Classification

SLM003 06/08/2018

References:

`ISL04` James G., Witten D., Hastie T., Tibshirani R. (2013) **Classification**. In: *An Introduction to Statistical Learning*. Springer Texts in Statistics, vol 103. Springer, New York, NY. doi: https://doi.org/10.1007/978-1-4614-7138-7_4 (https://doi.org/10.1007/978-1-4614-7138-7_4)

`ESL04` Hastie T., Tibshirani R., Friedman J. (2009) **Linear Methods for Classification**. In: *The Elements of Statistical Learning* (2nd ed.). Springer Series in Statistics. Springer, New York, NY. doi: https://doi.org/10.1007/978-0-387-84858-7_4 (https://doi.org/10.1007/978-0-387-84858-7_4)

Outline

1. Chapter summary
    A. Logistic regression
    B. Discriminant analysis
        a. Linear discriminant analysis (LDA)
        b. Quadratic discriminant analysis (QDA)
2. Discussion (exercises, implementation, applications)
3. sklearn basics (classification)

Objectives

- Understand the principles behind the methods
- Develop intuition of the mathematical formulation

Terminology cheat sheet

- **Supervised learning**: learn input(s)-output relationship by example (supervision)
- Classification predicts _**qualitative**_ (a.k.a. _categorical_, _discrete_) outputs
    - May be supervised or unsupervised
- Input: ***predictors*** (a.k.a. *features*, *independent variables*, X)
    - May be quantitative and/or qualitative
- Output: ***response*** (a.k.a. *target*, *dependent variable*, y)
    - Different *response levels*, *targets*, ***classes***, *categories*

Logistic regression

Goal: Describe predictor-response relationship using a **logistic model**. Predict by thesholding probability.

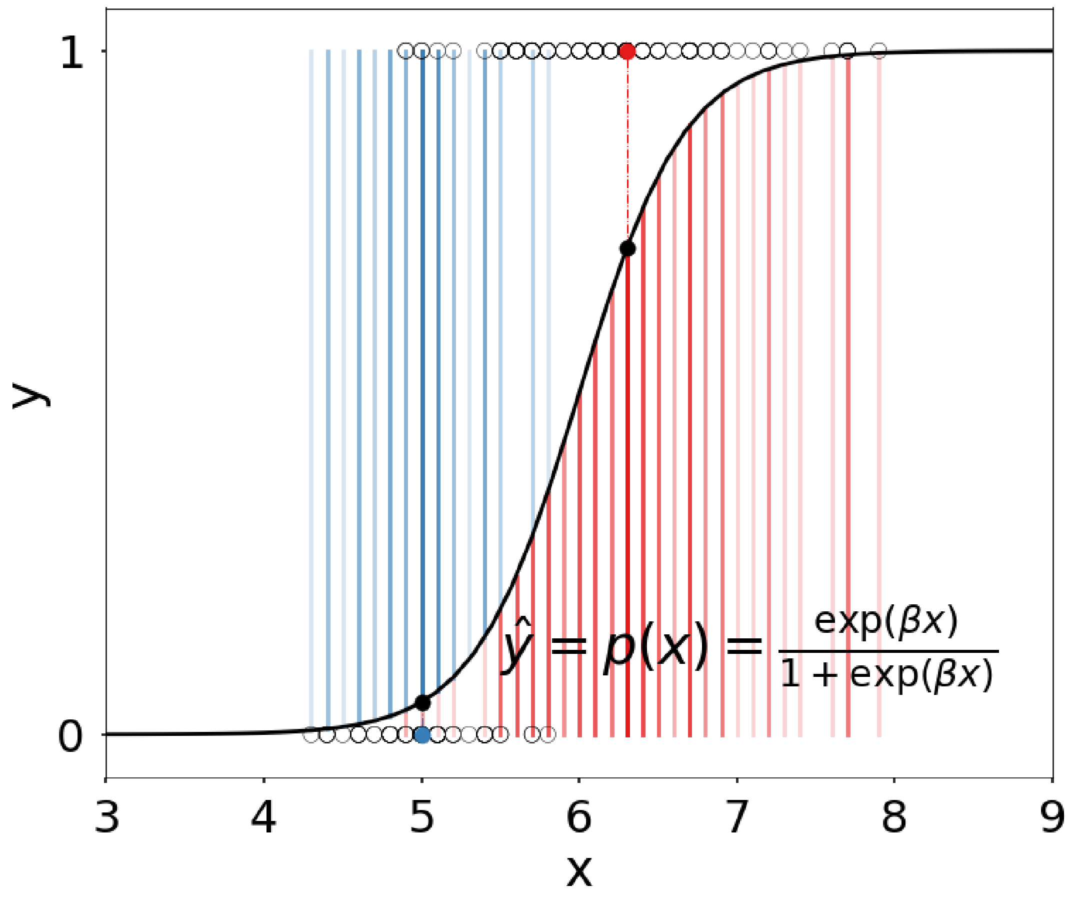
The *logistic function* (a.k.a. *sigmoid curve*) is defined as:

$$p(X) = \frac{\exp(\beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p)}{1 + \exp(\beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p)} \tag{4.6}$$

$p(X)$: probability of positive response (binary) | X_i: predictors | β_i: parameters of the model

How to fit the model? i.e. How to determine the appropriate β_i to describe our training data?

Fitting a logistic model using "maximum likelihood" ($k = 2$)



For a single training data point:

if $y_i = 1$, model plausibility at $x_i = p(x_i)$

if $y_i = 0$, model plausibility at $x_i = 1 - p(x_i)$

n.b. the closer $p(x_i)$ is to 0, i.e. y_i, the better

For all training data,
Model plausibility, i.e. "Likelikhood":

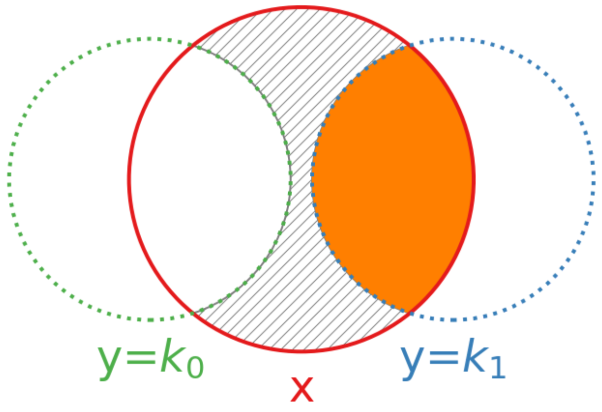
$$\mathrm{l} = \prod_{i:y_i=1} p(x_i) \prod_{i\prime:y_{i\prime}=0} (1 - p(x_{i\prime}))$$

Model is best-fitted when β maximises l.

Discriminant analysis

Goal: Describe **distribution statistics** (based on *training data* and/or prior knowledge about the population). Assign data to the most probable class.

Bayes' Theorem



$$P(x) \cdot P(y=k_1|x) = P(y=k_1) \cdot P(x|y=k_1)$$

$$P(y=k_1|x) = \frac{P(y=k_1) \cdot P(x|y=k_1)}{P(y=k_0) \cdot P(x|y=k_0) + P(y=k_1) \cdot P(x|y=k_1)}$$

$$\underbrace{P(y=k_i|x)}_{\text{posterior probability}} = \frac{\overbrace{P(y=k_i)} \cdot \overbrace{P(x|y=k_i)}}{\sum_{l=0}^{K} \underbrace{P(y=k_l)}_{\text{class prior}} \cdot \underbrace{P(x|y=k_l)}_{\text{class density } f(x)}}$$

Classification using discriminant analysis

To predict which class, actually no need to calculate the posterior $P(y = k_i|x)$, as long as we know which class k_i has the highest posterior

Thus, based on assumptions about the density function $P(x|y = k_l)$, we can define a *discriminant function* $\delta(x)$, such that:

$$\underset{k}{\operatorname{argmax}}\, \delta_k(x) = \underset{k}{\operatorname{argmax}}\, P(y = k|x)$$

Assume *Gaussian* (a.k.a. *normal*) density function,

- With **common** *predictor covariance* Σ shared by all classes, we can derive a *linear* discriminant (LDA):
$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \tfrac{1}{2} {\mu_k}^T \Sigma^{-1} \mu_k + \log \pi_k \tag{4.19}$$
- With **class-specific** *predictor covariance* Σ_k, we get a *quadratic* discriminant (QDA):
$$\delta_k(x) = -\tfrac{1}{2} x^T \Sigma_k^{-1} x + x^T \Sigma_k^{-1} \mu_k - \tfrac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k - \tfrac{1}{2} \log |\Sigma_k| \tag{4.23}$$

Errors are not born equal: Thresholding binary classification

As discussed so far, we threshold $\hat{p}(X)$ at 0.5, without distinguishing between different types of errors.

	Pos	Neg
Predict pos	True pos	False pos (Type I error)
Predict neg	False neg (Type II error)	True neg

$$\text{Sensitivity, Recall} = \frac{\text{True pos}}{\text{Pos}}$$

$$\text{Specificity} = 1 - \frac{\text{False pos}}{\text{Neg}} = \frac{\text{True neg}}{\text{Neg}}$$

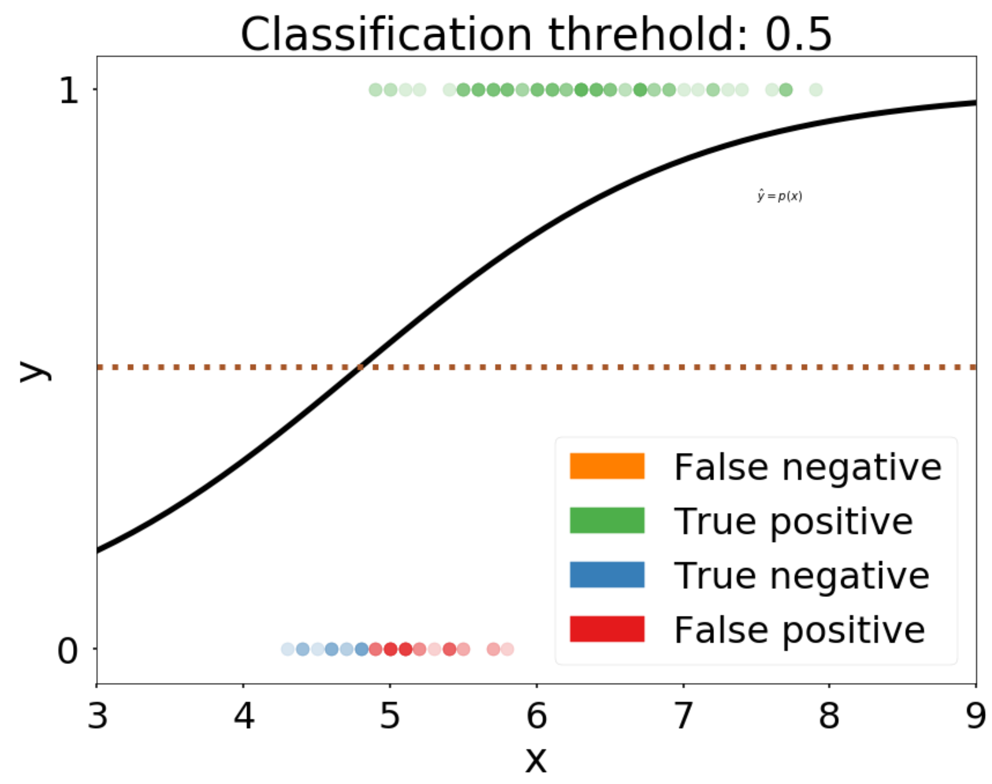
$$\text{Precision} = \frac{\text{True pos}}{\text{Predict pos}}$$

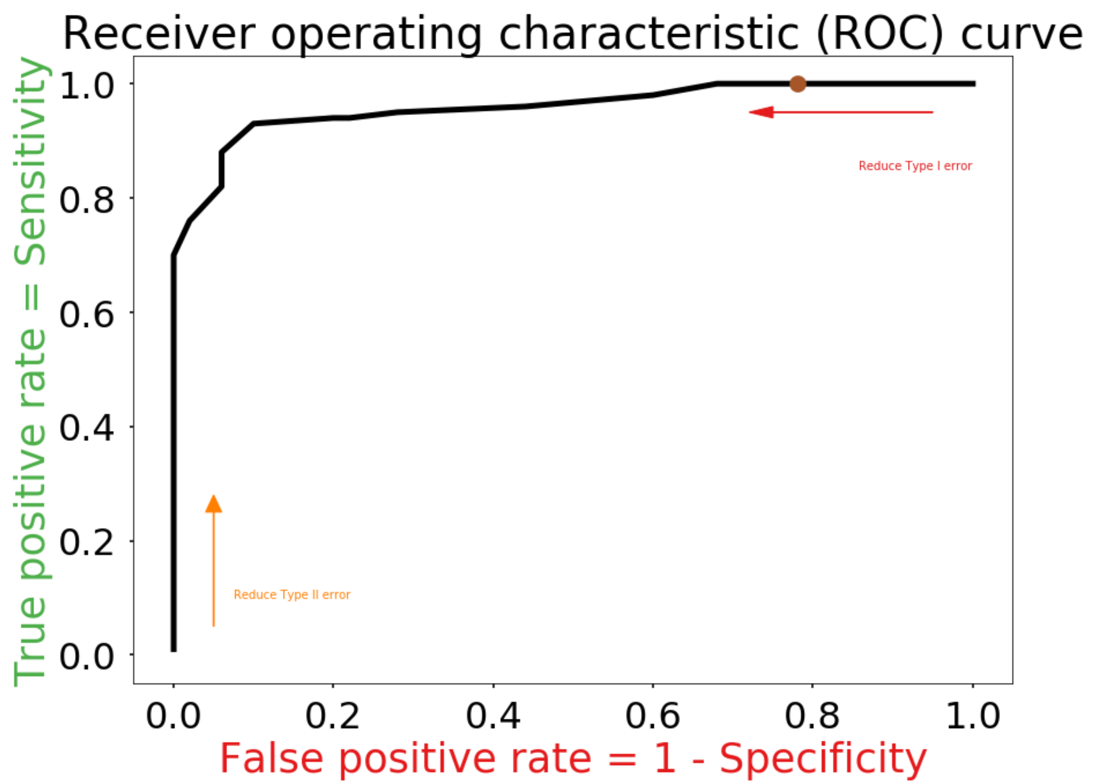
$$\text{Accuracy} = \frac{\text{True}}{\text{Total}}$$

Further reading: Wikipedia:Confusion_matrix (https://en.wikipedia.org/wiki/Confusion_matrix)

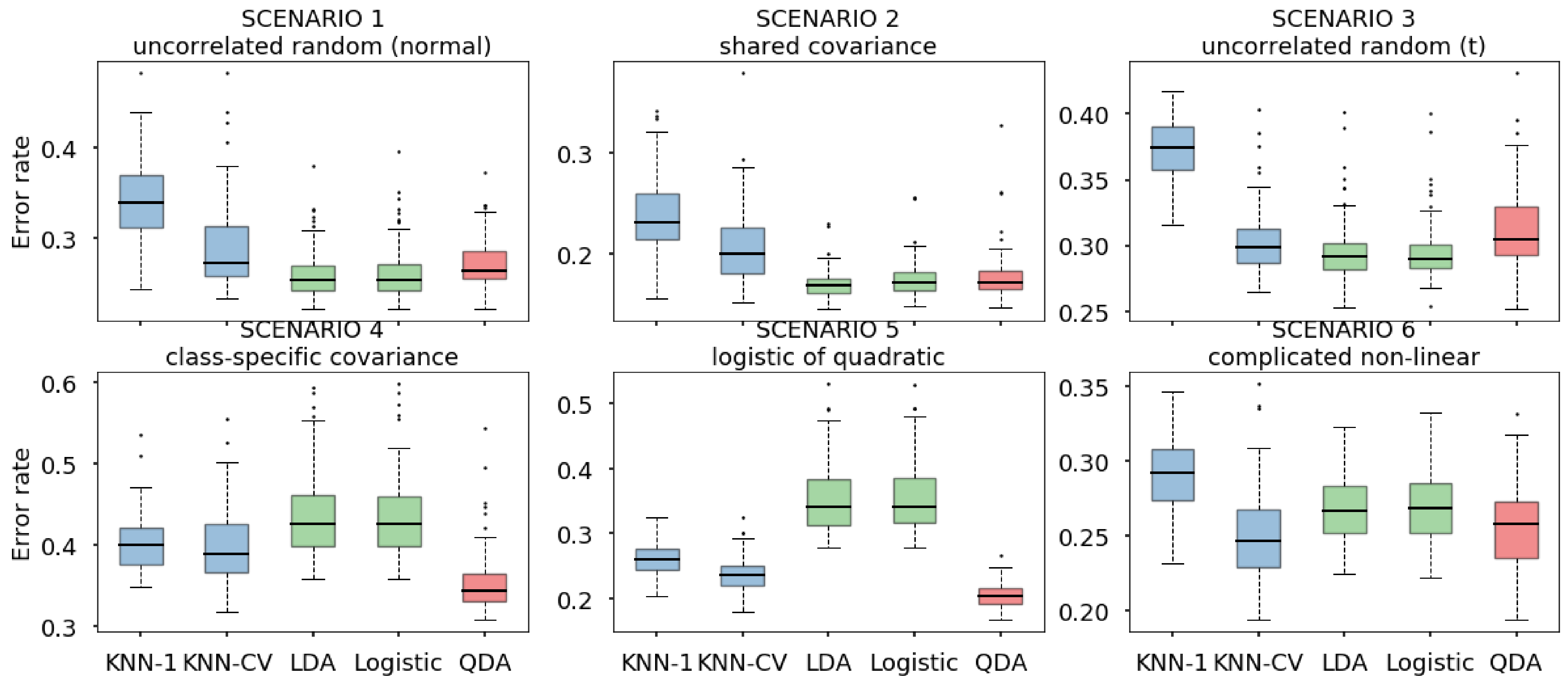
Choosing classification threshold based on the ROC curve

In [5]:
```
interactive(fig_threshold, page=(0,len(thresh_list)-1))
```





Comparison between different classifiers (reproducing Fig 4.10, 4.11)



Summary

- Linear decision boundary:
    - Logistic Regression: model each binary decision using a logistic form of *linear* regression, predict the binary response probability
    - LDA: model predictor distributions of each class as *Gaussian*, then based on Bayes' Theorem, that select response that is most probable
        - More stable than logistic regression when classes are well-separated
        - If Guassian, more stable than logistic regression even with small sample size
- Non-linear decision boundary:
    - QDA: same as LDA, but allow each class to have *different predictor covariances*
        - More suitable for fitting non-linear decision boundary, but risk overfitting if true boundary is linear

Discussion

scikit-Learn basics

Load example dataset

```
In [11]: from sklearn import datasets

         X, y = datasets.load_iris(return_X_y=True)

         X.shape, y.shape
```

```
Out[11]: ((150, 4), (150,))
```

sklearn estimator classes

- Regressor: `neighbors.KNeighborsRegressor`, `linear_model.LinearRegression`
- Classifier: `neighbors.KNeighborsClassifier`, `linear_model.LogisticRegression`
- Clusterer: `cluster.KMeans`, `cluster.AgglomerativeClustering`
- Transformer: `decomposition.PCA`, `manifold.TSNE`
- etc.

General usage

In [12]:
```
# 0. Import estimator constructor class
from sklearn.neighbors import KNeighborsClassifier

# 1. Initialise an estimator instance
estimator = KNeighborsClassifier()

# 3. Initalise an estimator instance with specific parameters
# Note that estimator instance has been overwritten
estimator = KNeighborsClassifier(n_neighbors=2)  # Jupyter: Shift + Tab inside brackets for docstrings; supports tab-c
ompletion

# 4. Modify parameters of existing estimator instance
estimator.set_params(n_neighbors=4)

# 5. Jupyter: tab-completion is your friend
# estimator.

# 2. Fitting (Jupyter: toggle comment with Ctrl + /)
estimator.fit(X, y)  # Also display estimator parmeters by default
```

Out[12]:
```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
           metric_params=None, n_jobs=1, n_neighbors=4, p=2,
           weights='uniform')
```

Classifier-specific usage

In [13]:
```
from sklearn.linear_model import LogisticRegression
logreg = LogisticRegression()
```

In [14]:
```
from sklearn.model_selection import train_test_split

# 1. Split data into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=30)

# 2. Fit with training data
logreg.fit(X_train, y_train)

# 3. Classify test data
logreg.predict(X_test)

# 4. Predict probability p_k(x=x_i), useful for thresholding/weighting
logreg.predict_proba(X_test).shape
np.argmax(logreg.predict_proba(X_test), axis=1) == logreg.predict(X_test)
np.argmax(logreg.predict_proba(X_test)*[1,2,1], axis=1) == logreg.predict(X_test)

# 5. Test accuracy
logreg.predict(X_test) == y_test
logreg.score(X_test, y_test)
```

Out[14]:
```
0.9666666666666667
```

Classifier attributes (model paramenters)

```
In [15]: # Store attributes are indicated by a trailing underscore
         print(logreg.classes_, '\n\n', logreg.coef_, '\n\n', logreg.intercept_)

         # Attributes are updated upon re-training
         X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=30)
         logreg.fit(X_train, y_train)
         print('\n\n', logreg.coef_, '\n\n', logreg.intercept_)
```

```
[0 1 2]

 [[ 0.42246987  1.35051861 -2.14480559 -0.95452713]
 [ 0.33231761 -1.37640461  0.43295424 -0.99460386]
 [-1.56735495 -1.41692793  2.2974056   2.26647004]]

 [ 0.25969649  0.85941538 -1.01267347]


 [[ 0.39709677  1.3914835  -2.17758643 -0.97797652]
 [ 0.58191457 -1.76581288  0.5512131  -1.36892025]
 [-1.52492997 -1.52941477  2.30289617  2.30936333]]

 [ 0.24666901  0.80446332 -1.114254  ]
```

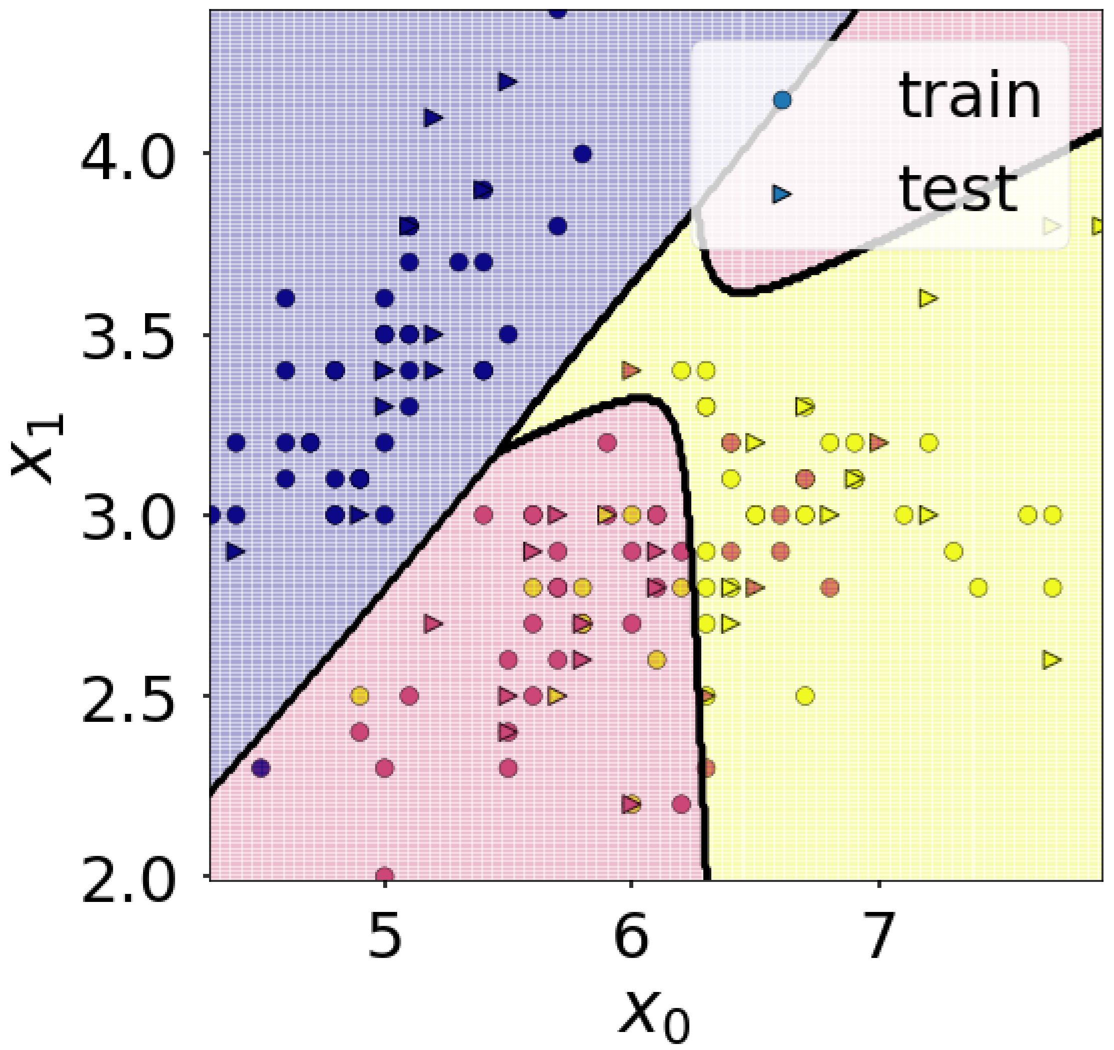
Plotting decision boundary of a trained classifier

```
In [16]: from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis

         qda = QuadraticDiscriminantAnalysis(store_covariance=True)
         X_train, X_test, y_train, y_test = train_test_split(X[:,:2], y, test_size=0.25)  # Limit to p=2
         qda.fit(X_train, y_train)
```

```
Out[16]: QuadraticDiscriminantAnalysis(priors=None, reg_param=0.0,
                        store_covariance=True, store_covariances=None, tol=0.0001)
```

In [17]:

```
%%capture stdout
import matplotlib.pyplot as plt
from util import make_mesh
fig, ax = plt.subplots(figsize=(8,8))

# 1. Plot train and test data with different markers
ax.scatter(X_train[:,0], X_train[:,1], c=y_train, \
           s=80, cmap='plasma', edgecolors='k', label='train')
ax.scatter(X_test[:,0], X_test[:,1], c=y_test, \
           s=80, cmap='plasma', edgecolors='k', marker='>', \
           lw=1, label='test')
ax.legend()
ax.set_xlabel('$x_0$')
ax.set_ylabel('$x_1$')

# 2. Make a grid of points
x_mesh, (X0, X1) = make_mesh(X, step_size=0.01)
print(x_mesh.shape, x_mesh[0, 0, :])

# 3. Evaluate response class at each grid point
grid_eval = qda.predict(x_mesh.reshape(-1,2)).reshape(\
                    x_mesh.shape[:2])
ax.pcolormesh(X0, X1, grid_eval, cmap='plasma', alpha=0.1)
ax.set_xlim(X0.min(), X0.max())
ax.set_ylim(X1.min(), X1.max())

# 4. Plot decision boundary
ax.contour(X0, X1, grid_eval, vmin=0, vmax=0.5, cmap="Greys")

plt.show()
```



train
test
4.0
3.5
3.0
2.5
2.0
x_1
5
6
7
x_0