5. Supervised Learning

KNN
SVM
Linear SVM
Non-linear SVM

KNN

Algorithm & Variants
Best K

KNN Algorithm & Variants

- For both classification and regression
 - A useful technique is to assign weights based on the neighbours.
 - The nearer neighbors contribute more to the average than the more distant ones.

Test data point

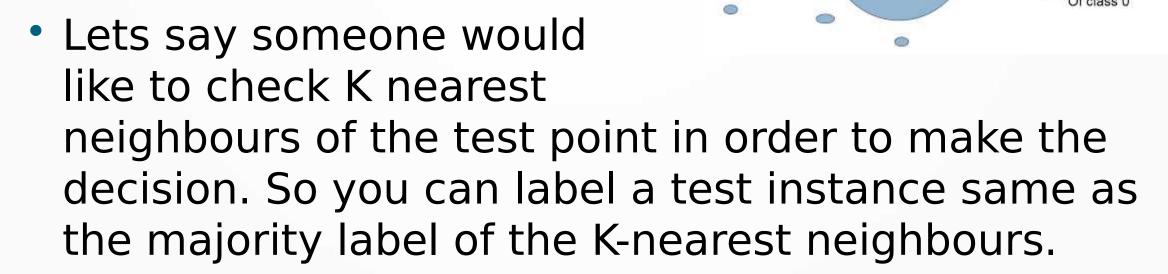
Fraining data point

raining data point

- The basic idea is to label the test data point is the same as the nearest neighbor.
- If a black circle as a test point falls into a region in which the closest point is a black ellipse with class label of 1, based on the nearest neighbor, we are going to label this new sample as class 1.

KNN Algorithm & Variants...

But also K in KNN can vary.



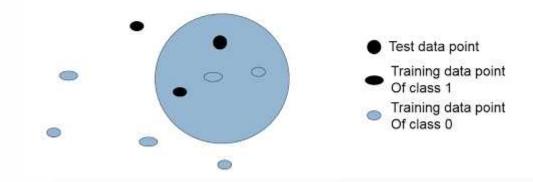
Test data point

Training data point

raining data point

The figure is an example a of 3—NN classification.

KNN Algorithm & Variants...



- As you saw in the figure, a new test point falls into the scope of two training points from class 0 and one from class 1.
- Obviously you trust the 0 class due to majority.

- How do you pick the variable K which holds the number of neighbours?
- How important is selecting the right K?
- You can think of K as controlling the shape of the decision boundary we talked about earlier.
- For small values of K, we are restraining the region of a given prediction and forcing our classifier to be more focused on the close regions and neighbours.
- We are asking the classifier not to care about fairly distant points.
- This will result in a low bias and high variance (why?)

- Higher values of K will have smoother decision boundaries which means lower variance but increased bias.
- So basically, higher values of K means asking for more and more information even from distant training points.
- Like most of machine learning problems, finding hyperparameters such as K is not really straightforward.

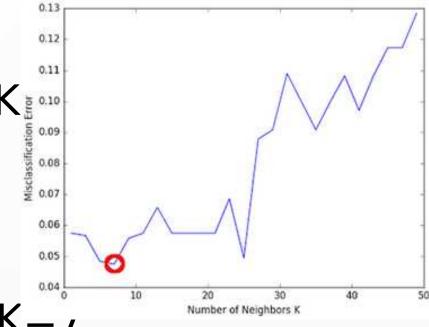
- Finding the best answer is not always possible.
- But as a simple and handy method, you can use Crossvalidation (see week 2 of course 3, Model Selection) to partition your data into test and training samples and evaluate your model with different ranges of K values.
- For example you can consider the number of neighbours to be $K=1,..,K_{max}$
- Now perform the Cross-validation for every possible number of K and evaluate the model based on the training and test data you have partitioned.

- You can use the misclassification error as a measurement of performance in your models.
- Finally, by exploring different values of K and their corresponding misclassification error, we can decide which K has the best performance based on our partitioned data.
- You can define K_{max} based on your training data points.
- There is no rule of thumb in selecting K_{max} since it depends on your desired rate of exploration for K

 For example when you are dealing with 1000 training data points, you may want to define K=1,...,50

• This figure illustrates a sample plot of Number of Neighbours (Kg on and misclassification error.

• As you can see the minimum value of the error occurs when K = 7.



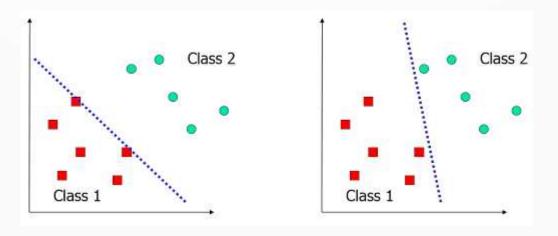
Support Vector Machine (SVM)

Support Vector Machine (SVM)

- SVMs can represent non-linear functions and they have an efficient training algorithm.
- With sufficiently large training data, SVMs can achieve high classification accuracy.
- For example, ≈99% accuracy for handwritten digits recognition.

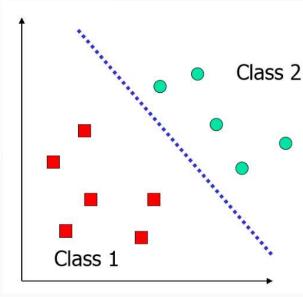
Support Vector Machine (SVM) Revisiting linear binary classification...

- Consider the following figure as an illustration of boundary in a two class binary classification problem.
- Many decision boundaries can separate these two classes as you can see in the figure.
- Which one should we choose?

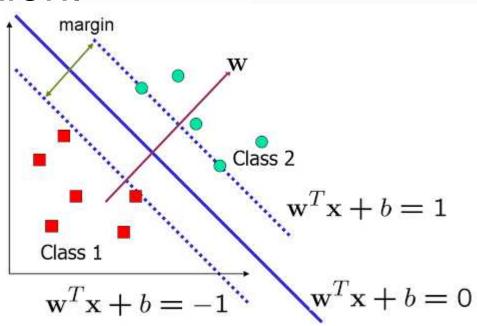


Support Vector Machine (SVM) Revisiting linear binary classification...

- In SVM, given the labelled data, we do not choose this line randomly.
- We aim for maximizing the margin for this boundary line.
- Consider the figure as another example.
- Can you see the difference now?
- The proposed line looks to be in the middle of the data points with different classes.
- That will lead us to the next topic about margins in SVM.

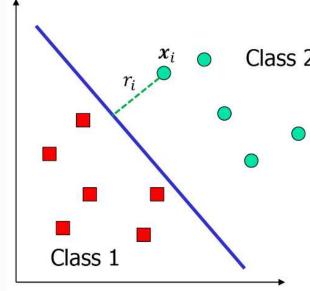


- The basic idea is that the decision boundary should be as far away from the data of both classes as possible.
- The aim is to minimise possible conflicts which may happen during classification.
- So we should maximise the margin (see figure).



- As you can see in the figure, we have three lines:
 - $\mathbf{w}^T \mathbf{x} + b = -1$ as the border line of class 1.
 - $\mathbf{w}^T \mathbf{x} + b = 1$ as the border lines of class 2
 - $\mathbf{w}^T \mathbf{x} + b = 0$ as the boundary with a specific margin
- Now let us denote our training instances as $\{x_i, y_i\}$, i = 1, ..., n where $y_i \in \{-1,1\}$.
- What is the Euclidean distance from a point x to the decision boundary?

- In the above figure, we have denoted this distance with.
- We know that the shortest distance between a point and a hyperplane is perpendicular to the plane, and hence, parallel to



So the distance of to the separating hyperplane
 is:

$$r_i = y_i \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|}$$

- Let us assume that the minimum distance of the hyperplane from any instance is.
- Thus for each instance we have: $r_i = y_i \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|} \ge r$
- Instances that are closest to the hyperplane are called support vectors and are at distance from the hyperplane.
- So the margin is defined as the distance between the support vectors and is given as $m = 2r = \frac{2}{\|\mathbf{w}\|}$ (why?)

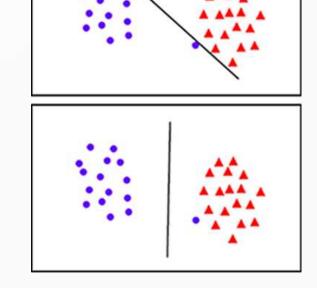
- Because we would like to have equal distances for both sides of data points ().
- Thus we have $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$
- we know: $r_i = y_i \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|} \ge r$
- So we know that $2r = \frac{2}{\|\mathbf{w}\|}$ then $r = \frac{1}{\mathbf{w}}$
- Then, $y_i \frac{\mathbf{w}^T \mathbf{x}_i + b}{\|\mathbf{w}\|} \ge \frac{1}{\|\mathbf{w}\|} = y_i (\mathbf{w}^T \mathbf{x}_i + b) \ge 1$

- SVM aims to find a hyperplane (w,b) so that the margin $\frac{z}{\|\mathbf{w}\|}$ is maximised while satisfying the constraint $y_i(\mathbf{w}^T\mathbf{x}_i+b) \geq 1$
- SVM formulation therefore solves the following optimisation problem: $\min_{Minimize} \frac{1}{2} \|\mathbf{w}\|^2$

subject to
$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \ge 1 \quad \forall i$$

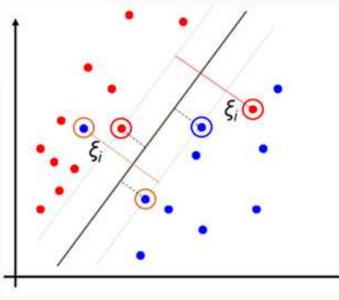
- Remember the problem of maximising $\frac{2}{\|\mathbf{w}\|}$ is the same as minimising $\frac{1}{5}\|\mathbf{w}\|^2$
- We need to optimise a quadratic function in subject to linear constraints.

- In SVM, we have so far assumed that data is linearly separable. What approach should we take when data is not linearly separable?
- Sometimes, data can be linearly separable but with a narrow margin.
- At other times, due to noise, some of the instances may not be linearly separable (see the figure for noisy data).



- It is generally preferred not to interfere with the boundary even with small noisy data points or outliers.
- It is acceptable to have large margins even though some of the constraints are violated.
- In practice, we need a trade-off between the margin and the number of errors in classifying the training instances.

- This trade-off brings us to the soft margin concept.
- Consider the following figure; the soft margin concept is defined when the training instances are not linearly separable.
- Slack variables are added to allow mis-classification of outliers, noisy or difficult to classify instances.
- So basically we are allowing some of the data points to cross the borders and to be in the wrong side of the boundary or to be mis-classified.



- Although we allow some of the training instances to be mis-classified, we still want to minimize the sum of slack variables.
- So for those data points which their ζ_i value is non-zero, we can infer that they are mis-classified, and the amount of mis-classification is also presented in ζ_i .
- SVM with soft margin uses the following formulation:

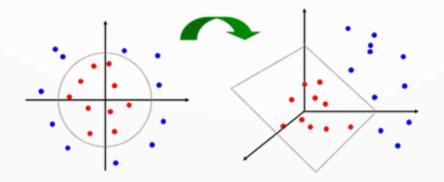
```
Find \mathbf{w} and \mathbf{b} such that  \Phi(\mathbf{w}) = \mathbf{w}^{\mathsf{T}} \mathbf{w} + C \sum_{i} \xi_{i} \text{ is minimized}  and for all (\mathbf{x}_{i}, y_{i}), i=1..n: y_{i} (\mathbf{w}^{\mathsf{T}} \mathbf{x}_{i} + b) \ge 1 - \xi_{i}, \xi_{i} \ge 0
```

- The parameter can be used as a way to achieve the trade-off between large margin and fitting training data.
 - For the high values of , we highly penalize the misclassification.
 - But for the small values of , we allow more misclassifications.
- That is how SVM handles this trade-off around misclassification.

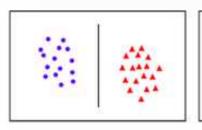
Linear SVM Linear SVM: Summary

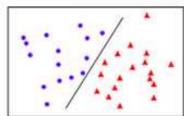
- In the previous step, we investigated how an SVM handles perfectly separable data points.
- In this, we looked into how it handles almost separable data points.
- In the next part, we are going to review nonlinear SVMs.

- You may encounter data points which are not linearly separable;
- in that case, can we project them to another space in which they could be linearly separable?



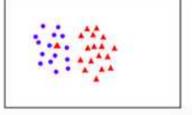
• in the first two cases, we can see that the separable data points are easily linearly separable.

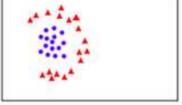




 In the bottom left image, a single noisy data point exists; but by ignoring that points we can still draw a proper linear boundary for the data.







- since there are no linear separable lines you can understand the complexity of the classification.
- The data points and their great numbers, conclude that these are not just noisy outputs.
- So we probably need a nonlinear boundary for this.

- When faced with data points that are not linearly separable, can we project them to another space in which they are linearly separable?
- The key idea:
 - To handle non-linearity, we can transform the features to a higher dimensional space where data is linearly separable (see figure below).
 - This figure illustrates a 2D space in which the data points can only be separated through a nonlinear curve.
 - However by transforming these data points to a 3D space, it looks that data points are now linearly separable!

- SVM performs the required transformation $\Phi : \mathbf{x} \to \phi(\mathbf{x})$ implicitly by using <u>kernels</u>.
- We call this <u>implicit</u> because we do not need to compute φ(x)
- Since data participates (see the previous lesson) in computations only in the form of dot products, all the computations are performed via kernels.

- The dot product of instances in transformed space becomes $\phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$
- which is directly computed through a kernel function $k(\mathbf{x}_i, \mathbf{x}_j)$
- This is known as a kernel trick.
- There are kernels (e.g. radial basis function kernel) which allows transformations to even infinite dimensional feature spaces.
- A kernel function is a function that is used to compute dot products in a high dimensional feature space.

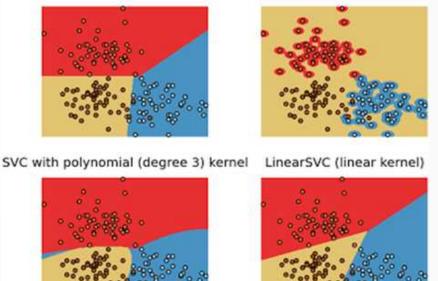
Nonlinear SVM Kernel function...

- Some popular kernel functions where $k(\mathbf{x}_i, \mathbf{x}_j) = \phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$
 - Linear Kernel: $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j, Mapping$ $\phi(\mathbf{x}) = x$
 - Polynomial Kernel with degree p: $k(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$
 - Radial basis function (RBF) kernel: $k(\mathbf{x}_i, \mathbf{x}_j) = e^{-\frac{\|\mathbf{x}_i \mathbf{x}_j\|^2}{2\sigma^2}}$

Mapping $\phi(x)$ is infinite dimensional.

Nonlinear SVM Kernel function...

- SVM fits a linear hyperplane in high dimensional space;
- but in original space the boundaries are nonlinear
- In the figure, SVC means Support Vector Classification.
- Also you can see while using the linear kernel you are getting linear boundaries,
- however in polynomial kernel with degree 3, the SVM came up with curve boundaries.



VC with RBF kernel

All these outputs are on the Iris data set which is a multivariate data set introduced by the British statistician and biologist Ronald Fisher.

Python Program

KNN SVM (Linear, poly and RBF kernel)

KNN

- The K Nearest Neighbour (KNN) algorithm as one of the most interesting and powerful machine learning methods.
- In this practical, you will apply them to classification problems that are possibly non-linearly separable.
- For this practical, we use the simple but extremely popular <u>Iris data set</u>.
- This <u>dataset contains 50 samples</u> of the iris flower varieties:(Iris setosa, Iris virginica and Iris versicolor).
- <u>Each row contains four features</u>: the length and the width of the sepals and petals, in centimetres.
- This data is commonly use to build classification models that take these four measurements as input and predict the species of Iris flower (setosa/ virginica/versicolor).

KNN

 We can import the iris dataset from this package using the following code:

print('First 5 rows of our data: {}'.format(X[:5, :]))

print('Unique labels: {}'.format(np.unique(y)))

```
from matplotlib import pyplot as plt
import numpy as np
                                                        X is of type: <class 'numpy.ndarray'>
# Import the Iris data set
                                                        y is of type: <class 'numpy.ndarray'>
from sklearn import datasets
                                                        First 5 rows of our data: [[5.1 3.5 1.4 0.2]
iris = datasets.load iris()
                                                         [4.9 3. 1.4 0.2]
                                                         [4.7 3.2 1.3 0.2]
# divide this data into features and labels
                                                         [4.6 3.1 1.5 0.2]
X = iris.data
                                                         [5. 3.6 1.4 0.2]]
                                                        Unique labels: [0 1 2]
y = iris.target
print('X is of type: {}'.format(type(X)))
print('y is of type: {}'.format(type(y)))
# How does our data look
```

KNN

 Let us now split our data into 80% training and 20% testing.

```
from sklearn.model selection import train test split
#Split the data into 80% Training and 20% Testing sets
Xtrain, Xtest, ytrain, ytest = train_test_split(X,y, test_size=0.2, random_state=42)
                                                      First 5 rows of our data: [[5.1 3.5]
print (Xtrain.shape)
                                                       [4.9 3.]
print (ytrain.shape)
                                                       [4.7 3.2]
print (Xtest.shape)
                                                       [4.6 3.1]
print (ytest.shape)
                                                       [5. 3.6]]
                                                      (120, 2)
Xtrain[:5,:] # first 5 rows of training data
                                                      (120,)
                                                      (30, 2)
                                                      (30,)
                                                      array([[4.6, 3.6],
                                                             [5.7, 4.4],
                                                             [6.7, 3.1],
                                                             [4.8, 3.4],
                                                             [4.4, 3.2]])
```

KNN: Advanced Visualization

 We now define a function to plot the true data points and the calculated decision boundaries of a given classifier model (also called estimator).

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn import metrics

# Build a kNN using 5 neighbor nodes
knn_model = KNeighborsClassifier(n_neighbors=5)

#Fit the model using our training data
knn_model.fit(Xtrain, ytrain)

#Training Accuracy:
knn_acc = metrics.accuracy_score(ytrain, knn_model.predict(Xtrain))
print ("KNN Training Accuracy: {}".format(knn_acc))

#visualize the decision bounday. The points represent the true data.
plot_estimator(knn_model, Xtrain, ytrain)
```

KNN: Advanced Visualization

- In this plot, the points represent the true data, the decision boundary is plotted as background color.
- We can immediately see that one class is linearly separable from the rest.
- Lets now look at the testing accuracy:

```
#Testing Accuracy:
knn_acc_test = metrics.accuracy_score(ytest, knn_model.predict(Xtest))
print ("KNN Testing Accuracy: {}".format(knn_acc_test))
KNN Testing Accuracy: 0.8
```

SVM

- Load a nonlinearly separable classification dataset
- Using the dataset, run SVM with both linear and nonlinear kernels (polynomial, RBF) and assess its prediction accuracy.
- Study the effects of C parameter and other kernel parameters and plot the performance.
- Plot the support vectors.

SVM...

- same as before:
 - importing libraries and dataset
 - drop last 2 columns for easy visualization
 - train-test split
- to do:
 - extend this code by building a support vector machine classification model for this data using a linear kernel.

 Let's start with a linear kernel with the default parameters.

```
from sklearn import svm
from sklearn import metrics

# Fit an SVM using linear kernel
svm_model = svm.SVC(kernel='linear')
svm_model.fit(Xtrain, ytrain)

#Training/Testing Accuracy:
svm_acc = metrics.accuracy_score(ytrain, svm_model.predict(Xtrain))
print("SVM Training Accuracy: {}".format(svm_acc))
plot_estimator(svm_model,Xtrain,ytrain)
```

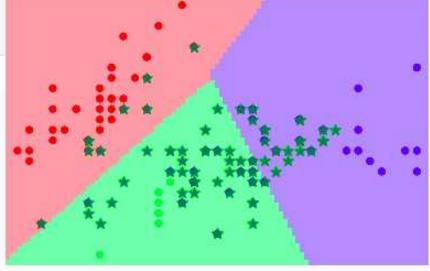
SVM Training Accuracy: 0.8

 The decision boundary is calculated using the support vectors learnt from training data.

 We can get these support vector data points using support vectors parameter in the SVM

model.

 We will now plot the support vectors in * shape after plotting the decision boundary.



- Test accuracy.
- As we have seen Linear kernel gave us a linear decision boundary: the separation boundary is a straight line between the two categories.

- In order to facilitate the visualization, let's consider the iris data set Class 1 and Class 2 samples.
- These two types are not linearly separable, so we can see something more interesting.
- Here we use the in1d function in numpy to do this easily.

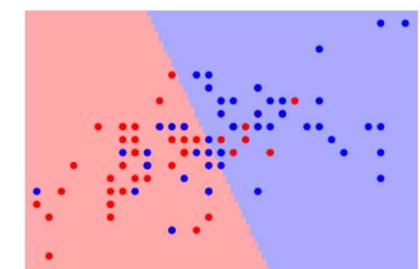
- In order to facilitate the visualization, let's consider the iris data set Class 1 and Class 2 samples.
- These two types are not linearly separable, so we can see something more interesting.
- Here we use the in1d function in numpy to do this easily.

```
(80, 2)
(80,)
(20, 2)
(20,)
```

Training.

```
# Fit SVM using linear kernel on training data
svc_model = svm.SVC(kernel='linear')
svc_model.fit(Xtrain, ytrain)

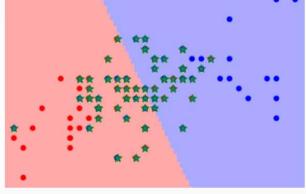
#Training/Testing Accuracy:
svc_acc = metrics.accuracy_score(ytrain, svc_model.predict(Xtrain))
print("SVM Training Accuracy: {}".format(svc_acc))
plot_estimator(svc_model,X,y)
SVM Training Accuracy: 0.7125
```



support vectors and testing.

```
# Plotting support vectors
plot_estimator(svc_model,X,y)
plt.scatter(svc_model.support_vectors_[:, 0], svc_model.support_vectors_[:, 1],
plt.show()

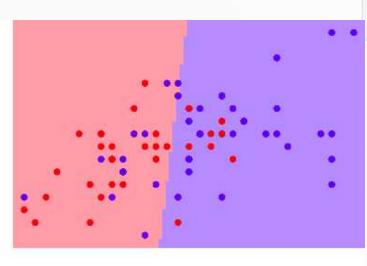
#Testing Accuracy:
svc_acc_test = metrics.accuracy_score(ytest, svc_model.predict(Xtest))
print("SVM Testing Accuracy: {}".format(svc_acc_test))
```



SVM Testing Accuracy: 0.7

- C is 1 by default and it's a reasonable default choice.
- If you have a lot of noisy observations you should decrease it.
- It corresponds to regularize more the estimation.
- It is similar to the L2 regularization parameter.
- Lets start with a high C value.
- This corresponds to high penalty for mis-classification.
- Hence the learnt margin will be narrow, resulting in small number of support vectors.

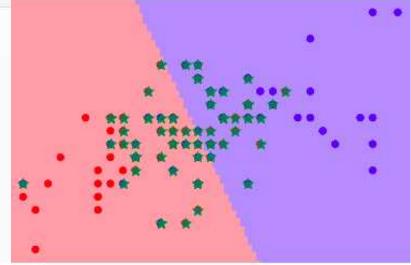
code



Data has a total of 55 support vectors Training accuracy: 0.725 Testing accuracy: 0.7

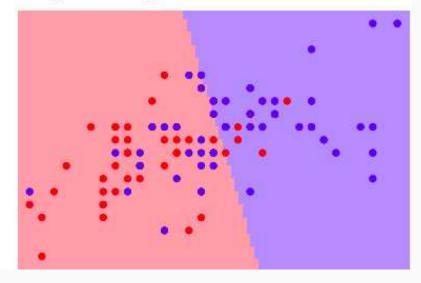
support vectors

High C values: small number of support vectors



- If we have a low C value, we get no regularization, low penalty for misclassification.
- Hence we find a bigger margin with more support vectors.

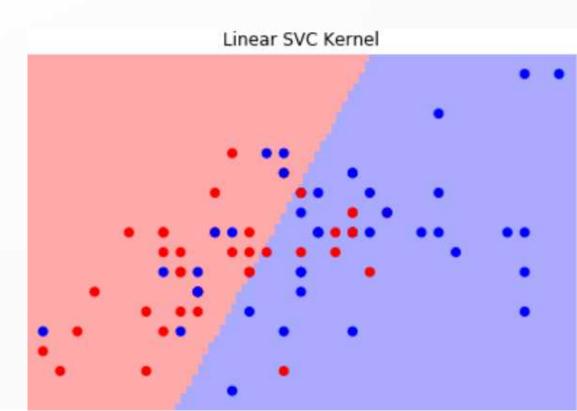
Data has a total of 76 support vectors Training accuracy: 0.7 Testing accuracy: 0.65



- Notice that the decision boundary has changed for the model, decreasing the testing accuracy.
- Also now almost all the points become support vectors. This
 is one of the issues with small sample data.

- In sklearn, LinearSVC is another implementation of Linear kernel.
- It has more flexibility in terms of parameters.

```
svc_model = svm.LinearSVC()
plot_estimator(svc_model, Xtrain, ytrain)
plt.title('Linear SVC Kernel')
plt.show()
```



SVM: Polynomial kernel SVM with Polynomial Kernel

- Here, you fit a polynomial kernel with varying degrees.
- The degree of the polynomial kernel can be specified using "degree" parameter.

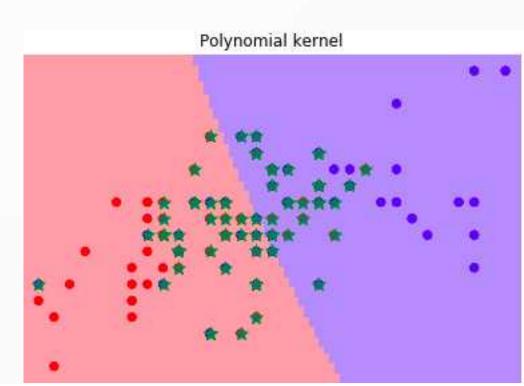
 Training accuracy: 0.7125

Testing accuracy: 0.7

Polynomial kernel

SVM: Polynomial kernel SVM with Polynomial Kernel

- Here, you fit a polynomial kernel with varying degrees.
- The degree of the polynomial kernel can be specified using "degree" parameter.



SVM: Polynomial kernel SVM in Python - RBF kernel

- You can specify RBF Kernel using two parameters C and gamma.
- Intuitively, the gamma parameter defines how far the influence of a single training example reaches, with low values meaning 'far' and high values meaning 'close'.
- The gamma parameters can be seen as the inverse of the radius of influence of samples selected by the model as support vectors.
- The C parameter trades off misclassification of training examples against simplicity of the decision surface.
- A low C makes the decision surface smooth, while a high C aims at classifying all training examples correctly by giving the model freedom to select more samples as support vectors.

SVM: Polynomial kernel SVM in Python - RBF kernel

For this dataset, lets look at the influence of gamma.

.format(metrics.accuracy_score(ytrain, svc_model.predict(Xtrain))))

.format(metrics.accuracy_score(ytest, svc_model.predict(Xtest))))

print("Testing accuracy : {}"\

 You can set gamma as 10, 100, 1000 and see the differences to the decision surface and accuracy. Training accuracy: 0.8875

Testing accuracy: 0.85

RBF kernel

```
svc_model = svm.SVC(kernel='rbf', gamma=le2)

svc_model.fit(X,y)
plot_estimator(svc_model, X, y)
plt.title('RBF kernel')
#Training accuracy:
print("Training accuracy: {}"\
```

SVM: Polynomial kernel SVM in Python - RBF kernel

plot support vectors

