

This notebook was put together by [Jake Vanderplas](http://www.vanderplas.com). Source and license info is on [GitHub](https://github.com/jakevdp/sklearn_tutorial/).

Supervised Learning In-Depth: Support Vector Machines

Previously we introduced supervised machine learning. There are many supervised learning algorithms available; here we'll go into brief detail one of the most powerful and interesting methods: **Support Vector Machines (SVMs)**.

```
In [19]: %matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
from scipy import stats

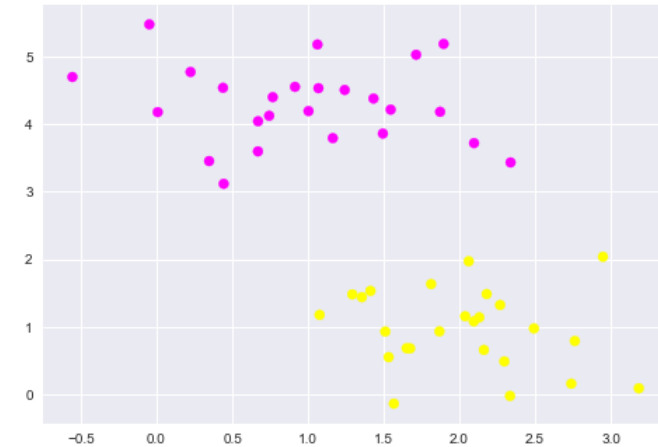
plt.style.use('seaborn')
```

Motivating Support Vector Machines

Support Vector Machines (SVMs) are a powerful supervised learning algorithm used for **classification** or for **regression**. SVMs are a **discriminative** classifier: that is, they draw a boundary between clusters of data.

Let's show a quick example of support vector classification. First we need to create a dataset:

```
In [20]: from sklearn.datasets.samples_generator 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='spring');
```

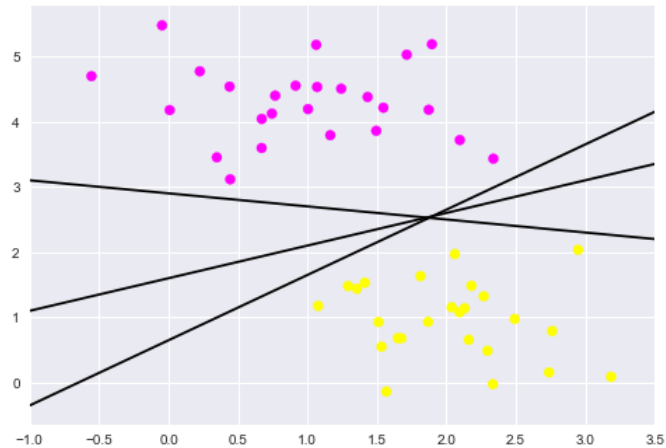


A discriminative classifier attempts to draw a line between the two sets of data. Immediately we see a problem: such a line is ill-posed! For example, we could come up with several possibilities which perfectly discriminate between the classes in this example:

```
In [21]: xfit = np.linspace(-1, 3.5)
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='spring')

for m, b in [(1, 0.65), (0.5, 1.6), (-0.2, 2.9)]:
    plt.plot(xfit, m * xfit + b, '-k')

plt.xlim(-1, 3.5);
```



These are three very different separators which perfectly discriminate between these samples. Depending on which you choose, a new data point will be classified almost entirely differently!

How can we improve on this?

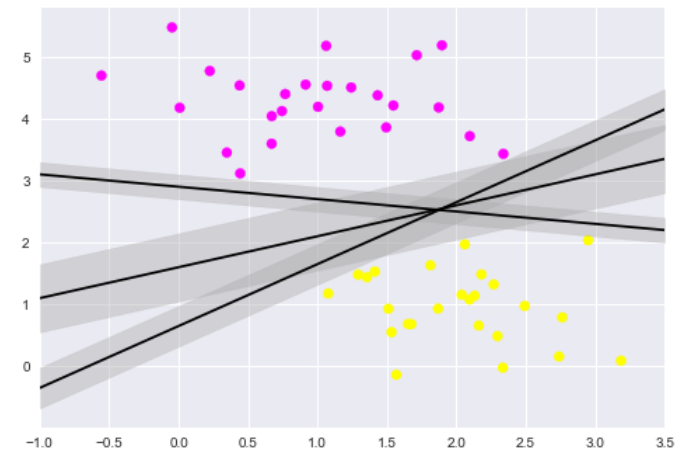
Support Vector Machines: Maximizing the *Margin*

Support vector machines are one way to address this. What support vector machines do is to not only draw a line, but consider a *region* about the line of some given width. Here's an example of what it might look like:

```
In [22]: xfit = np.linspace(-1, 3.5)
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='spring')

for m, b, d in [(1, 0.65, 0.33), (0.5, 1.6, 0.55), (-0.2, 2.9, 0.2)]:
    yfit = m * xfit + b
    plt.plot(xfit, yfit, '-k')
    plt.fill_between(xfit, yfit - d, yfit + d, edgecolor='none', color='#AAAAAA', alpha=0.4)

plt.xlim(-1, 3.5);
```



Notice here that if we want to maximize this width, the middle fit is clearly the best. This is the intuition of **support vector machines**, which optimize a linear discriminant model in conjunction with a **margin** representing the perpendicular distance between the datasets.

Fitting a Support Vector Machine

Now we'll fit a Support Vector Machine Classifier to these points. While the mathematical details of the likelihood model are interesting, we'll let you read about those elsewhere. Instead, we'll just treat the scikit-learn algorithm as a black box which accomplishes the above task.

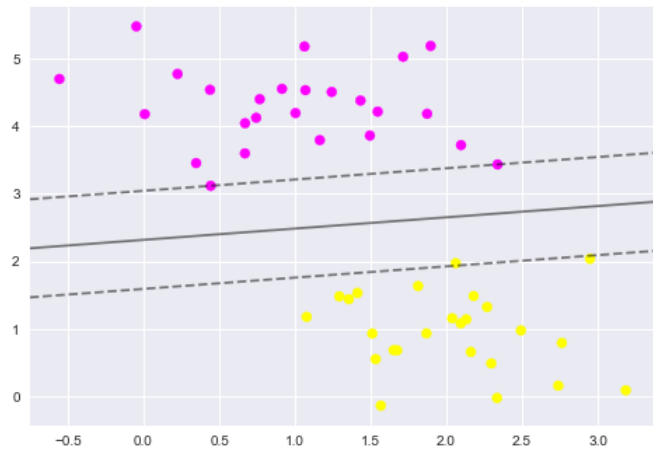
```
In [23]: from sklearn.svm import SVC # "Support Vector Classifier"
clf = SVC(kernel='linear')
clf.fit(X, y)
```

```
Out[23]: SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape='ovr', degree=3, gamma='auto_deprecate
d',
  kernel='linear', max_iter=-1, probability=False, random_state=
None,
  shrinking=True, tol=0.001, verbose=False)
```

To better visualize what's happening here, let's create a quick convenience function that will plot SVM decision boundaries for us:

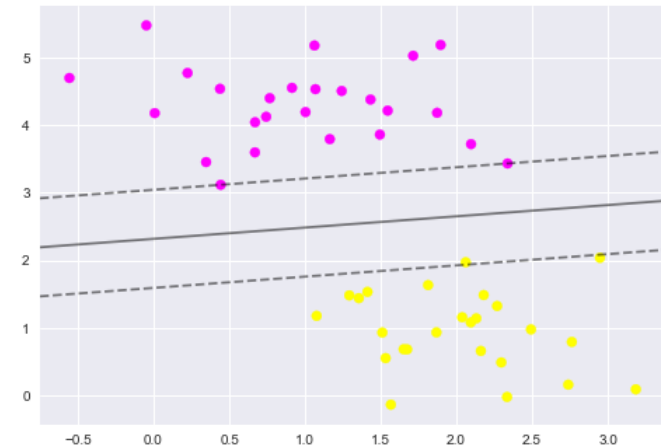
```
In [24]: def plot_svc_decision_function(clf, ax=None):
  """Plot the decision function for a 2D SVC"""
  if ax is None:
    ax = plt.gca()
  x = np.linspace(plt.xlim()[0], plt.xlim()[1], 30)
  y = np.linspace(plt.ylim()[0], plt.ylim()[1], 30)
  Y, X = np.meshgrid(y, x)
  P = np.zeros_like(X)
  for i, xi in enumerate(x):
    for j, yj in enumerate(y):
      P[i, j] = clf.decision_function([[xi, yj]])
  # plot the margins
  ax.contour(X, Y, P, colors='k',
    levels=[-1, 0, 1], alpha=0.5,
    linestyles=['--', '-', '--'])
```

```
In [25]: plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='spring')
plot_svc_decision_function(clf);
```



Notice that the dashed lines touch a couple of the points: these points are the pivotal pieces of this fit, and are known as the *support vectors* (giving the algorithm its name). In scikit-learn, these are stored in the `support_vectors_` attribute of the classifier:

```
In [26]: plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='spring')
plot_svc_decision_function(clf)
plt.scatter(clf.support_vectors_[:, 0], clf.support_vectors_[:, 1],
  s=200, facecolors='none');
```



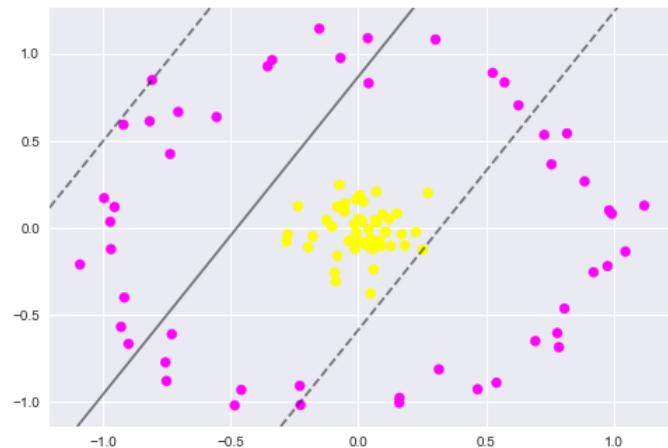
Going further: Kernel Methods

Where SVM gets incredibly exciting is when it is used in conjunction with *kernels*. To motivate the need for kernels, let's look at some data which is not linearly separable:

```
In [27]: from sklearn.datasets.samples_generator 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='spring')
plot_svc_decision_function(clf);
```



Clearly, no linear discrimination will ever separate these data. One way we can adjust this is to apply a **kernel**, which is some functional transformation of the input data.

For example, one simple model we could use is a **radial basis function**

```
In [28]: r = np.exp(-(X[:, 0] ** 2 + X[:, 1] ** 2))
```

If we plot this along with our data, we can see the effect of it:

```
In [29]: from mpl_toolkits import mplot3d
import ipywidgets as widgets
from ipywidgets import interact, interact_manual

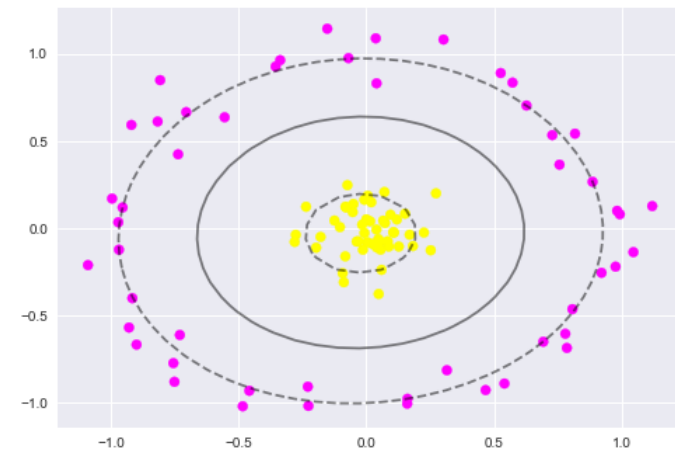
def plot_3D(elev=30, azim=30):
    ax = plt.subplot(projection='3d')
    ax.scatter3D(X[:, 0], X[:, 1], r, c=y, s=50, cmap='spring')
    ax.view_init(elev=elev, azim=azim)
    ax.set_xlabel('x')
    ax.set_ylabel('y')
    ax.set_zlabel('r')

interact(plot_3D, elev=(-90, 90), azip=(-180, 180));
```

We can see that with this additional dimension, the data becomes trivially linearly separable! This is a relatively simple kernel; SVM has a more sophisticated version of this kernel built-in to the process. This is accomplished by using `kernel='rbf'`, short for *radial basis function*:

```
In [30]: clf = SVC(kernel='rbf', gamma='auto')
clf.fit(X, y)

plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='spring')
plot_svc_decision_function(clf)
plt.scatter(clf.support_vectors_[:, 0], clf.support_vectors_[:, 1],
            s=200, facecolors='none');
```



Here there are effectively N basis functions: one centered at each point! Through a clever mathematical trick, this computation proceeds very efficiently using the "Kernel Trick", without actually constructing the matrix of kernel evaluations.

```
In [ ]:
```