Lecture 26 - SVM continued

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
plt.style.use('seaborn-colorblind')
from IPython.display import Image
```

In order to solve this constrained optimization problem, we introduce *Lagrange multipliers* $a_n \geq 0$, with one multiplier an for each of the constraints, giving the Lagrangian function

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

- Note the minus sign in front of the Lagrange multiplier term, because we are minimizing with respect to w and b, and maximizing with respect to a.

Setting the derivatives of $L(w, b, a)$ with respect to w and b equal to zero, we obtain the following two conditions:

$$w = \sum_{n=1}^{N} a_n t_n \phi(x_n)$$
$$0 = \sum_{n=1}^{N} a_n t_n$$

Eliminating w and b from $L(w, b, a)$ using these conditions then gives the *dual representation* of the maximum margin problem in which we maximize

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

with respect to a subject to the constraints

$$a_n \geq 0, n = 1, 2, \ldots, N$$
$$\sum_{n=1}^{N} a_n t_n = 0$$

Here the kernel function is defined by $k(x, y) = \phi(x)^T \phi(y)$.

- This takes the form of a quadratic programming problem in which we optimize a quadratic function of a subject to a set of inequality constraints.
- The solution to a quadratic programming problem in M variables in general has computational complexity that is $O(M^3)$. In going to the dual formulation we have turned the original optimization problem into the dual problem, which has N variables.
  - For a fixed set of basis functions whose number M is smaller than the number N of data points, the move to the dual problem appears disadvantageous. However, it allows the model to be reformulated using kernels, and so the maximum margin classifier can be applied efficiently to feature spaces whose dimensionality exceeds the number of data points, including infinite feature spaces.
  - The kernel formulation also makes clear the role of the constraint that the kernel function $k(x, y)$ be positive definite, because this ensures that the Lagrangian function $\tilde{L}(a)$ is bounded below, giving rise to a well defined optimization problem.

In order to classify new data points using the trained model, we evaluate the sign of $y(x) = w^T \phi(x) + b$. This can be expressed in terms of the parameters $\{a_n\}$ and the kernel function by substituting for w to give

$$y(x) = \sum_{n=1}^{N} a_n t_n k(x, x_n) + b$$

- A constrained optimization of this form satisfies the Karush-Kuhn-Tucker (KKT) conditions, which in this case require that the following three properties hold

$$a_n \geq 0$$
$$t_n y(x_n) - 1 \geq 0$$
$$a_n \left(t_n y(x_n) - 1\right) = 0$$

Thus for every data point, either $a_n = 0$ or $t_n y(x_n) = 1$.

- Any data point for which $a_n = 0$ will not appear in the sum of $y(x)$ and hence plays no role in making predictions for new data points.
- The remaining data points are called **support vectors**, and because they satisfy $t_n y(x_n) = 1$, they correspond to points that lie on the maximum margin hyperplanes in feature space.
- Once the model is trained, a significant proportion of the data points can be discarded and only the support vectors retained!

Having solved the quadratic programming problem and found a value for a, we can then determine the value of the threshold parameter b by noting that any support vector x_n satisfies $t_n y(x_n) = 1$.

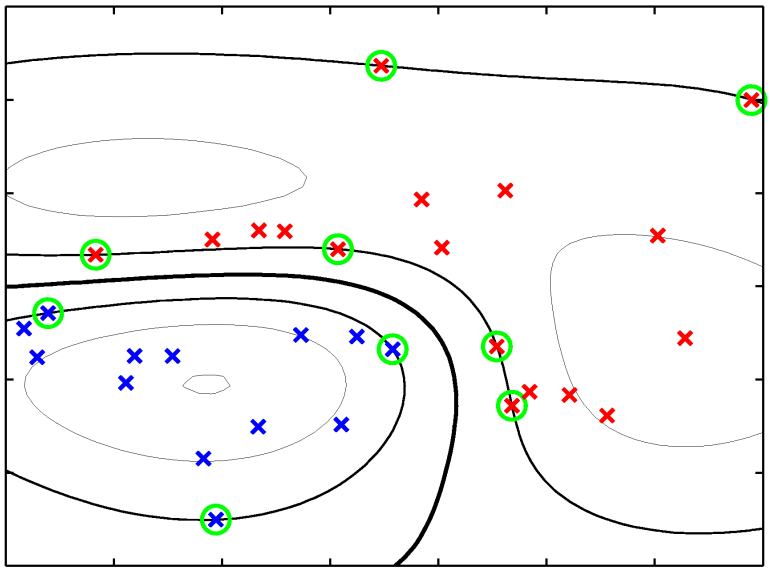
$$t_n \left(\sum_{m \in S} a_m t_m k(x_n, x_m) + b \right) = 1$$

where S denotes the set of indices of the support vectors. Although we can solve this equation for b using an arbitrarily chosen support vector x_n, a numerically more stable solution is obtained by first multiplying through by t_n, making use of $t_n^2 = 1$, and then averaging these equations over all support vectors and solving for b to give

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

In [2]:
```
Image("figures/Figure7.2.png", width=400)
```

Out[2]:



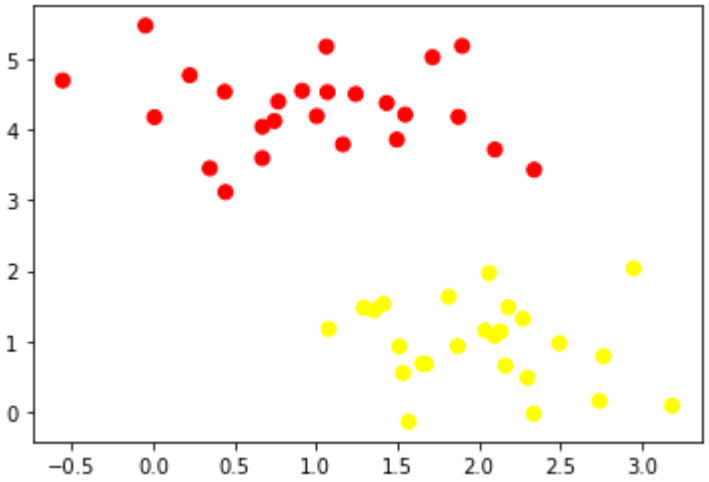
This figure (7.2 from the Bishop textbook) is an example of the classification resulting from training a support vector machine on a simple synthetic data set using a Gaussian kernel.

Although the data set is not linearly separable in the two-dimensional data space x, it is linearly separable in the nonlinear feature space defined implicitly by the nonlinear kernel function. Thus the training data points are perfectly separated in the original data space.

This example also provides a geometrical insight into the origin of sparsity in the SVM. The maximum margin hyperplane is defined by the location of the support vectors. Other data points can be moved around freely (so long as they remain outside the margin region) without changing the decision boundary, and so the solution will be independent of such data points.

Example

In [2]:
```
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');
```

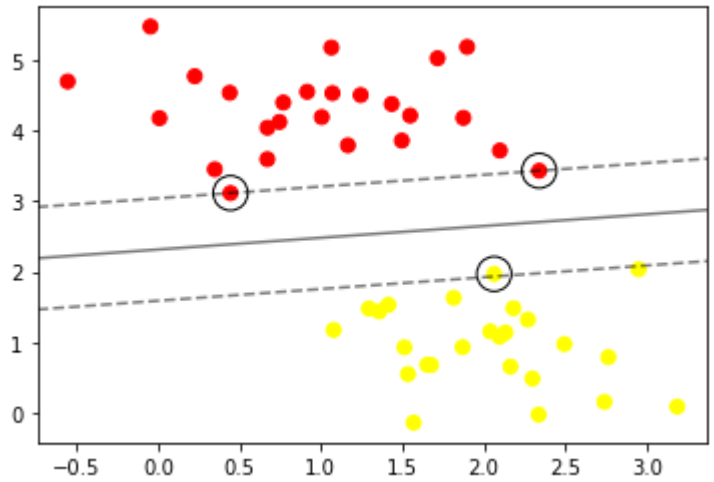


In [4]:
```
from sklearn.svm import SVC # "Support vector classifier"
model = SVC(kernel='linear')
model.fit(X, y)
```

Out[4]:
```
SVC(kernel='linear')
```

In [5]:
```
"Source: 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);
```

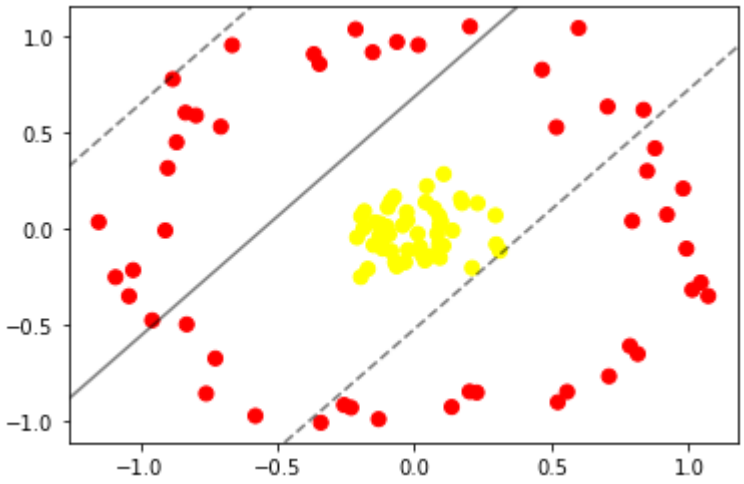


In [7]:
```
model.support_vectors_
```

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));
```

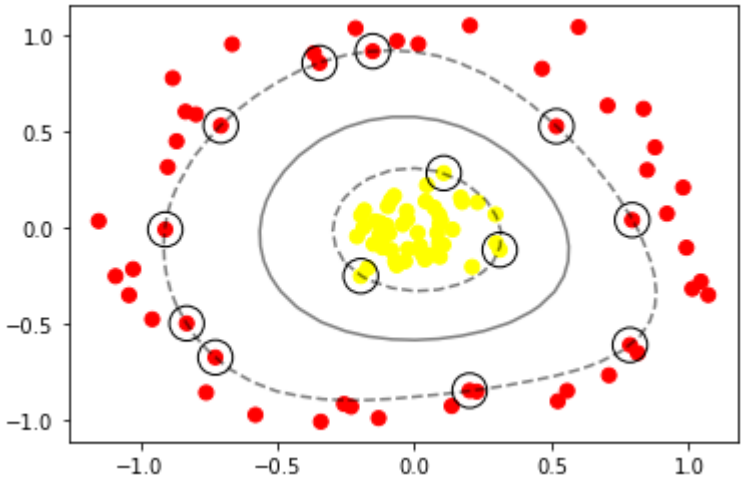
In [9]:
```
from sklearn.datasets import make_circles
X, y = make_circles(100, factor=.1, noise=.1)

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');
```



Support Vector Machines: Overlapping Classes (Softening Margin)

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

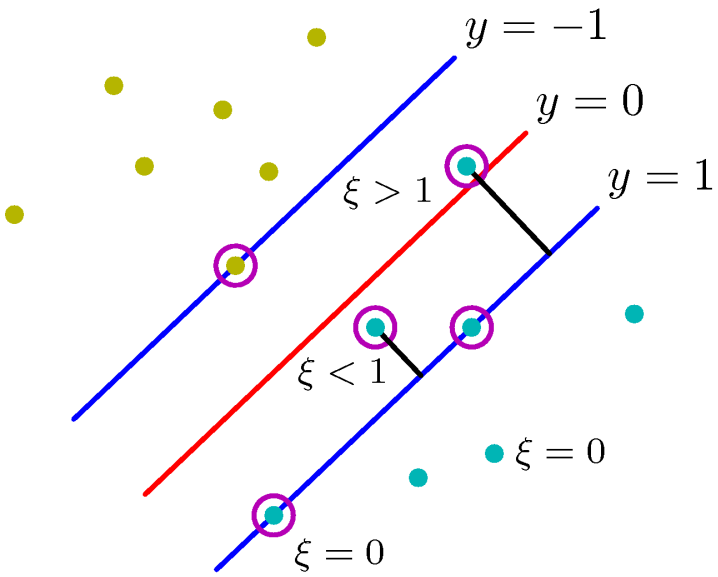
$$t_n y(x_n) \geq 1 - \xi_n, n = 1, \ldots, N$$

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 [3]:
```
Image("figures/Figure7.3.png", width=400)
```

Out[3]:



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:

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

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 $\{a_n \geq 0\}$ and $\{\mu_n \geq 0\}$ 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

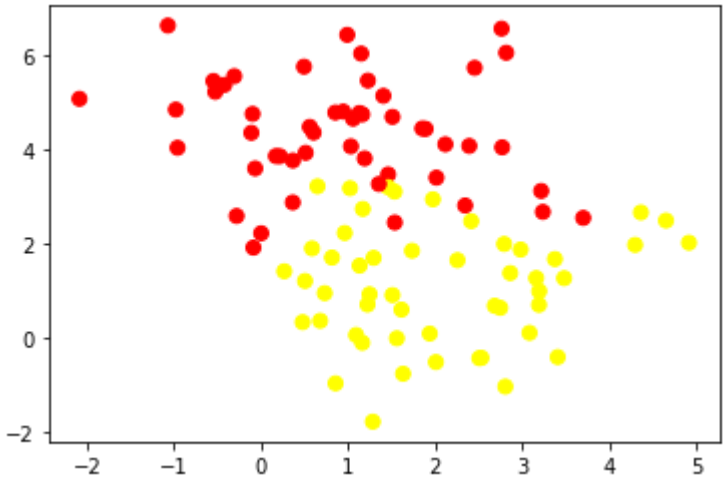
$$b = \frac{1}{N_M} \sum_{n \in M} \left(t_n - \sum_{m \in S} a_m t_m k(x_n, x_m) \right)$$

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**.

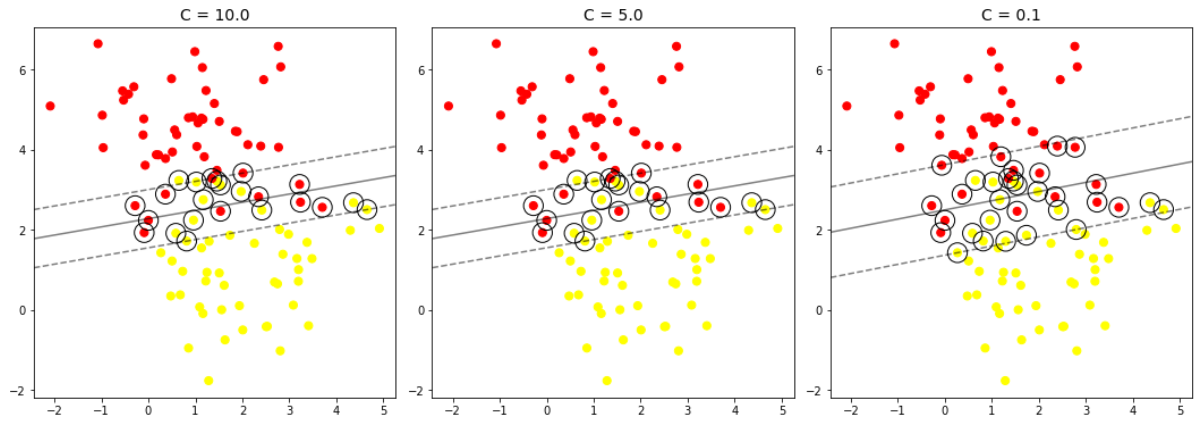
We first note that the objective function $\tilde{L}(a)$ is quadratic and so any local optimum will also be a **global**

In [12]:
```
X, y = make_blobs(n_samples=100, centers=2,
                  random_state=0, cluster_std=1.2)
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn');
```



In [ ]:
```
# X, y = make_blobs(n_samples=100, centers=2,
#                   random_state=0, cluster_std=0.8)
```

In [13]:
```
fig, ax = plt.subplots(1, 3, figsize=(16, 6))
fig.subplots_adjust(left=0.0625, right=0.95, wspace=0.1)

for axi, C in zip(ax, [10, 5, 0.1]):
    model = SVC(kernel='linear', C=C).fit(X, y)
    axi.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='autumn')
    plot_svc_decision_function(model, axi)
    axi.scatter(model.support_vectors_[:, 0],
                model.support_vectors_[:, 1],
                s=300, lw=1, facecolors='none');
    axi.set_title('C = {0:.1f}'.format(C), size=14)
```



The optimal value for the C parameter will depend on your dataset, and should be tuned using cross-validation or a similar procedure.

Example: Face Recognition

See Section [In-Depth: Support Vector Machines (https://jakevdp.github.io/PythonDataScienceHandbook/05.07-support-vector-machines.html)](https://jakevdp.github.io/PythonDataScienceHandbook/05.07-support-vector-machines.html) from **Python Data Science Handbook** textbook

In [ ]:
```
```