

# Homework Assignment 6

## 1 (8 points) Conceptual Questions

1. Which one below best describes what support vectors are:

A. The decision boundary.

B. The positive and the negative planes.

C. The training samples that determine the positive and the negative planes.

D. The test samples that determine the positive and the negative planes.

2. When tuning the hyper-parameters of a model, we find the hyper-parameters that

A. minimize error on the test set

B. minimize error on the test set

C. maximize the margin of the classifier

D. minimize error on the validation set

3. Select all that apply. k-fold cross validation is

A. Not necessary when you have huge amounts of labelled data

B. A way to do model selection while minimizing over-fitting

C. The only way to do hyper-parameter tuning

D. Subject to the bias-variance trade-off

4. When you increase the k in cross-validation while keeping the dataset the same, you

A. Get a decrease in both the generalization error and the validation error

B. Get an increase both the generalization error and the validation error

C. Get a decrease in the variability of the validation error across folds

D. Get an increase in the variability of the validation error across folds

## 2 (10 points) Cross-Validation

Given a training dataset  $S_{\text{training}} = \{(x_i, y_i)\}, i = 1, \dots, 6\}$  where  $x_i \in \mathbb{R}$  is the feature scalar and  $y_i \in \{-1, +1\}$  is the corresponding label. The data points in the dataset  $S_{\text{training}}$  are given below:

$$(x_1, y_1) = (2, -1), (x_2, y_2) = (7, -1), (x_3, y_3) = (4, +1), \\ (x_4, y_4) = (1, -1), (x_5, y_5) = (3, +1), (x_6, y_6) = (6, +1).$$

Suppose you are training a linear classifier  $f(x; a, b) = \text{sign}(ax + b)$  with 2-fold cross-validation where  $\text{sign}(z)$  is defined as:

$$\text{sign}(z) = \begin{cases} 1, & z \geq 0 \\ -1, & z < 0 \end{cases}$$

- You have split the dataset  $S_{\text{training}}$  into:

$$S_1 = \{(x_1, y_1), (x_2, y_2), (x_3, y_3)\} \\ S_2 = \{(x_4, y_4), (x_5, y_5), (x_6, y_6)\}$$

- After training the classifier  $f(x; a, b)$  on  $S_1$ , you have obtained the parameters  $a_1 = -1, b_1 = 5$  and then try to validate the classifier on  $S_2$ .
- After training the classifier  $f(x; a, b)$  on  $S_2$ , you have obtained the parameters  $a_2 = 2, b_2 = -3$  and then try to validate the classifier on  $S_1$ .

Please finish the tasks below:

1. Calculate the **average training error** in the 2-fold cross-validation.

**Note:** The definition of average training error is the mean of the error of classifier  $f(x; a_1, b_1)$  on  $S_1$  and the error of classifier  $f(x; a_2, b_2)$  on  $S_2$ .

$$S_1 = \frac{1}{3} \text{ and } S_2 = \frac{0}{3} = 0$$

$\text{Average Training Error} \Rightarrow \frac{1}{6}$
---

2. Calculate the **average validation error** (i.e. the cross-validation error) in the 2-fold cross-validation.

$\text{Average validation error} \Rightarrow \frac{2}{3}$
---

### 3 (12 points) Shattering

In this problem, consider a classifier  $f(x; a, b) = \text{sign}(ax^T x - b)$  where the feature vector  $x = [x_1, x_2]^T \in \mathbb{R}^2$  and its prediction  $f(x; a, b) \in \{-1, +1\}$ . Besides,  $a, b \in \mathbb{R}$  are the model parameters and  $\text{sign}(z)$  is defined as:

$$\text{sign}(z) = \begin{cases} 1, & z \geq 0 \\ -1, & z < 0 \end{cases}$$

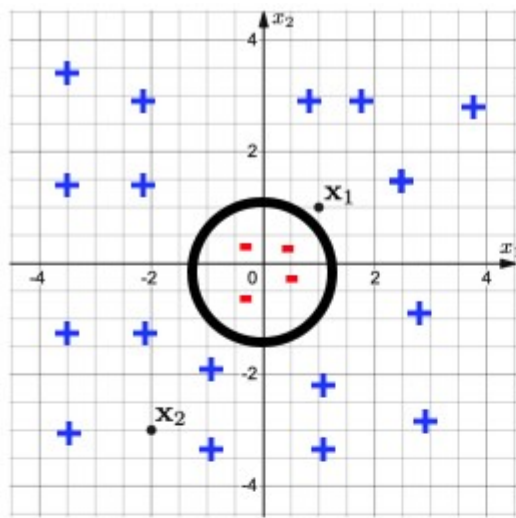
The classifier  $f(x; a, b)$  performs a binary classification on an input feature vector  $x$  under model parameters  $a, b \in \mathbb{R}$  that can be learned.

In this question, please attempt to show that if the classifier  $f(x; a, b)$  can shatter two points,  $x_1 = [1, 1]^T$  and  $x_2 = [-2, -3]^T$ .

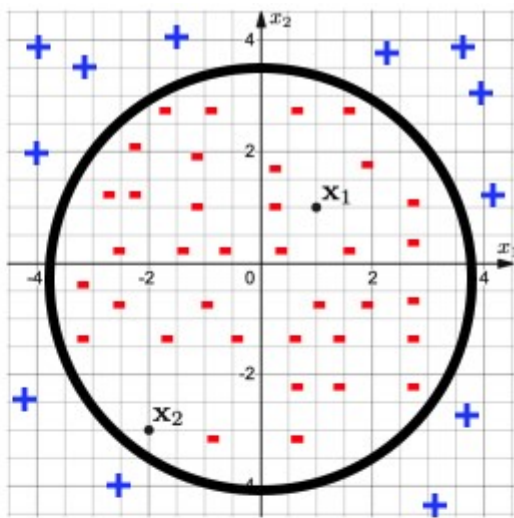
- If you think  $f(x; a, b)$  can shatter  $x_1$  and  $x_2$ , you need to show that for each possible label configuration  $(y_1, y_2) \in \{(+1, +1), (-1, -1), (+1, -1), (-1, +1)\}$  of  $x_1$  and  $x_2$ , there exists a classifier  $f(x; a, b)$  that classifies the  $x_1$  and  $x_2$  correctly, and you should illustrate each classifier by the following steps:

- Draw the decision boundary of the classifier.
- Shade the area where the classifier makes the positive prediction

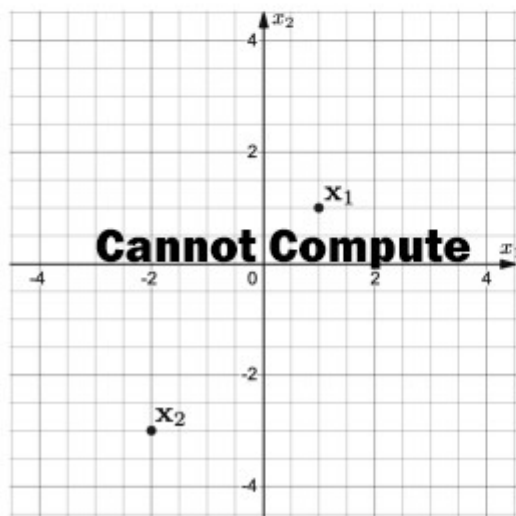
- If you think classifier  $f(x; a, b)$  cannot shatter  $x_1$  and  $x_2$ , please explain the reason.



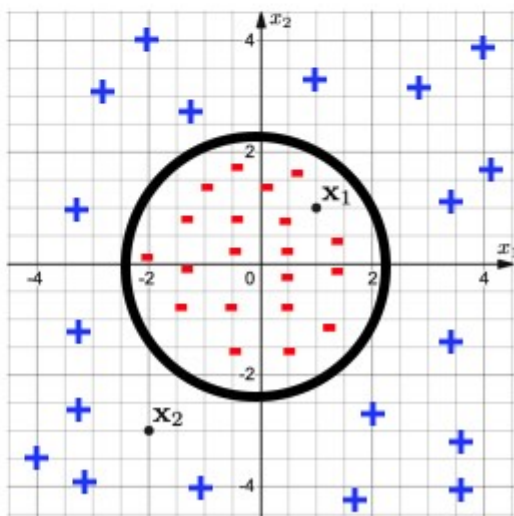
$$(y_1, y_2) = (+1, +1)$$



$$(y_1, y_2) = (-1, -1)$$



$$(y_1, y_2) = (+1, -1)$$



$$(y_1, y_2) = (-1, +1)$$

**Answer:**  $f(x; a, b)$  cannot be shattered since there is no way to classify  $(y_1, y_2) = (+1, -1)$ . That is, we are unable to draw a circle that allows  $x_1$  to have a +1 classification and  $x_2$  to have -1 classification

## 4 (10 points) SVM: Gradient

Given a training dataset  $S_{\text{training}} = \{(x_i, y_i)\}, i = 1, \dots, n\}$ , we wish to optimize the loss  $\mathcal{L}(w, b)$  of a linear SVM classifier:

$$\mathcal{L}(w, b) = \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^n (1 - y_i(w^T x_i + b))_+ \quad (1)$$

where  $(z)_+ = \max(0, z)$  is called the rectifier function and  $C$  is a scalar constant

The optimal weight vector  $w^*$  and the bias  $b^*$  used to build the SVM classifier are defined as follows:

$$w^*, b^* = \operatorname{argmin}_{w, b} \mathcal{L}(w, b) \quad (2)$$

In this problem, we attempt to obtain the optimal parameters  $w^*$  and  $b^*$  by using a standard gradient descent algorithm.

**Hint:** To derive the derivative of  $\mathcal{L}(w, b)$ , please consider two cases:

- (a)  $1 - y_i(w^T x_i + b) \geq 0$ ,
- (b)  $1 - y_i(w^T x_i + b) < 0$

1. Derive the derivative:  $\frac{\partial \mathcal{L}(w, b)}{\partial w}$

$$\frac{\mathcal{L}(w, b)}{\partial w} = w + C \sum_{i=1}^n \begin{cases} 0, & \text{if } y_i(w^T x_i + b) \geq 1 \\ -y_i x_i, & \text{otherwise} \end{cases}$$

2. Derive the derivative:  $\frac{\partial \mathcal{L}(w, b)}{\partial b}$

$$\frac{\mathcal{L}(w, b)}{\partial b} = C \sum_{i=1}^n \begin{cases} 0, & \text{if } y_i(w^T x_i + b) \geq 1 \\ -y_i, & \text{otherwise} \end{cases}$$

## 5 (10 points) SVM: Margin

As shown in the Figure 3, we have the decision boundary (marked as a black line) defined as Eq. 3 given  $w, b$ :

$$w^T x + b = 0 \quad (3)$$

In parallel to the decision boundary, we have the positive plane (marked as a red line) defined as Eq. 4 and the negative plane (marked as a blue line) defined as Eq. 5:

$$w^T x + b = +1 \quad (4)$$

$$w^T x + b = -1 \quad (5)$$

We pick an arbitrary point  $x^-$  on the negative plane, and draw a purple line that passes  $x^-$  and is perpendicular to the negative plane. The intersection between this purple line and the positive plane can be denoted as  $x^+$ . Thus, we have the following Eq. 6 that indicates the relation between  $x^+$  and  $x^-$ :

$$x^+ = x^- + \lambda w \quad (6)$$

where  $\lambda \in \mathbb{R}$  is an undetermined scalar. The margin  $M$  is defined as the distance between the positive and the negative planes, which can be calculated from Eq. 7:

$$M = \|x^+ - x^-\|_2 = \sqrt{\langle \lambda w, \lambda w \rangle} \quad (7)$$

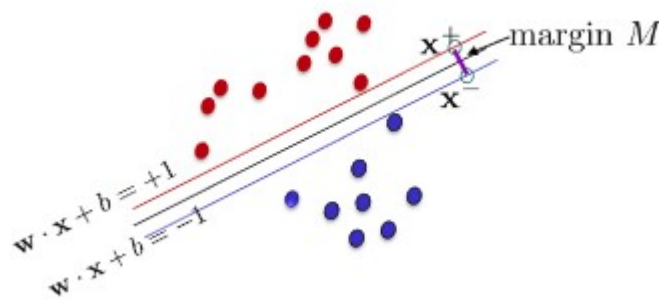


Figure 3: The decision boundary, the positive plane and the negative plane.

Please derive the following according to Eq. 7:

$$M = \frac{2}{\sqrt{\langle w, w \rangle}}$$

**Hint:** You can firstly represent  $\lambda$  in the form of  $w$  by using Eq. 4, 5, 6

$$(4) \Rightarrow x^+ = \frac{1-b}{w}, \quad (5) \Rightarrow x^- = \frac{-b-1}{w}$$

$$(6) \Rightarrow \lambda = \frac{x^+ - x^-}{w}$$

plugging  $x^+$  and  $x^-$  into  $\lambda$

$$\begin{aligned} \Rightarrow \lambda &= \frac{\frac{1-b}{w} - \frac{-b-1}{w}}{w} \\ \Rightarrow \lambda &= \frac{2}{ww} \end{aligned}$$

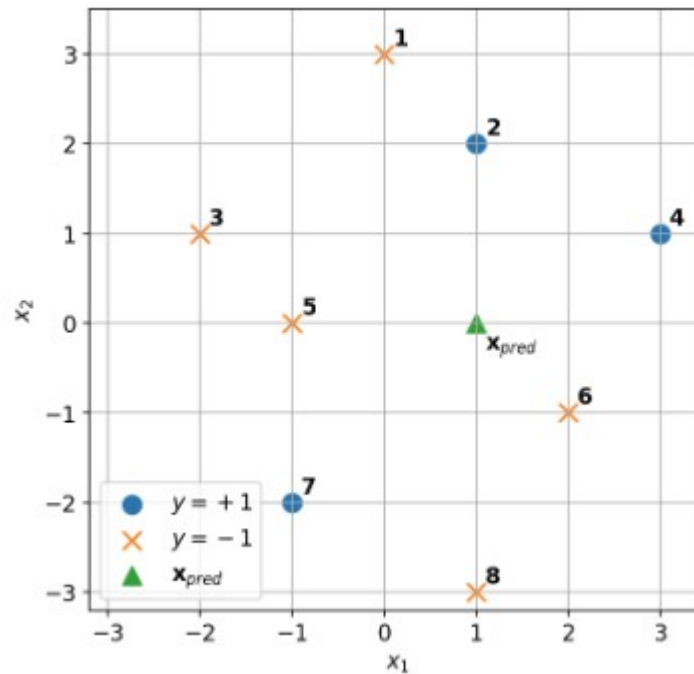
$$M = \sqrt{\langle \lambda w, \lambda w \rangle} \dots (7)$$

plugging  $\lambda$  in (7),

$$\begin{aligned} \Rightarrow M &= \sqrt{\left(\frac{2w}{ww}\right)\left(\frac{2w}{ww}\right)^T} \\ \Rightarrow M &= \sqrt{\frac{4}{w^t w}} \\ \Rightarrow M &= \frac{2}{\sqrt{w^T w}} \\ \Rightarrow M &= \frac{2}{\sqrt{\langle w, w \rangle}} \end{aligned}$$

## 6 (10 points) K Nearest Neighbors

Consider a training dataset  $S_{\text{training}} = \{(x_i, y_i), i = 1, 2, \dots, 9\}$  where each data point  $(x, y)$  has a feature vector  $x = [x_1, x_2]^T$  and the corresponding label  $y \in \{-1, +1\}$ . The points with the corresponding labels in the dataset are shown in the figure below.



In the figure above, the index  $i$  for each training example  $x_i$  is given in **bold** near the point. You are asked to predict the label of a point  $x_{\text{pred}} = [1, 0]^T$  shown in the figure as a triangle using  $k$  nearest neighbors ( $k$ -NN) method under **Euclidean distance**.

1. List the indices of all the data points in  $S_{\text{training}}$  and their corresponding labels.

$$\begin{aligned}
 (x_1, y_1) &\Rightarrow x_1 = [0, 3], y_1 = -1 \\
 (x_2, y_2) &\Rightarrow x_2 = [1, 2], y_2 = +1 \\
 (x_3, y_3) &\Rightarrow x_3 = [-2, 1], y_3 = -1 \\
 (x_4, y_4) &\Rightarrow x_4 = [3, 1], y_4 = +1 \\
 (x_5, y_5) &\Rightarrow x_5 = [-1, 0], y_5 = -1 \\
 (x_6, y_6) &\Rightarrow x_6 = [2, -1], y_6 = -1 \\
 (x_7, y_7) &\Rightarrow x_7 = [-1, -2], y_7 = +1 \\
 (x_8, y_8) &\Rightarrow x_8 = [1, -3], y_8 = -1
 \end{aligned}$$

2. Determine the predicted label for  $x_{\text{pred}}$  using the  $k$ -NN with different  $k$ .



(a)  $k=1 \Rightarrow$  label is - 1

(b)  $k=3 \Rightarrow$  label is - 1

(c)  $k=5 \Rightarrow$  label is + 1

## 7 (20 points) Coding: K Nearest Neighbors

In this problem, you need to implement the  $k$  nearest neighbors (k-NN) algorithm and apply it to the binary classification. Here we use the modified Iris dataset  $S = \{(x_i, y_i)\}$  where each feature vector  $x \in R^2$  and label  $y \in \{-1, +1\}$ . You are not allowed to use `sklearn.neighbors.KNeighborsClassifier()` in your code, but you can use it to validate your implementation.

- Load the modified Iris dataset. The dataset  $S$  is split to three subsets: The training set  $S_{\text{training}}$ , the validation set  $S_{\text{validation}}$  and the test set  $S_{\text{test}}$ . In the code, we use  $X_{\text{train}}$ ,  $Y_{\text{train}}$  for the feature vectors and labels of the training set respectively. Similar notations are also used for the validation and the test sets.
- Implement k-NN algorithm in 3 steps.

1. For each feature vector  $x$  you are predicting a label, you need to calculate the distances between this feature vector  $x$  and all the feature vectors in the training set  $S_{\text{training}}$ .

2. Then sort all distances in ascending order and pick the labels for the  $k$  minimum distances.

3. Count the number of negative labels  $N_{y=-1}$ , and the number of the positive labels  $N_{y=+1}$  from  $k$  labels picked in step 2. Use the following decision rule to predict label  $\hat{y}$  for each feature vector  $x$ :

$$\hat{y} = \begin{cases} +1, & N_{y=-1} < N_{y=+1}, \\ -1, & N_{y=-1} \geq N_{y=+1} \end{cases}$$

Here we assume **Euclidean distance** as the distance metric. For more details, please refer to the code and the corresponding part in the slides.

- Use the validation set to obtain optimal  $k^*$ . In k-NN, there is a hyper-parameter  $k$  which adjusts the number of nearest neighbors. You would need to perform a grid search on the following list of  $k$ :

$$k \in \{1, 2, 3\}$$

For each  $k$ , you need to form a k-NN classifier with the training set  $S_{\text{training}}$ . Then, use the classifier to make predictions on the validation set  $S_{\text{validation}}$  and calculate the error  $e_{\text{validation}}$ . We aim to obtain the best hyper-parameter  $k^*$  corresponding to the minimum validation error  $e_{\text{validation}}^*$  among all  $k$ s.

- Use the obtained classifier corresponding to the best hyper-parameter  $k^*$  to calculate the test error  $e_{\text{test}}$  on test set  $S_{\text{test}}$ .

```
In [1]: %config InlineBackend.figure_format = 'retina'
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets
import scipy
from matplotlib.colors import ListedColormap
from functools import partial
```

## Load the modified Iris dataset

```

In [2]: # Iris dataset.
iris = datasets.load_iris()      # Load Iris dataset.

X = iris.data                    # The shape of X is (150, 4), which means
                                # there are 150 data points, each data
                                # point
                                # has 4 features.

Y = (iris.target > 1.5).reshape(-1,1).astype(np.float) # The shape of Y
is (150, 1), which means
                                # there are 150 data points, each data
                                # point
                                # has 1 target value.
Y[Y==0] = -1                     # Convert labels from {0, 1} to {-1, 1}

X_and_Y = np.hstack((X, Y))     # Stack them together for shuffling.
np.random.seed(1)               # Set the random seed.
np.random.shuffle(X_and_Y)      # Shuffle the data points in X_and_Y array

print(X.shape)
print(Y.shape)
print(X_and_Y[0])              # Should be: [5.8 4. 1.2 0.2 -1. ].

(150, 4)
(150, 1)
[ 5.8  4.  1.2  0.2 -1. ]

```

```

In [3]: # Divide the data points into training set and test set.
X_shuffled = X_and_Y[:, :4]
Y_shuffled = X_and_Y[:, 4]

X_train = X_shuffled[:50][:, [3,1]]      # Shape: (50,2)
Y_train = Y_shuffled[:50]                # Shape: (50,)
X_val    = X_shuffled[50:100][:, [3,1]]  # Shape: (50,2)
Y_val    = Y_shuffled[50:100]            # Shape: (50,)
X_test   = X_shuffled[100:][:, [3,1]]    # Shape: (50,2)
Y_test   = Y_shuffled[100:]              # Shape: (50,)

print(X_train.shape)
print(Y_train.shape)
print(X_val.shape)
print(Y_val.shape)
print(X_test.shape)
print(Y_test.shape)

(50, 2)
(50,)
(50, 2)
(50,)
(50, 2)
(50,)

```

## Visualization

```
In [4]: def vis(X, Y, knn_classifier=None):
        # Visualize k-NN.
        if knn_classifier is not None:
            # Calculate min, max and create grids.
            h = .02
            x0_min, x0_max = X[:, 0].min() - 0.1, X[:, 0].max() + 0.1
            x1_min, x1_max = X[:, 1].min() - 0.1, X[:, 1].max() + 0.1
            x0s, x1s = np.meshgrid(np.arange(x0_min, x0_max, h),
                                   np.arange(x1_min, x1_max, h))
            xs = np.stack([x0s, x1s], axis=-1).reshape(-1, 2)

            # Predict class using kNN classifier and data.
            ys_pred = np.array([knn_classifier(x) for x in xs])
            ys_pred = ys_pred.reshape(x0s.shape)

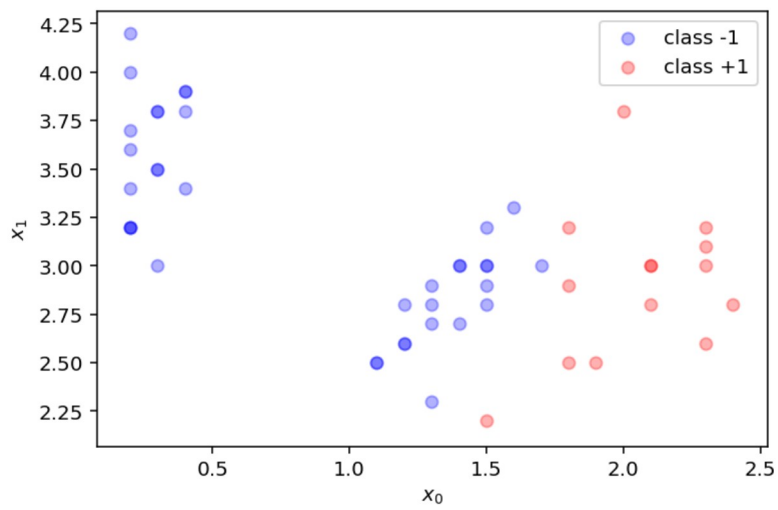
            # Put the result into a color plot.
            # Color map: #00AAFF - blue, #FFAAAA - red, #AAFFAA - green

            cmap_light = ListedColormap(['#00AAFF', '#FFAAAA'])
            plt.pcolormesh(x0s, x1s, ys_pred, cmap=cmap_light, alpha=0.3)

            indices_neg1 = (Y == -1).nonzero()[0]
            indices_pos1 = (Y == 1).nonzero()[0]
            plt.scatter(X[:,0][indices_neg1], X[:,1][indices_neg1],
                        c='blue', label='class -1', alpha=0.3)
            plt.scatter(X[:,0][indices_pos1], X[:,1][indices_pos1],
                        c='red', label='class +1', alpha=0.3)
            plt.legend()
            plt.xlabel('$x_0$')
            plt.ylabel('$x_1$')

            plt.show()
```

```
In [5]: # Visualize training set.  
vis(X_train, Y_train)  
# Note that some points have darker color since there can be  
# multiple points at the same location.
```



## k Nearest Neighbors

```

In [6]: # Euclidean distance.
def calc_distance(x1, x2):
    dist = np.square(x1-x2).sum()
    return np.sqrt(dist)

# k nearest neighbor predictor.
def f_knn(x, X_train, Y_train, k):
    # Create the list of (distance, label) pairs.
    dist_label_pairs = []
    for xi, yi in zip(X_train, Y_train):
        # Calculate the distance.
        dist = calc_distance(xi, x)
        # Add a (distance, label) pair to the list.
        dist_label_pairs.append((dist, yi))

    # Sort the pairs by distance (ascending).
    sorted_dist_label_pairs = sorted(dist_label_pairs, key=lambda x:x
[0])

    # Obtain the first k pairs (corresponding to k smallest distances).
    k_dist_label_pairs = sorted_dist_label_pairs[:k] ##### To
be filled. #####

    # Extract the labels of the k pairs.
    k_labels = np.array(k_dist_label_pairs)[:,-1] ##### To
be filled. #####

    # Count the number of +1 predictions and -1 predictions.
    pos1_in_k_labels = 0
    neg1_in_k_labels = 0
    for label in k_labels:
        if label == +1:
            pos1_in_k_labels += 1
        elif label == -1:
            neg1_in_k_labels += 1

    # Make the prediction based on counts.
    if pos1_in_k_labels > neg1_in_k_labels:
        y_pred = +1
    else:
        y_pred = -1

    return y_pred

# Judge function: 1(a != b). It supports scalar, vector and matrix.
def judge(a, b):
    return np.array(a != b).astype(np.float32)

# Calculate error given feature vectors X and labels Y.
def calc_error(X, Y, knn_classifier):
    e = 0
    n = len(X)
    for (xi, yi) in zip(X, Y):
        e += judge(yi, knn_classifier(xi))
    e = 1.0 * e / n

```

```
return e
```

## Visualize the results

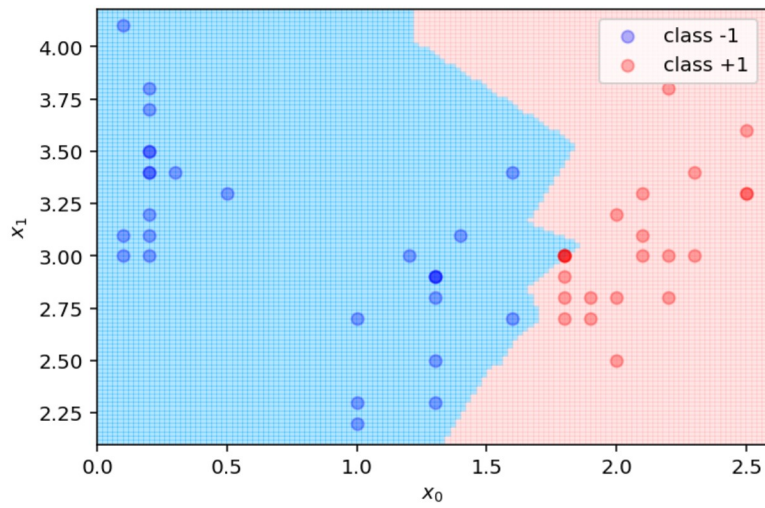
```
In [7]: opt_val_error = 1.0
        opt_k = None

        # Try different k(s).
        for k in [1,2,3]:
            # Visualize
            # 1. Validation set (as points).
            # 2. Decision boundary from training set (as background).
            print("k={}".format(k))
            # Create a k-NN classifier with training set.
            knn_classifier = partial(f_knn, X_train=X_train, Y_train=Y_train, k
=k)

            # Visualization.
            vis(X_val, Y_val, knn_classifier)
            # Calculate validation error.
            val_error = calc_error(X_val, Y_val, knn_classifier)
            print("Validation error: {}".format(val_error))
            if val_error < opt_val_error:
                opt_val_error = val_error
                opt_k = k
                opt_knn_classifier = knn_classifier
```

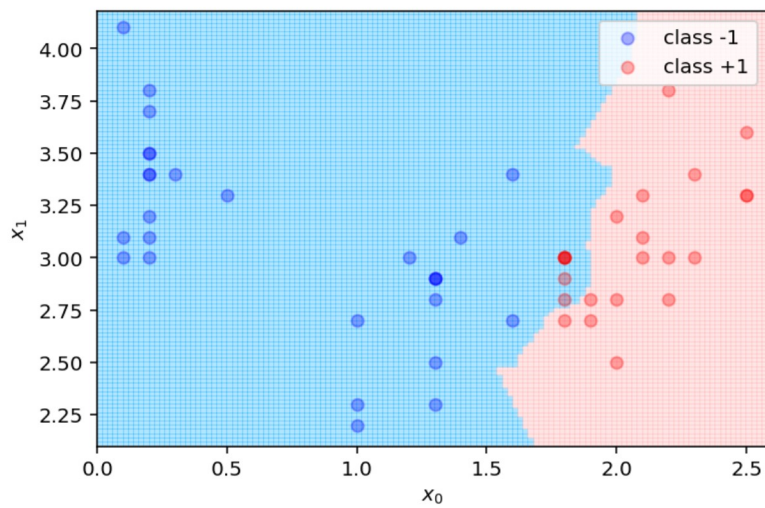


k=1



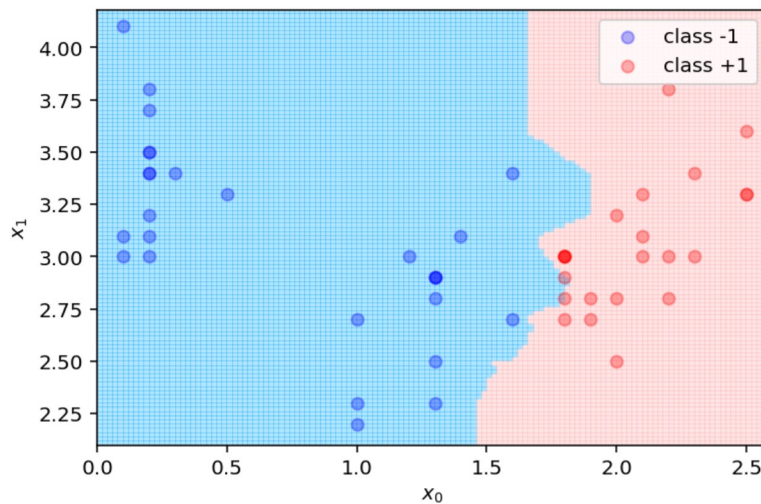
Validation error: 0.08

k=2



Validation error: 0.12

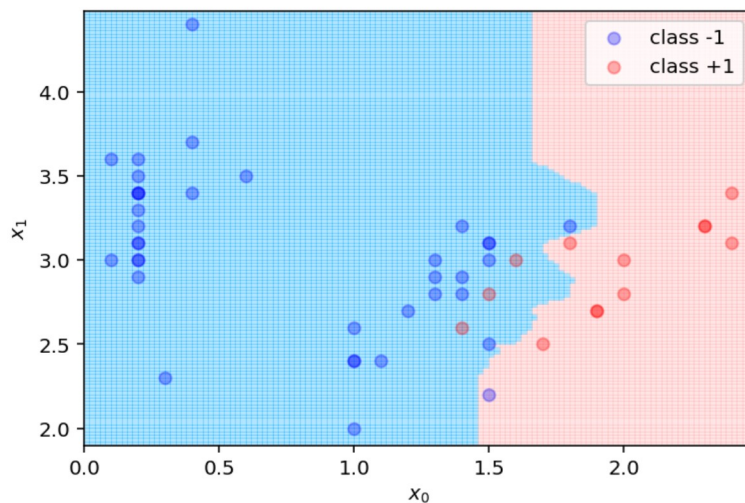
k=3



Validation error: 0.02

```
In [8]: print("Best k={}".format(opt_k))
test_error = calc_error(X_test, Y_test, opt_knn_classifier)
vis(X_test, Y_test, opt_knn_classifier)
print("Test error: {}".format(test_error))
```

Best k=3



Test error: 0.08

## 8 (20 points) Coding: Decision Tree

In this problem, you need to implement the decision tree algorithm and apply it to the binary classification. Here we use the lonosphere dataset  $S = \{(x_i, y_i)\}$  where each feature vector  $x \in \mathbb{R}^{3,4}$  and label  $y \in \{-1, +1\}$ . You are allowed to use the functions from scikit-learn in this question.

- Load the Ionosphere dataset. The dataset  $S$  is split to two subsets: The training set  $S_{\text{training}}$  and the test set  $S_{\text{test}}$ . In the code, we use  $X_{\text{train}}$ ,  $Y_{\text{train}}$  for the feature vectors and labels of the training set respectively. Similar notations are also used for the test set.
- Train the decision tree classifier with the entropy criterion. In the decision tree, there is a hyper-parameter  $D$  which controls the maximum depth. You would need to perform a grid search on the following list of  $D$ :

$$D \in \{1, 2, 3, 4, 5\}$$

For each  $D$ , you need to form a decision tree classifier with the training set  $S_{\text{training}}$ . Specifically, you need to conduct a 10-fold cross-validation on  $S_{\text{training}}$  and calculate the cross-validation error  $\bar{e}$  (i.e. average validation error over the splits in cross-validation). We aim to obtain the best hyper-parameter  $D^*$  corresponding to the minimum cross-validation error  $\bar{e}^*$  among all  $D$ s.

- Use the obtained classifier corresponding to the best hyper-parameter  $D^*$  to calculate the test error  $e_{\text{test}}$  on test set  $S_{\text{test}}$ .

## Decision Tree with Scikit-Learn

```
In [9]: %config InlineBackend.figure_format = 'retina'
import scipy.io as sio
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns
from sklearn import tree
from sklearn import datasets
from sklearn.metrics import accuracy_score
from sklearn.model_selection import GridSearchCV
```

### Load the Ionosphere dataset

```
In [10]: # Ionosphere dataset.
X_and_Y = np.load('ionosphere.npy').astype(np.float32) # Load data from
file.

np.random.seed(1) # Set the random seed.
np.random.shuffle(X_and_Y) # Shuffle the data.
X = X_and_Y[:, 0:-1] # First column to second last column: F
eatures.
Y = X_and_Y[:, -1] # Last column: Labels.
Y[Y==0] = -1 # Convert labels from {0, 1} to {-1,
1}.

print(X.shape) # (351, 34)
print(Y.shape) # (351,)
print(X_and_Y[0])
# The result should be:
# [ 1.          0.        -0.205    0.2875    0.23        0.1        0.2825    0.31
75
# 0.3225    0.35        0.36285 -0.34617  0.0925    0.275    -0.095    0.21
# -0.0875    0.235    -0.34187  0.31408 -0.48        -0.08        0.29908  0.33
176
# -0.58     -0.24        0.3219   -0.28475 -0.47        0.185    -0.27104 -0.31
228
# 0.40445  0.0305    1.         ]

(351, 34)
(351,)
[ 1.          0.        -0.205    0.2875    0.23        0.1        0.2825    0.31
75
0.3225    0.35        0.36285 -0.34617  0.0925    0.275    -0.095    0.21
-0.0875    0.235    -0.34187  0.31408 -0.48        -0.08        0.29908  0.33
176
-0.58     -0.24        0.3219   -0.28475 -0.47        0.185    -0.27104 -0.31
228
0.40445  0.0305    1.         ]
```

```
In [11]: # Divide the data points into training set and test set.
X_shuffled = X
Y_shuffled = Y
X_train = X_shuffled[:200] # Shape: (200, 34)
Y_train = Y_shuffled[:200] # Shape: (200,)
X_test = X_shuffled[200:] # Shape: (151,4)
Y_test = Y_shuffled[200:] # Shape: (151,)

print(X_train.shape)
print(Y_train.shape)
print(X_test.shape)
print(Y_test.shape)

(200, 34)
(200,)
(151, 34)
(151,)
```

## Decision Tree Using Scikit-Learn

```
In [12]: # Perform grid search for best max depth.

# 1. Create a decision tree classifier.
#     Hint: You can use tree.DecisionTreeClassifier()
#           We use "entropy" as the criterion. The random state should be
#           set to 1 for consistent results. Other options are left at default.
estimator = tree.DecisionTreeClassifier(criterion='entropy', random_state=1)

##### To be filled. #####
# 2. Create a grid searcher with cross-validation.
D_list = [1, 2, 3, 4, 5]
param_grid = {'max_depth': D_list}
#     Hint: You can use GridSearchCV()
#           Please set a 10-fold cross-validation.
grid_search = GridSearchCV(estimator, param_grid, cv=10) ##### To be filled. #####
# 3. Use the grid searcher to fit the training set.
#     - This grid searcher will try every max depth in the list.
#     - For each max depth, a cross-validation is applied to the training set,
#       that is, it creates several (training subset, validation subset) pairs.
#     Note: Sometimes the validation subset is called as "test" subset, but it
#           is not the subset of real test set.
#     - For each pair, a decision tree classifier will be trained on the
#       training subset and evaluated on validation subset.
#     - The average validation scores will be kept.
#     Hint: You can simply use .fit() function of the grid searcher.
grid_search.fit(X_train, Y_train) ##### To be filled. #####
```

```
Out[12]: GridSearchCV(cv=10,
                      estimator=DecisionTreeClassifier(criterion='entropy',
                                                         random_state=1),
                      param_grid={'max_depth': [1, 2, 3, 4, 5]})
```

## Visualize the Results

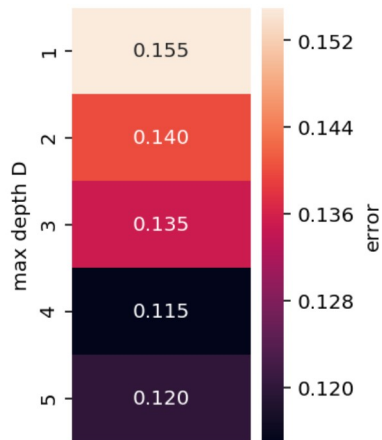
```
In [13]: print(grid_search.cv_results_['mean_test_score'])

[0.845 0.86  0.865 0.885 0.88 ]
```

```
In [14]: # Draw heatmaps for result of grid search.
def draw_heatmap(errors, D_list, title):
    plt.figure(figsize = (2,4))
    ax = sns.heatmap(errors, annot=True, fmt='.3f', yticklabels=D_list,
xticklabels=[])
    ax.collections[0].colorbar.set_label('error')
    ax.set(ylabel='max depth D')
    bottom, top = ax.get_ylim()
    ax.set_ylim(bottom + 0.5, top - 0.5)
    plt.title(title)
    plt.show()

# Draw heatmaps of cross-validation errors (in cross-validation).
# Hint: You can use .cv_results_['mean_test_score'] to obtain
#       cross-validation accuracy (that is, average validation accuracy
over
#       different splits in the cross-validation). You need to convert
it
#       to the error.
#       Note that you need to reshape the results to shape (?, 1), whic
h is
#       needed by draw_heatmap().
cross_val_errors = (1 - grid_search.cv_results_['mean_test_score']).res
hape(5,1)
draw_heatmap(cross_val_errors, D_list, title='cross-validation error w.
r.t D')
```

cross-validation error w.r.t D



```
In [15]: # Show the best max depth.
# Hint: You can use the .best_params_ of the grid searcher
#         to obtain the best parameter(s).
best_max_depth = grid_search.best_params_##### To be filled. #####
#
print("Best max depth D: {}".format(best_max_depth))

# Calculate the test error.
# Hint: You can use .best_estimator_.predict() to make predictions.

#test_error = (((grid_search.best_estimator_.predict(X_test) -Y_test)/
2)**2).sum()/len(Y_test)##### To be filled. #####
test_error = 1 - accuracy_score(y_true=Y_test, y_pred=grid_search.predict(X_test))
print("Test error: {}".format(test_error))
```

Best max depth D: {'max\_depth': 4}

Test error: 0.1258278145695364