Exercise 7 – Evaluation III

Introduction to Machine Learning

Hint: Useful libraries

R

```
# Consider the following libraries for this exercise sheet:

library(ggplot2)
```

Python

```
# Consider the following libraries for this exercise sheet:

import numpy as np
import matplotlib.pyplot as plt
from sklearn import metrics
```

Exercise 1: ROC metrics

Learning goals

1. Create confusion matrices and compute associated evaluation metrics
2. Compute ROC coordinates and AUC
3. Understand relationship between ROC curve & classification threshold

Consider a binary classification algorithm that yielded the following results:

ID	True class	Prediction
1	0	0.33
2	0	0.27
3	0	0.11
4	1	0.38
5	1	0.17
6	1	0.63
7	1	0.62
8	1	0.33
9	0	0.15
10	0	0.57

Create a confusion matrix assuming a threshold of 0.5. Point out which values correspond to true positives (`TP`), true negatives (`TN`), false positives (`FP`), and false negatives (`FN`).

Solution

First, sort the table:

ID	True class	Score	Predicted class
6	1	0.63	1
7	1	0.62	1
10	0	0.57	1
4	1	0.38	0
1	0	0.33	0
8	1	0.33	0
2	0	0.27	0
5	1	0.17	0
9	0	0.15	0
3	0	0.11	0

This translates to:

		Truth	
		1	**0**
Prediction	**1**	2	1
	0	3	4

So we get:

#FN	#FP	#TN	#TP
3	1	4	2

Calculate: PPV, NPV, TPR, FPR, ACC, MCE and $F1$ measure.

Solution

$$\rho_{\text{PPV}} = \frac{\#\text{TP}}{\#\text{TP} + \#\text{FP}} = \frac{2}{3}$$

$$\rho_{\text{NPV}} = \frac{\#\text{TN}}{\#\text{TN} + \#\text{FN}} = \frac{4}{7}$$

$$\rho_{\text{TPR}} = \frac{\#\text{TP}}{\#\text{TP} + \#\text{FN}} = \frac{2}{5}$$

$$\rho_{\text{FPR}} = \frac{\#\text{FP}}{\#\text{TN} + \#\text{FP}} = \frac{1}{5}$$

$$\rho_{\text{ACC}} = \frac{\#\text{TP} + \#\text{TN}}{\#\text{TP} + \#\text{TN} + \#\text{FP} + \#\text{FN}} = \frac{6}{10}$$

$$\rho_{\text{MCE}} = \frac{\#\text{FP} + \#\text{FN}}{\#\text{TP} + \#\text{TN} + \#\text{FP} + \#\text{FN}} = \frac{4}{10}$$

$$\rho_{F1} = \frac{2 \cdot \rho_{\text{PPV}} \cdot \rho_{\text{TPR}}}{\rho_{\text{PPV}} + \rho_{\text{TPR}}} = 0.5$$

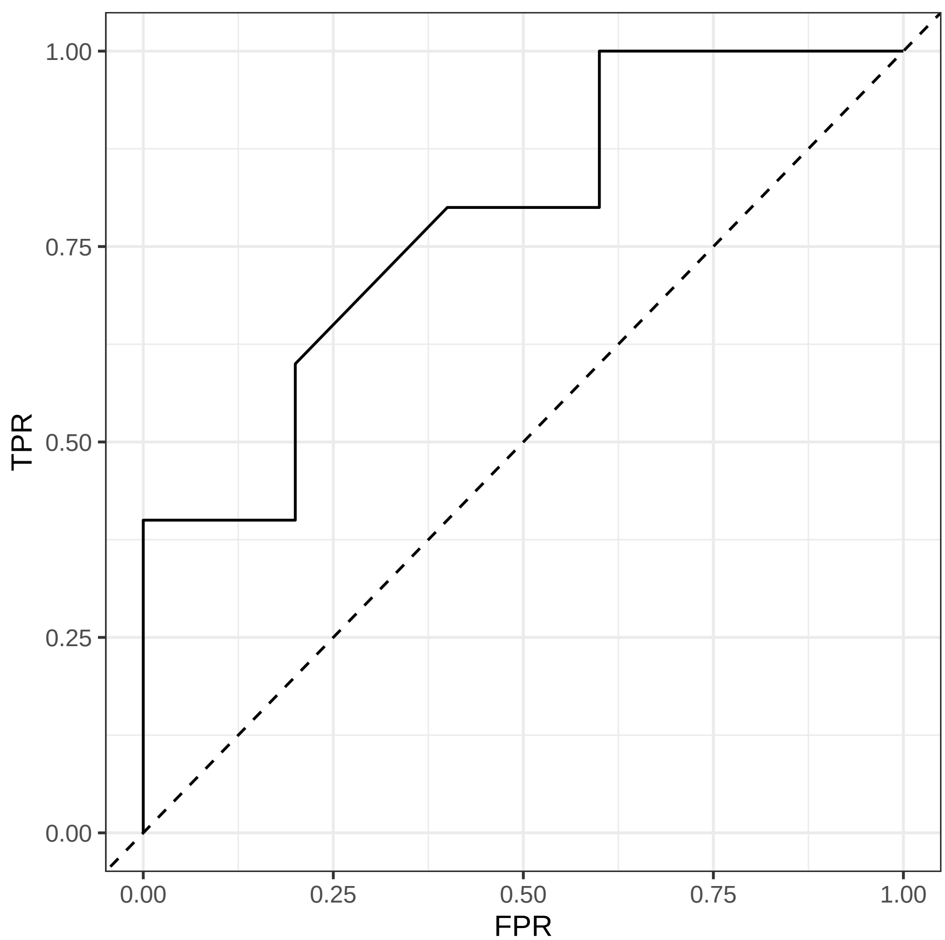
Draw the ROC curve and interpret it.

Solution

We need the table sorted by score (descending). Finding that $\frac{1}{n_+} = \frac{1}{n_-} = 0.2$, we follow the algorithm described in the lecture slides:

1. $c = 1 \implies$ we start in $(0, 0)$ and predict everything as negative, so TPR 0 and FPR 0.

2. $c = 0.625 \implies$ TPR $0 + \frac{1}{n_+} = 0.2$ and FPR 0 (obs 6 correctly classified).
3. $c = 0.6 \implies$ TPR $0.2 + \frac{1}{n_+} = 0.4$ and FPR 0 (obs 7 correctly classified).
4. $c = 0.5 \implies$ TPR 0.4 and FPR $0 + \frac{1}{n_-} = 0.2$ (obs 10 misclassified).
5. $c = 0.35 \implies$ TPR $0.4 + \frac{1}{n_+} = 0.6$ and FPR 0.2 (obs 4 correctly classified).
6. $c = 0.3 \implies$ TPR $0.6 + \frac{1}{n_+} = 0.8$ and FPR $0.2 + \frac{1}{n_-} = 0.4$ (obs 8 correct but obs 1 misclassified).
7. $c = 0.2 \implies$ TPR 0.8 and FPR $0.4 + \frac{1}{n_-} = 0.6$ (obs 2 misclassified).
8. $c = 0.16 \implies$ TPR $0.8 + \frac{1}{n_+} = 1$ and FPR 0.6 (obs 5 correctly classified).
9. $c = 0.14 \implies$ TPR 1 and FPR $0.6 + \frac{1}{n_-} = 0.8$ (obs 9 misclassified)
10. $c = 0.09 \implies$ TPR 1 and FPR 1 (obs 3 misclassified).



We see that the resulting ROC curve is distinct from the diagonal marking a purely random classifier, but also not too great. The step function character is clearly visible for so few observations (the non-axis-parallel part in the middle is due to the fact that we have two observations with the same score but different true class, so both TPR and FPR go up when we move from $c = 0.35$ to $c = 0.3$).

Calculate the AUC.

Solution

We can compute the AUC by adding rectangular and triangular areas, s.t.

$$\rho_{\text{AUC}} = 0.2 \cdot 0.4 + 0.2 \cdot 0.6 + \tfrac{1}{2} \cdot 0.2 \cdot 0.2 + 0.2 \cdot 0.8 + 0.4 \cdot 1 = 0.78.$$

How would the ROC curve change if you had chosen a different threshold in a)?

Solution

Not at all, because the ROC curve is drawn by iterating through *all* thresholds, and the corresponding AUC does not depend on a particular choice of c.

Exercise 2: k-NN

> Learning goals
>
> 1. Perform k-NN by visual means
> 2. Perform k-NN with pen and paper, possibly using weighted distances

Let the two-dimensional feature vectors in the following figure be instances of two different classes (triangles and circles). Classify the point (7, 6) – represented by a square in the picture – with a k-NN classifier using $L1$ norm (Manhattan distance):

$$d_{\text{Manhattan}}(\mathbf{x}, \tilde{\mathbf{x}}) = \sum_{j=1}^{p} |x_j - \tilde{x}_j|.$$

As a decision rule, use the unweighted number of the individual classes in the k-neighborhood, i.e., assign the point to the class that represents most neighbors.

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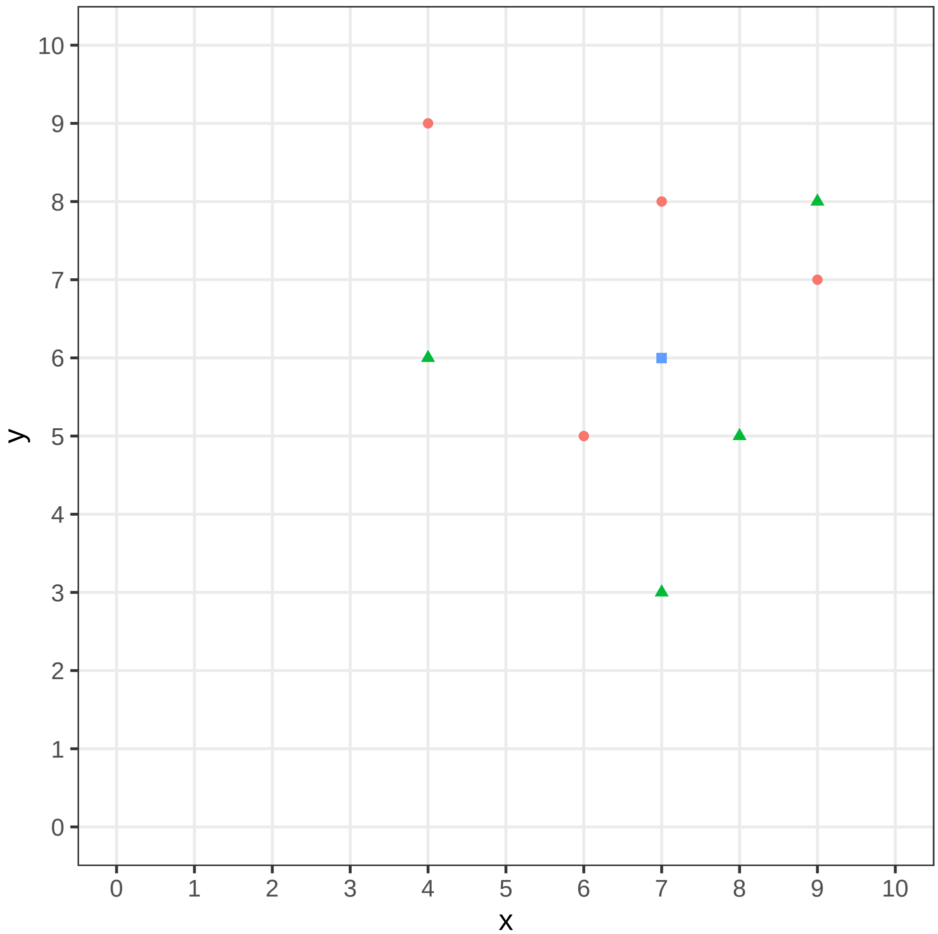
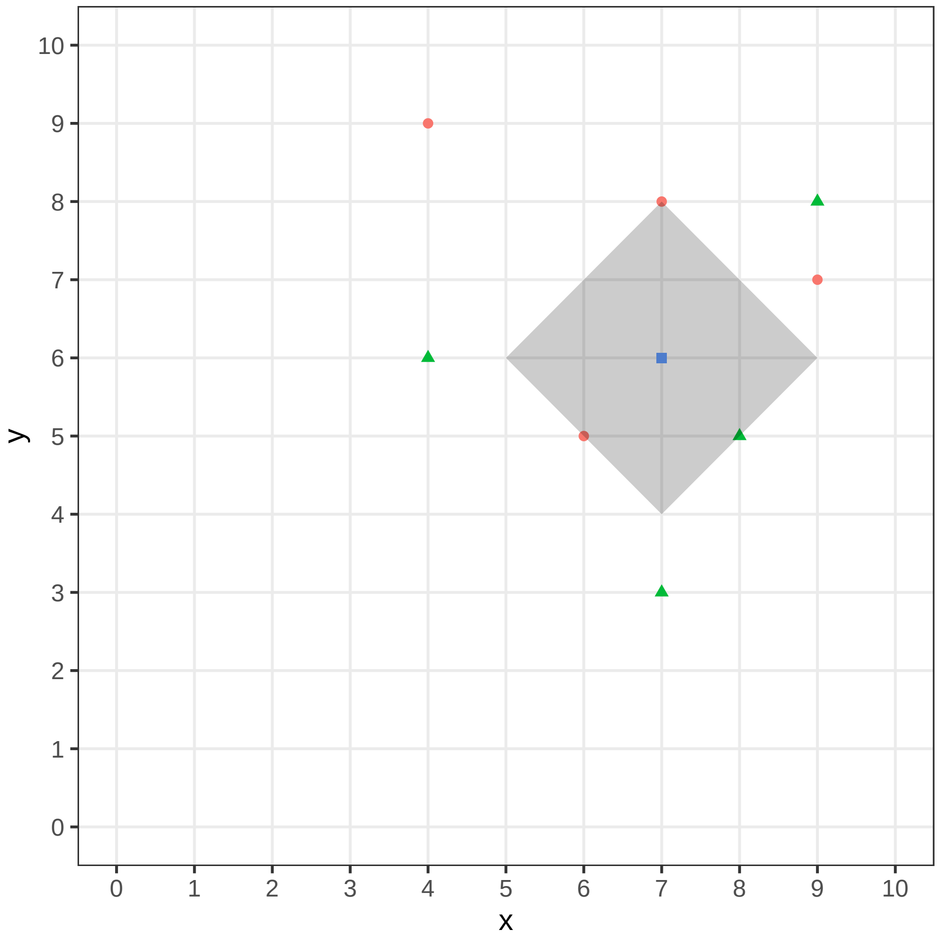
i. $k = 3$



10
9
8
7
6
5
4
3
2
1
0
y
0 1 2 3 4 5 6 7 8 9 10
x



10
9
8
7
6
5
4
3
2
1
0
y
0 1 2 3 4 5 6 7 8 9 10
x

Solution

$\Longrightarrow$ 2 circles and 1 triangle, so we predict "circle":

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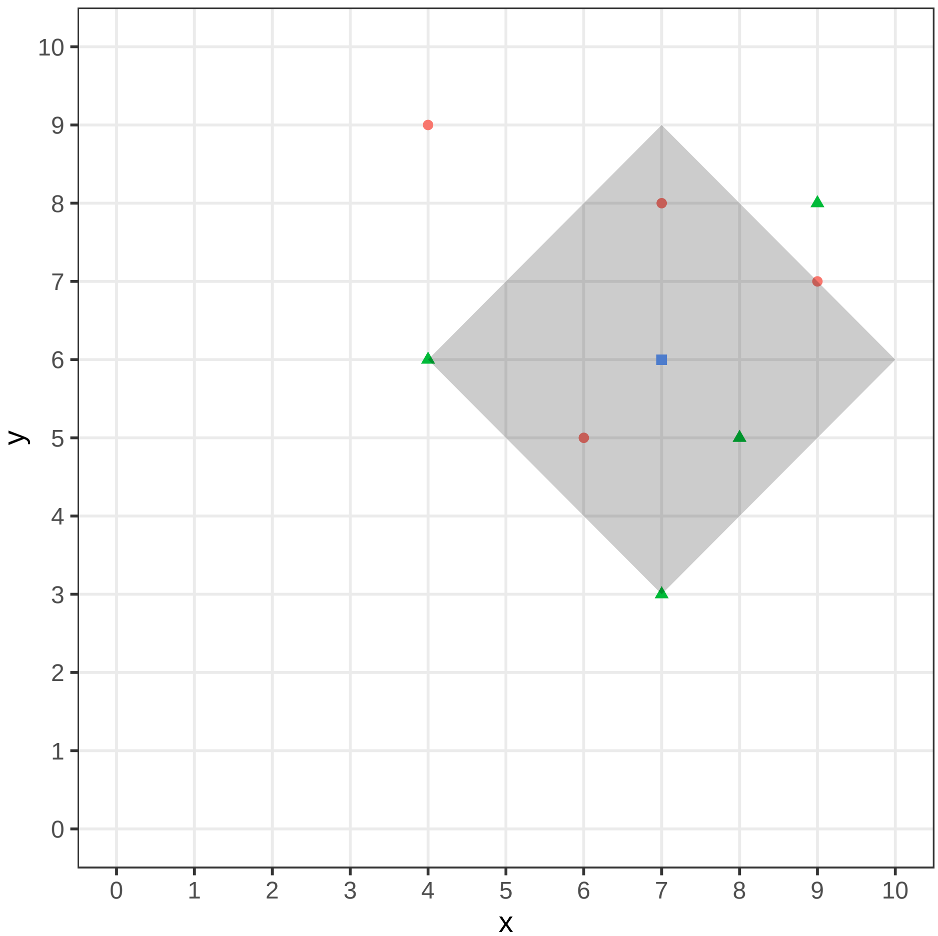
ii. $k = 5$

Solution



$\Longrightarrow$ 3 circles and 3 triangles, we have to specify beforehand what to do in case of a tie.

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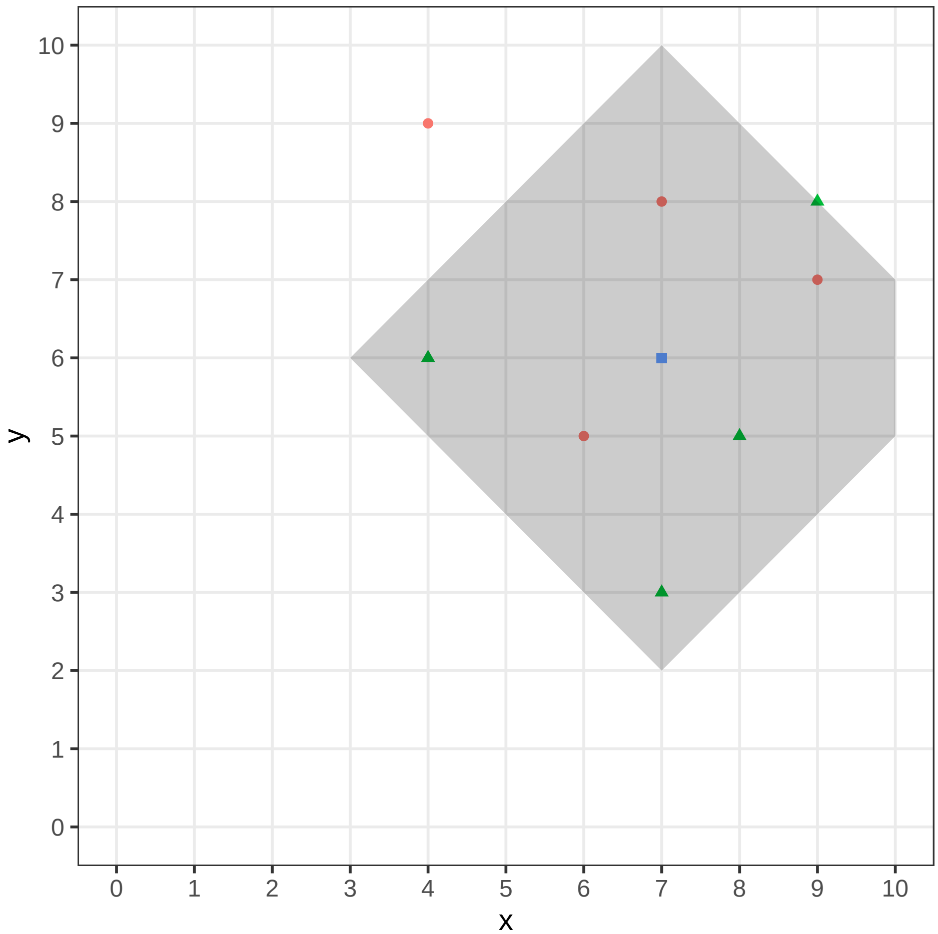
iii. $k = 7$



10
9
8
7
6
5
4
3
2
1
0
y
0
1
2
3
4
5
6
7
8
9
10
x

Solution

$\Longrightarrow$ 3 circles and 4 triangles, so we predict "triangle".

Now consider the same constellation but assume a regression problem this time, where the circle-shaped points have a target value of 2 and the triangles have a value of 4.

Again, predict for the square point (7, 9), using both the *unweighted* and the *weighted* mean in the neighborhood (still with Manhattan distance).

Hint

We now consider both *unweighted* and *weighted* predictions. Recall that weights are computed based on the distance between the point of interest and its respective neighbors. With the Manhattan, or "city block" metric, the distance can be read from the plot by walking along the grid lines (shortest way). For example, in the 3-neighborhood, all points have a distance of 2 from our square, so all get weights $\frac{1}{2}$.

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i. $k = 3$

Solution

$$\hat{y} = \frac{2 + 2 + 4}{3} = \frac{8}{3} \approx 2.67$$

$$\hat{y}_{\text{weighted}} = \frac{\frac{1}{2} \cdot 2 + \frac{1}{2} \cdot 2 + \frac{1}{2} \cdot 4}{\frac{3}{2}} = \frac{8}{3} \approx 2.67$$

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ii. $k = 5$

Solution

$$\hat{y} = \frac{3 \cdot 2 + 3 \cdot 4}{6} = 3$$

$$\hat{y}_{\text{weighted}} = \frac{\frac{1}{2} \cdot 2 + \frac{1}{2} \cdot 2 + \frac{1}{3} \cdot 2 + \frac{1}{2} \cdot 4 + \frac{1}{3} \cdot 4 + \frac{1}{3} \cdot 4}{\frac{5}{2}} = \frac{44}{15} \approx 2.93$$

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iii. $k = 7$

Solution

$$\hat{y} = \frac{3 \cdot 2 + 4 \cdot 4}{7} = \frac{22}{7} \approx 3.14$$

$$\hat{y}_{\text{weighted}} = \frac{\frac{1}{2} \cdot 2 + \frac{1}{2} \cdot 2 + \frac{1}{3} \cdot 2 + \frac{1}{2} \cdot 4 + \frac{1}{3} \cdot 4 + \frac{1}{3} \cdot 4 + \frac{1}{4} \cdot 4}{\frac{11}{4}} = \frac{100}{33} \approx 3.03$$