Lecture 33 - Slack Variables; Soft-Margin SVM

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
plt.style.use('bmh')
```

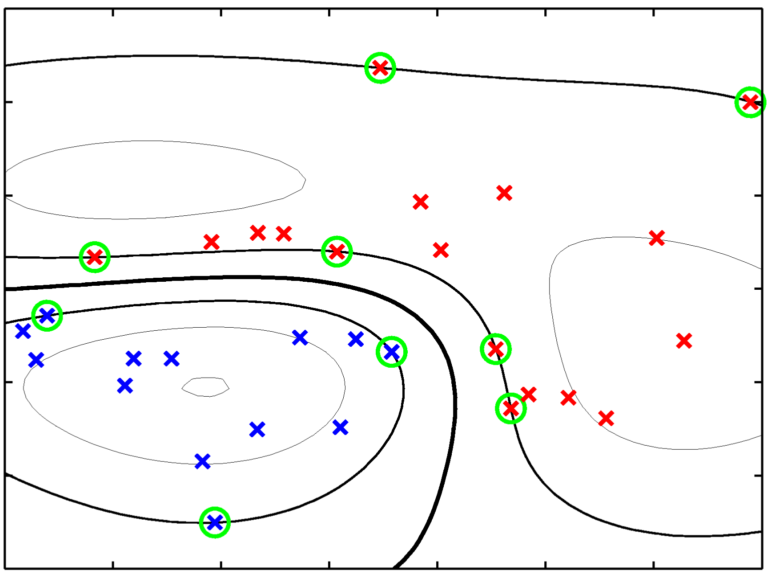
Example of Hard-Margin SVM

Linearly-separable classes in the feature space spanned by the transformation $\phi(x)$ may form a non-linear decision boundary in the input space.

In [2]:

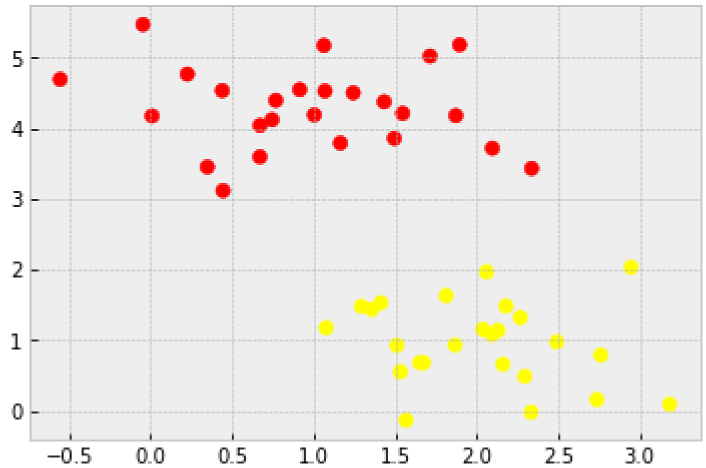
```
from IPython.display import Image
Image("figures/Figure7.2.png", width=400)
```

Out[2]:



In [3]:

```
from sklearn.datasets import make_blobs
X, y = make_blobs(n_samples=50, centers=2,
                  random_state=0, cluster_std=0.60)
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn');
```



In [4]:

```
from sklearn.svm import SVC # "Support vector classifier"

model = SVC(kernel='linear')
model.fit(X, y)
```

Out[4]:

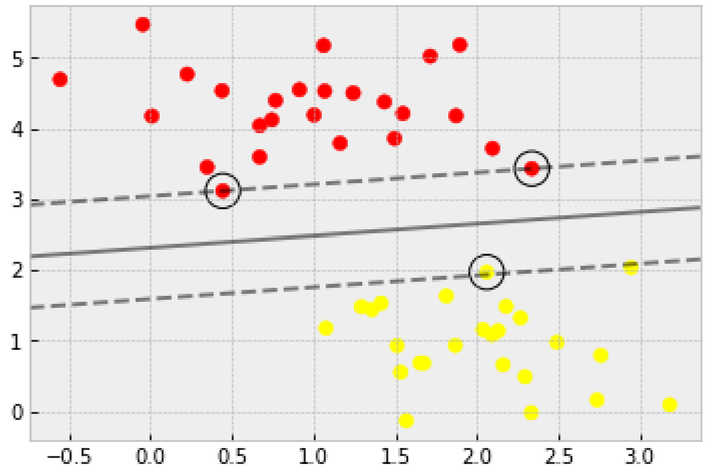
```
SVC(kernel='linear')
```

In [5]:

```
# Python Data Science Handbook

def plot_svc_decision_function(model, ax=None, plot_support=True):
    """Plot the decision function for a 2D SVC"""
    if ax is None:
        ax = plt.gca()
    xlim = ax.get_xlim()
    ylim = ax.get_ylim()

    # create grid to evaluate model
    x = np.linspace(xlim[0], xlim[1], 30)
    y = np.linspace(ylim[0], ylim[1], 30)
    Y, X = np.meshgrid(y, x)
    xy = np.vstack([X.ravel(), Y.ravel()]).T
    P = model.decision_function(xy).reshape(X.shape)

    # plot decision boundary and margins
    ax.contour(X, Y, P, colors='k',
               levels=[-1, 0, 1], alpha=0.5,
               linestyles=['--', '-', '--'])

    # plot support vectors
    if plot_support:
        ax.scatter(model.support_vectors_[:, 0],
                   model.support_vectors_[:, 1],
                   s=300, linewidth=1, edgecolors='black',facecolors='none');
    ax.set_xlim(xlim)
    ax.set_ylim(ylim)
```

In [6]:

```
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn')
plot_svc_decision_function(model);
```



In [7]:

```
model.support_vectors_
```

Out[7]:

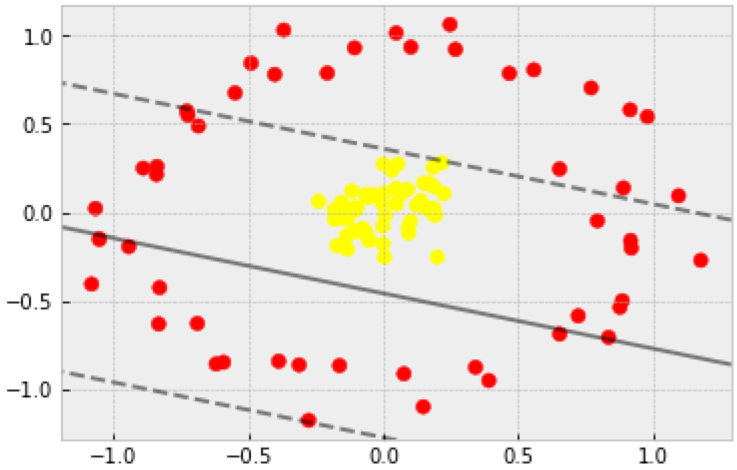
```
array([[0.44359863, 3.11530945],
       [2.33812285, 3.43116792],
       [2.06156753, 1.96918596]])
```

In [8]:

```
def plot_svm(N=10, ax=None):
    X, y = make_blobs(n_samples=200, centers=2,
                      random_state=0, cluster_std=0.60)
    X = X[:N]
    y = y[:N]
    model = SVC(kernel='linear', C=1E10)
    model.fit(X, y)

    ax = ax or plt.gca()
    ax.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn')
    ax.set_xlim(-1, 4)
    ax.set_ylim(-1, 6)
    plot_svc_decision_function(model, ax)

from ipywidgets import interact, fixed
interact(plot_svm, N=[10, 30, 60, 100, 200], ax=fixed(None));
```

In [9]:

```
from sklearn.datasets import make_circles
X, y = make_circles(100, factor=.1, noise=.1)

clf = SVC(kernel='linear').fit(X, y)

plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn')
plot_svc_decision_function(clf, plot_support=False);
```



In [10]:

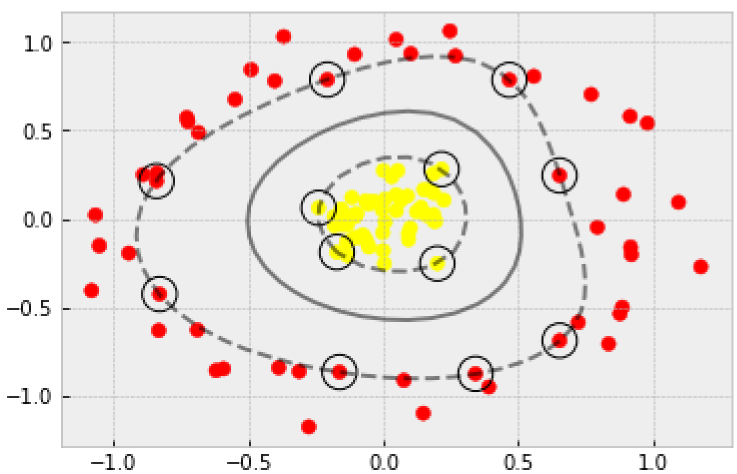
```
clf = SVC(kernel='rbf', C=1E6)
clf.fit(X, y)
```

Out[10]:

```
SVC(C=1000000.0)
```

In [11]:

```
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn')
plot_svc_decision_function(clf)
plt.scatter(clf.support_vectors_[:, 0], clf.support_vectors_[:, 1],
            s=300, lw=1, facecolors='none');
```



Soft-Margin Support Vector Machine (SVM): Overlapping Classes

To handle this case, the SVM implementation has a bit of a fudge-factor which "softens" the margin: that is, it allows some of the points to creep into the margin if that allows a better fit. The hardness of the margin is controlled by a tuning parameter, most often known as **slack varible** $\xi_n \geq 0$, $n = 1, \ldots, N$, with one slack variable for each training data point. For very large ξ, the margin is hard, and points cannot lie in it. For smaller ξ, the margin is softer, and can grow to encompass some points.

A **slack variable** is defined as $\xi_n = 0$ for data points that are on or inside the correct margin boundary and $\xi_n = |t_n - y(x_n)|$ for other points. Thus a data point that is on the decision boundary $y(x_n) = 0$ will have $\xi_n = 1$, and points with $\xi_n > 1$ will be misclassified. The exact classification constraints are then replaced with

$$t_n y(x_n) \geq 1 - \xi_n, n = 1, \ldots, N$$

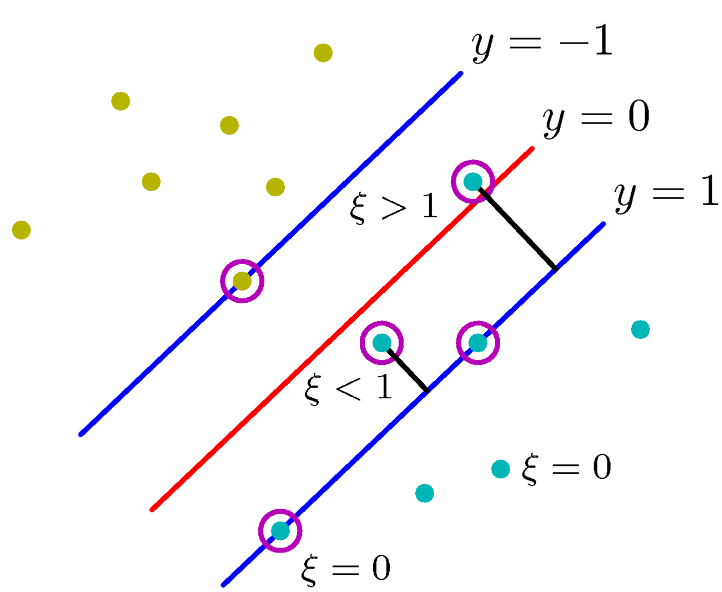
in which the slack variables are constrained to satisfy $\xi_n \geq 0$.

- Data points for which $\xi_n = 0$ are correctly classified and are either on the margin or on the correct side of the margin.
- Points for which $0 < \xi_n \leq 1$ lie inside the margin, but on the correct side of the decision boundary.
- And those data points for which $\xi_n > 1$ lie on the wrong side of the decision boundary and are misclassified.

In [12]:

```
Image('figures/Figure7.3.png', width=400)
```

Out[12]:



Our goal is now to maximize the margin while softly penalizing points that lie on the wrong side of the margin boundary. We therefore minimize:

$$\arg_{w,b} \min C \sum_{n=1}^{N} \xi_n + \frac{1}{2} \|w\|^2$$
$$\text{subject to } t_n y(x_n) \geq 1 - \xi_n, n = 1, \ldots, N$$
$$\text{and } \xi_n \geq 0, n = 1, \ldots, N$$

where the parameter $C > 0$ controls the trade-off between the slack variable penalty and the margin.

- Because any point that is misclassified has $\xi_n > 1$, it follows that $\sum_n \xi_n$ is an upper bound on the number of misclassified points.

- The parameter C is therefore analogous to (the inverse of) a regularization coefficient because it controls the trade-off between minimizing training errors and controlling model complexity.
- In the limit $C \to \infty$, we will recover the earlier support vector machine for separable data.

The Lagrangian is given by:

$$L(w, b, a) = \frac{1}{2}\|w\|^2 + C\sum_{n=1}^{N} \xi_n - \sum_{n=1}^{N} a_n \left(t_n y(x_n) - 1 + \xi_n\right) - \sum_{n=1}^{N} \mu_n \xi_n$$

where $\{a_n \geq 0\}_{n=1}^{N}$ and $\{\mu_n \geq 0\}_{n=1}^{N}$ are Lagrange multipliers. The corresponding set of Karush–Kuhn–Tucker (KKT) conditions are given by

$$\begin{aligned} a_n &\geq 0 \\ t_n y(x_n) - 1 + \xi_n &\geq 0 \\ a_n(t_n y(x_n) - 1 + \xi_n) &\geq 0 \\ \mu_n &\geq 0 \\ \xi_n &\geq 0 \\ \mu_n \xi_n &= 0 \end{aligned}$$

where $n = 1, \ldots, N$.

We now optimize for w, b and $\{\xi_n\}$:

$$\begin{aligned} \frac{\partial L}{\partial w} &= 0 \Rightarrow w = \sum_{n=1}^{N} a_n t_n \phi(x_n) \\ \frac{\partial L}{\partial b} &= 0 \Rightarrow \sum_{n=1}^{N} a_n t_n = 0 \\ \frac{\partial L}{\partial \xi_n} &= 0 \Rightarrow a_n = C - \mu_n \Rightarrow a_n \leq C \end{aligned}$$

The dual Lagrangian is then given by:

$$\tilde{L}(a) = \sum_{n=1}^{N} a_n - \sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(x_n, x_m)$$

which is identical to the separable case, except that the constraints are somewhat different. We therefore have to minimize $\tilde{L}(a)$ with respect to the dual variables $\{a_n\}$ subject to

$$0 \leq a_n \leq C$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

As before, a subset of the data points may have $a_n = 0$, in which case they do not contribute to the predictive model. The remaining data points constitute the support vectors. These have $a_n > 0$ and hence $t_n y(x_n) = 1 - \xi_n$.

- If $a_n < C$, then $\mu_n > 0$, which requires $\xi_n = 0$ and hence such points lie on the margin.

- Points with $a_n = C$ can lie inside the margin and can either be correctly classified if $\xi_n \leq 1$ or misclassified if $\xi_n > 1$.

To determine the parameter b, we note that those support vectors for which $0 < a_n < C$ have $\xi_n = 0$ so that $t_n y(x_n) = 1$ and hence will satisfy

$$t_n \left(\sum_{m \in S} a_m t_m k(x_n, x_m) + b \right) = 1$$

Again, a numerically stable solution is obtained by averaging to give

$$b = \frac{1}{N_M} \sum_{n \in M} \left(t_n - \sum_{m \in S} a_m t_m k(x_n, x_m) \right)$$

where M denotes the set of indices of data points having $0 < a_n < C$.

Although predictions for new inputs are made using only the support vectors, the training phase (i.e., the determination of the parameters a and b) makes use of the whole data set, and so it is important to have **efficient algorithms for solving the quadratic programming problem**.

We first note that the objective function $\tilde{L}(a)$ is quadratic and so any local optimum will also be a **global optimum** provided the constraints define a convex region (which they do as a consequence of being linear).