))
```

```
average accuracy : 0.975
average std : 0.049999999999999996
```

In [46]:

```
kernel_model.fit(X_train,y_train)
print("test accuracy :",kernel_model.score(X_val,y_val))
```

```
test accuracy : 0.95
```

Grid Search for hyperparameter tuning, changing hyperparameters in the kernel as given by the Grid Search for best results

In [47]:

```
grid = GridSearchCV(SVC(),param_grid,refit=True,verbose=2)
grid.fit(X_train,y_train)
```

```
Fitting 5 folds for each of 48 candidates, totalling 240 fits
```

```
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
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[CV] END .....C=0.1, gamma=1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.1, kernel=sigmoid; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=rbf; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=0.1, gamma=0.01, kernel=poly; total time= 0.0s
```

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```
[CV] END .....C=100, gamma=0.01, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.01, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=rbf; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=poly; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
[CV] END .....C=100, gamma=0.001, kernel=sigmoid; total time= 0.0s
```

Out[47]:

```

  ▸ GridSearchCV
    ▸ estimator: SVC
      ▸ SVC

```

In [48]:

```
print(grid.best_estimator_)
```

SVC(C=10, gamma=1)

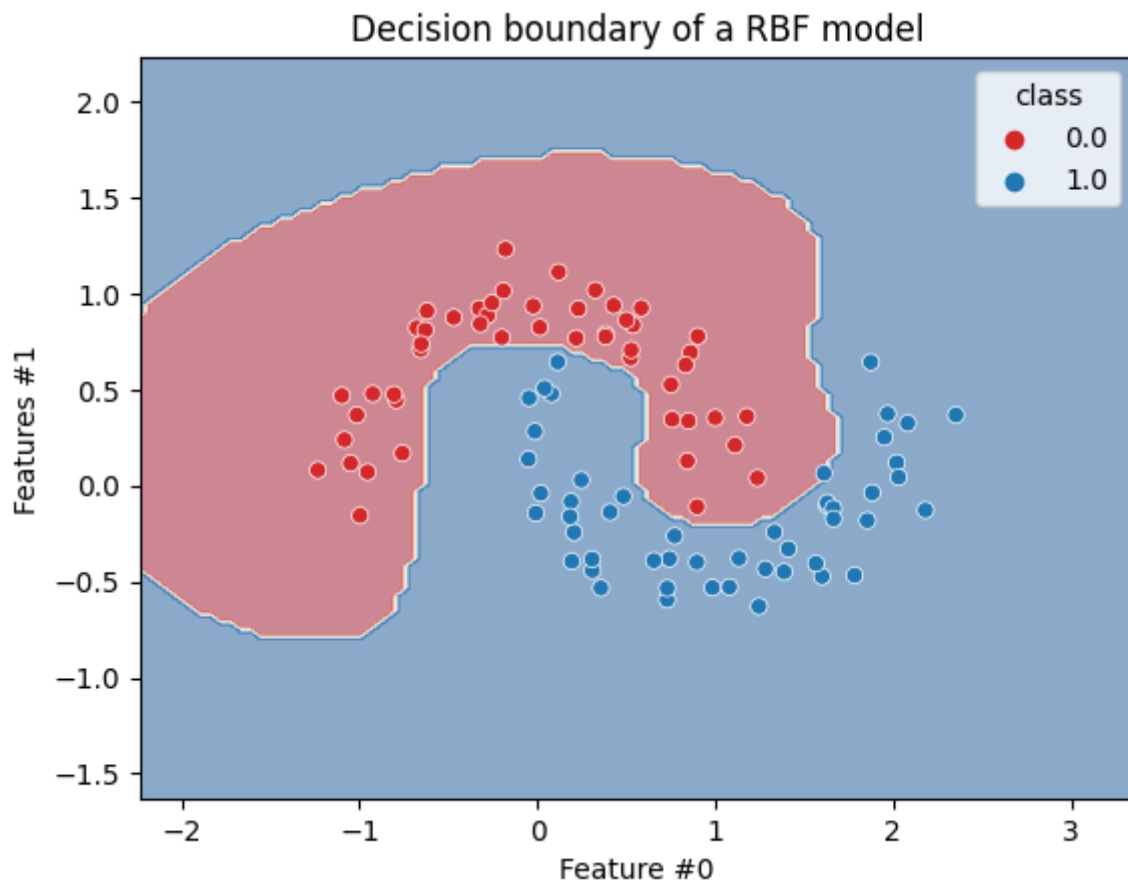
In [49]:

```

#kernel_model.fit(data_moons, target_moons)
DecisionBoundaryDisplay.from_estimator(kernel_model, data_moons, response_method
sns.scatterplot(data=moons, x=feature_names[0], y=feature_names[1], hue=target_m
plt.title("Decision boundary of a RBF model")

```

Out[49]: Text(0.5, 1.0, 'Decision boundary of a RBF model')



The RBF kernel performs well in making a non-linear decision boundary ( sort of like a semi-circle boundary ) around the blue data points separating them from the red ones.

Citations:

1. [https://inria.github.io/scikit-learn-mooc/python\\_scripts/logistic\\_regression\\_non\\_linear.html](https://inria.github.io/scikit-learn-mooc/python_scripts/logistic_regression_non_linear.html)
2. [https://nthu-datalab.github.io/ml/labs/07\\_SVM\\_Pipeline/07\\_SVM\\_Pipeline.html](https://nthu-datalab.github.io/ml/labs/07_SVM_Pipeline/07_SVM_Pipeline.html)
3. <https://www.vebuso.com/2020/03/svm-hyperparameter-tuning-using-gridsearchcv/>
4. <https://isheunesu48.medium.com/cross-validation-using-k-fold-with-scikit-learn-cfc44bf1ce6>

## Ans 3.

### MLP for Half Circles data

Importing the libraries

```
In [50]: from sklearn.model_selection import train_test_split
from sklearn.neural_network import MLPClassifier
from sklearn.metrics import confusion_matrix
```

Splitting the data into train and validation sets

```
In [51]: train_set, validation_set = train_test_split(circles, test_size=0.2, random_stat
```

## Splitting the dependent and independent variables

```
In [52]: X_train = train_set.iloc[:,0:-1].values
y_train = train_set.iloc[:, -1].values
X_val = validation_set.iloc[:, 0:-1].values
y_val = validation_set.iloc[:, -1].values
```

## Defining the accuracy function

```
In [53]: def accuracy(confusion_matrix):
    dialog_sum = confusion_matrix.trace()
    sum_of_all_elements = confusion_matrix.sum()
    return dialog_sum / sum_of_all_elements
```

## Defining the classifier

```
In [86]: classifier = MLPClassifier(hidden_layer_sizes= (100, 100, 50), max_iter=165, act
```

## K fold cross validation on train data set

```
In [87]: accuracies=cross_val_score(estimator=classifier,X=X_train,y=y_train,cv=10)
accuracies
```

```
Out[87]: array([0.6 , 0.75, 0.75, 0.75, 0.75, 0.5 , 1. , 0.5 , 0.75, 1. ])
```

```
In [88]: print("average accuracy :",np.mean(accuracies))
print("average std :",np.std(accuracies))
```

```
average accuracy : 0.735
average std : 0.16439282222773596
```

```
In [89]: classifier.fit(X_train,y_train)
print("test accuracy :",classifier.score(X_val,y_val))
```

```
test accuracy : 0.7272727272727273
```

## Grid Search

```
In [91]: mlp_gs = MLPClassifier(max_iter=165)
parameter_space = {
    'hidden_layer_sizes': [(100, 100, 50)],
    'activation': ['tanh', 'relu'],
    'solver': ['sgd', 'adam'],
    'alpha': [0.0001, 0.05],
    'learning_rate': ['constant', 'adaptive'],
}
clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=-1, cv=5)
clf.fit(X_train, y_train)
```

Out [91]:

```

  ▸ GridSearchCV
  ▸ estimator: MLPClassifier
    ▸ MLPClassifier

```

In [92]:

```
print('Best parameters found:\n', clf.best_params_)
```

Best parameters found:

```
{'activation': 'tanh', 'alpha': 0.0001, 'hidden_layer_sizes': (100, 100, 50),
 'learning_rate': 'constant', 'solver': 'adam'}
```

Predicting the y variable on the validation set

In [93]:

```
y_pred = classifier.predict(X_val)
```

Confusion matrix, calculating the accuracy

In [94]:

```
cm = confusion_matrix(y_pred, y_val)
print("Accuracy of MLP Classifier: ", accuracy(cm))
```

Accuracy of MLP Classifier: 0.7272727272727273

Plotting the decision boundary with the MLP classifier

In [95]:

```
h = 0.02
x_min = -4.8
x_max = 4.2
y_min = -6
y_max = 6
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
```

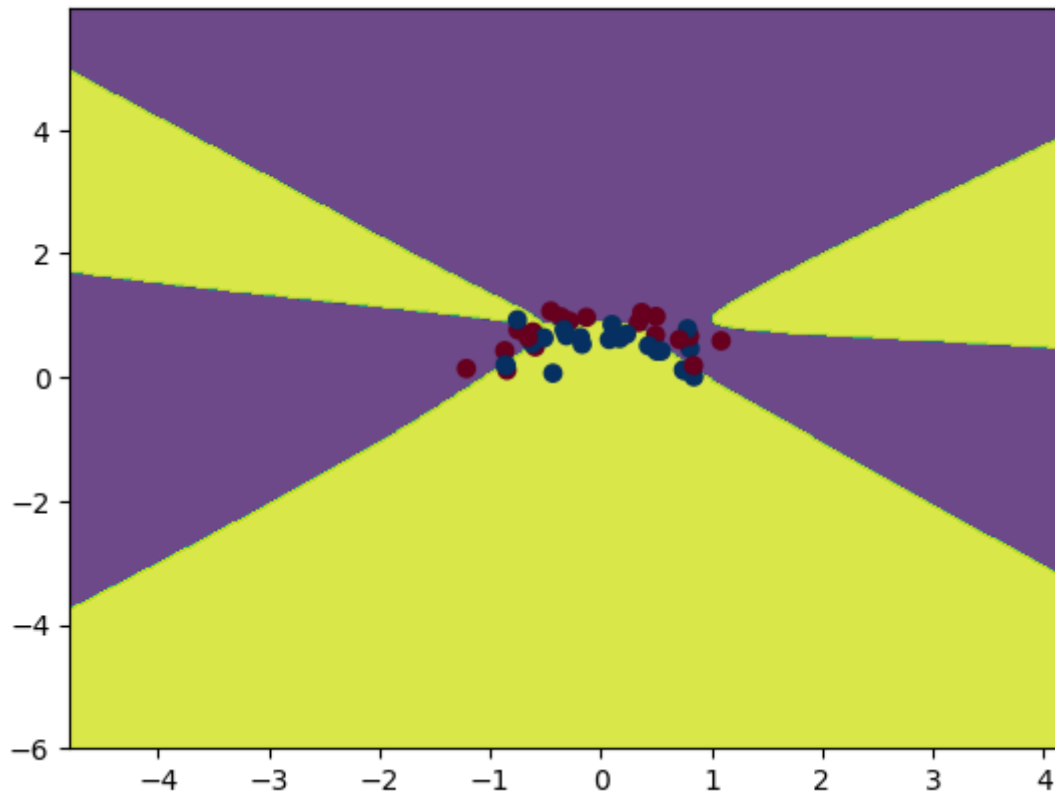
In [96]:

```
z = classifier.predict(np.c_[xx.ravel(), yy.ravel()])
```

In [97]:

```
z = z.reshape(xx.shape)
plt.contourf(xx, yy, z, alpha=0.8)
plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap="RdBu")
```

Out [97]: <matplotlib.collections.PathCollection at 0x7fd3735d96c0>



Rational for training process:

After importing the libraries, splitting the data into train, validation sets and the dependent and independent variables, defined the MLP classifier and performed K fold cross validation since we have less data and we don't want to overfit - we get the best model. Grid search is applied for obtaining the best hyperparameters. We check their accuracies on train and test data. Then the model with the best hyperparameters fits the train data. The decision boundary is then visualized and the decision boundary is observed.

Design parameters:

Using grid search the best hyperparameters are chosen. The activation function Tanh is chosen due to the non linear nature of the data. Adam optimizer is used as it works the best in this case.

## MLP for Moons data

Splitting the data into train and validation sets

```
In [107... train_set, validation_set = train_test_split(moons, test_size=0.2, random_state
```

Splitting the data into dependent and independent variables

```
In [108... x_train = train_set.iloc[:, 0:-1].values
x_val = validation_set.iloc[:, 0:-1].values
y_train = train_set.iloc[:, -1].values
y_val = validation_set.iloc[:, -1].values
```

## Defining the classifier

```
In [109... classifier = MLPClassifier(hidden_layer_sizes=(100, 100, 50), activation='relu',
```

## K fold cross validation on train data set

```
In [110... accuracies=cross_val_score(estimator=classifier,X=X_train,y=y_train,cv=10)
accuracies
```

```
Out[110... array([1.    , 1.    , 1.    , 1.    , 0.875, 1.    , 1.    , 1.    , 0.875,
        1.    ])
```

```
In [111... print("average accuracy :",np.mean(accuracies))
print("average std :",np.std(accuracies))
```

```
average accuracy : 0.975
average std : 0.049999999999999996
```

```
In [112... classifier.fit(X_train,y_train)
print("test accuracy :",classifier.score(X_val,y_val))
```

```
test accuracy : 1.0
```

## Grid Search

```
In [104... mlp_gs = MLPClassifier(max_iter=165)
parameter_space = {
    'hidden_layer_sizes': [(100, 100, 50)],
    'activation': ['tanh', 'relu'],
    'solver': ['sgd', 'adam'],
    'alpha': [0.0001, 0.05],
    'learning_rate': ['constant', 'adaptive'],
}
clf = GridSearchCV(mlp_gs, parameter_space, n_jobs=-1, cv=5)
clf.fit(X_train, y_train)
```

```
Out[104... ► GridSearchCV
► estimator: MLPClassifier
    ► MLPClassifier
```

```
In [105... print('Best parameters found:\n', clf.best_params_)
```

```
Best parameters found:
{'activation': 'relu', 'alpha': 0.0001, 'hidden_layer_sizes': (100, 100, 50),
 'learning_rate': 'constant', 'solver': 'adam'}
```

## Predicting the independent variable on the validation set

```
In [113... y_pred = classifier.predict(X_val)
```

## Confusion matrix, calculating the accuracy

```
In [114... cm = confusion_matrix(y_pred, y_val)
print("Accuracy of MLP Classifier: ", accuracy(cm))
```

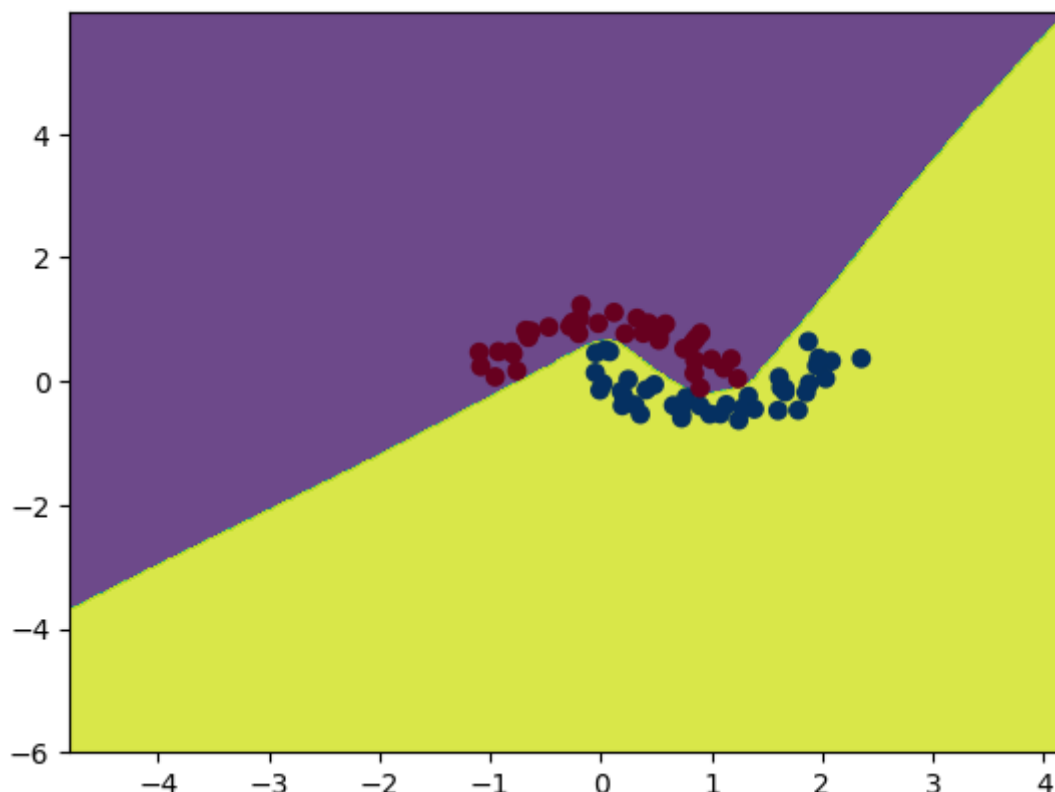
Accuracy of MLP Classifier: 1.0

```
In [115... h = 0.02
x_min = -4.8
x_max = 4.2
y_min = -6
y_max = 6
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
```

```
In [116... z = classifier.predict(np.c_[xx.ravel(), yy.ravel()])
```

```
In [117... z = z.reshape(xx.shape)
plt.contourf(xx, yy, z, alpha=0.8)
plt.scatter(X_train[:,0], X_train[:,1], c=y_train, cmap="RdBu")
```

Out[117... <matplotlib.collections.PathCollection at 0x7fd371e417e0>



Rational for training process:

After importing the libraries, splitting the data into train, validation sets and the dependent and independent variables, defined the MLP classifier and performed K fold cross validation since we have less data and we don't want to overfit - we get the best model. Grid search is applied for obtaining the best hyperparameters. We check their accuracies on train and test data. Then

the model with the best hyperparameters fits the train data. The decision boundary is then visualized and the decision boundary is observed.

Design parameters:

Using grid search the best hyperparameters are chosen. The activation function Tanh is chosen due to the non linear nature of the data. Adam optimizer is used as it works the best in this case.

## SVM vs MLP algorithms

SVMs

Both soft and hard margin SVMs are convex quadratic problems with linear constraints. Quadratic problems are usually computationally expensive combined with Gradient Descent. Hence, Stochastic Gradient Descent comes into play. It takes more steps and yet is more computationally efficient.

- The training time for SVM can be given as  $O(n \cdot d^2)$  if  $d < n$

d: dimensions

n: number of data points

- The run time ( predicting time ) can be given as  $O(k \cdot n)$

k: number of support vectors (  $0 < k \leq d$  )

My MLP code took longer to run than the SVM code hence the computation cost is higher.