CHAPTER

TWO

SCIKIT-LEARN TUTORIALS

2.1 An introduction to machine learning with scikit-learn

Section contents

In this section, we introduce the machine learning vocabulary that we use throughout scikit-learn and give a simple learning example.

2.1.1 Machine learning: the problem setting

In general, a learning problem considers a set of n samples of data and then tries to predict properties of unknown data. If each sample is more than a single number and, for instance, a multi-dimensional entry (aka multivariate data), it is said to have several attributes or **features**.

We can separate learning problems in a few large categories:

- supervised learning, in which the data comes with additional attributes that we want to predict (*Click here* to go to the scikit-learn supervised learning page).This problem can be either:
  - classification: samples belong to two or more classes and we want to learn from already labeled data how to predict the class of unlabeled data. An example of classification problem would be the handwritten digit recognition example, in which the aim is to assign each input vector to one of a finite number of discrete categories. Another way to think of classification is as a discrete (as opposed to continuous) form of supervised learning where one has a limited number of categories and for each of the n samples provided, one is to try to label them with the correct category or class.
  - regression: if the desired output consists of one or more continuous variables, then the task is called *regression*. An example of a regression problem would be the prediction of the length of a salmon as a function of its age and weight.
- unsupervised learning, in which the training data consists of a set of input vectors x without any corresponding target values. The goal in such problems may be to discover groups of similar examples within the data, where it is called clustering, or to determine the distribution of data within the input space, known as density estimation, or to project the data from a high-dimensional space down to two or three dimensions for the purpose of *visualization* (*Click here* to go to the Scikit-Learn unsupervised learning page).

Training set and testing set

Machine learning is about learning some properties of a data set and applying them to new data. This is why a common practice in machine learning to evaluate an algorithm is to split the data at hand into two sets, one that we call the **training set** on which we learn data properties and one that we call the **testing set** on which we test these properties.

2.1.2 Loading an example dataset

scikit-learn comes with a few standard datasets, for instance the iris and digits datasets for classification and the boston house prices dataset for regression.

In the following, we start a Python interpreter from our shell and then load the `iris` and `digits` datasets. Our notational convention is that `$` denotes the shell prompt while `>>>` denotes the Python interpreter prompt:

```
$ python
>>> from sklearn import datasets
>>> iris = datasets.load_iris()
>>> digits = datasets.load_digits()
```

A dataset is a dictionary-like object that holds all the data and some metadata about the data. This data is stored in the `.data` member, which is a `n_samples,n_features` array. In the case of supervised problem, one or more response variables are stored in the `.target` member. More details on the different datasets can be found in the *dedicated section*.

For instance, in the case of the digits dataset, `digits.data` gives access to the features that can be used to classify the digits samples:

```
>>> print(digits.data)
[[  0.   0.   5. ...,   0.   0.   0.]
 [  0.   0.   0. ...,  10.   0.   0.]
 [  0.   0.   0. ...,  16.   9.   0.]
 ...,
 [  0.   0.   1. ...,   6.   0.   0.]
 [  0.   0.   2. ...,  12.   0.   0.]
 [  0.   0.  10. ...,  12.   1.   0.]]
```

and `digits.target` gives the ground truth for the digit dataset, that is the number corresponding to each digit image that we are trying to learn:

```
>>> digits.target
array([0, 1, 2, ..., 8, 9, 8])
```

Shape of the data arrays

The data is always a 2D array, shape `(n_samples,n_features)`, although the original data may have had a different shape. In the case of the digits, each original sample is an image of shape `(8,8)` and can be accessed using:

```
>>> digits.images[0]
array([[  0.,   0.,   5.,  13.,   9.,   1.,   0.,   0.],
       [  0.,   0.,  13.,  15.,  10.,  15.,   5.,   0.],
       [  0.,   3.,  15.,   2.,   0.,  11.,   8.,   0.],
       [  0.,   4.,  12.,   0.,   0.,   8.,   8.,   0.],
       [  0.,   5.,   8.,   0.,   0.,   9.,   8.,   0.],
       [  0.,   4.,  11.,   0.,   1.,  12.,   7.,   0.],
       [  0.,   2.,  14.,   5.,  10.,  12.,   0.,   0.],
       [  0.,   0.,   6.,  13.,  10.,   0.,   0.,   0.]])
```

The *simple example on this dataset* illustrates how starting from the original problem one can shape the data for consumption in scikit-learn.

Loading from external datasets

To load from an external dataset, please refer to *loading external datasets*.

2.1.3 Learning and predicting

In the case of the digits dataset, the task is to predict, given an image, which digit it represents. We are given samples of each of the 10 possible classes (the digits zero through nine) on which we *fit* an estimator to be able to *predict* the classes to which unseen samples belong.

In scikit-learn, an estimator for classification is a Python object that implements the methods `fit(X,y)` and `predict(T)`.

An example of an estimator is the class `sklearn.svm.SVC` that implements support vector classification. The constructor of an estimator takes as arguments the parameters of the model, but for the time being, we will consider the estimator as a black box:

```
>>> from sklearn import svm
>>> clf = svm.SVC(gamma=0.001, C=100.)
```

Choosing the parameters of the model

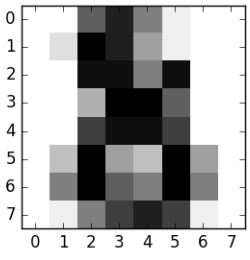
In this example we set the value of `gamma` manually. It is possible to automatically find good values for the parameters by using tools such as *grid search* and *cross validation*.

We call our estimator instance `clf`, as it is a classifier. It now must be fitted to the model, that is, it must *learn* from the model. This is done by passing our training set to the `fit` method. As a training set, let us use all the images of our dataset apart from the last one. We select this training set with the `[:-1]` Python syntax, which produces a new array that contains all but the last entry of `digits.data`:

```
>>> clf.fit(digits.data[:-1], digits.target[:-1])
SVC(C=100.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma=0.001, kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

Now you can predict new values, in particular, we can ask to the classifier what is the digit of our last image in the `digits` dataset, which we have not used to train the classifier:

```
>>> clf.predict(digits.data[-1:])
array([8])
```

The corresponding image is the following:  As you can see, it is a challenging task: the images are of poor resolution. Do you agree with the classifier?

A complete example of this classification problem is available as an example that you can run and study: *Recognizing hand-written digits*.

2.1.4 Model persistence

It is possible to save a model in the scikit by using Python's built-in persistence model, namely pickle:

```
>>> from sklearn import svm
>>> from sklearn import datasets
>>> clf = svm.SVC()
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
>>> clf.fit(X, y)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)

>>> import pickle
>>> s = pickle.dumps(clf)
>>> clf2 = pickle.loads(s)
>>> clf2.predict(X[0:1])
array([0])
>>> y[0]
0
```

In the specific case of the scikit, it may be more interesting to use joblib's replacement of pickle (`joblib.dump` & `joblib.load`), which is more efficient on big data, but can only pickle to the disk and not to a string:

```
>>> from sklearn.externals import joblib
>>> joblib.dump(clf, 'filename.pkl')
```

Later you can load back the pickled model (possibly in another Python process) with:

```
>>> clf = joblib.load('filename.pkl')
```

Note: `joblib.dump` and `joblib.load` functions also accept file-like object instead of filenames. More information on data persistence with Joblib is available here.

Note that pickle has some security and maintainability issues. Please refer to section *Model persistence* for more detailed information about model persistence with scikit-learn.

2.1.5 Conventions

scikit-learn estimators follow certain rules to make their behavior more predictive.

Type casting

Unless otherwise specified, input will be cast to `float64`:

```
>>> import numpy as np
>>> from sklearn import random_projection

>>> rng = np.random.RandomState(0)
>>> X = rng.rand(10, 2000)
>>> X = np.array(X, dtype='float32')
>>> X.dtype
dtype('float32')

>>> transformer = random_projection.GaussianRandomProjection()
>>> X_new = transformer.fit_transform(X)
>>> X_new.dtype
dtype('float64')
```

In this example, `X` is `float32`, which is cast to `float64` by `fit_transform(X)`.

Regression targets are cast to `float64`, classification targets are maintained:

```
>>> from sklearn import datasets
>>> from sklearn.svm import SVC
>>> iris = datasets.load_iris()
>>> clf = SVC()
>>> clf.fit(iris.data, iris.target)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)

>>> list(clf.predict(iris.data[:3]))
[0, 0, 0]

>>> clf.fit(iris.data, iris.target_names[iris.target])
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)

>>> list(clf.predict(iris.data[:3]))
['setosa', 'setosa', 'setosa']
```

Here, the first `predict()` returns an integer array, since `iris.target` (an integer array) was used in `fit`. The second `predict()` returns a string array, since `iris.target_names` was for fitting.

Refitting and updating parameters

Hyper-parameters of an estimator can be updated after it has been constructed via the *sklearn.pipeline.Pipeline.set_params* method. Calling `fit()` more than once will overwrite what was learned by any previous `fit()`:

```
>>> import numpy as np
>>> from sklearn.svm import SVC

>>> rng = np.random.RandomState(0)
>>> X = rng.rand(100, 10)
>>> y = rng.binomial(1, 0.5, 100)
>>> X_test = rng.rand(5, 10)

>>> clf = SVC()
>>> clf.set_params(kernel='linear').fit(X, y)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
>>> clf.predict(X_test)
array([1, 0, 1, 1, 0])

>>> clf.set_params(kernel='rbf').fit(X, y)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
>>> clf.predict(X_test)
array([0, 0, 0, 1, 0])
```

Here, the default kernel `rbf` is first changed to `linear` after the estimator has been constructed via `SVC()`, and changed back to `rbf` to refit the estimator and to make a second prediction.

Multiclass vs. multilabel fitting

When using *multiclass classifiers*, the learning and prediction task that is performed is dependent on the format of the target data fit upon:

```
>>> from sklearn.svm import SVC
>>> from sklearn.multiclass import OneVsRestClassifier
>>> from sklearn.preprocessing import LabelBinarizer

>>> X = [[1, 2], [2, 4], [4, 5], [3, 2], [3, 1]]
>>> y = [0, 0, 1, 1, 2]

>>> classif = OneVsRestClassifier(estimator=SVC(random_state=0))
>>> classif.fit(X, y).predict(X)
array([0, 0, 1, 1, 2])
```

In the above case, the classifier is fit on a 1d array of multiclass labels and the `predict()` method therefore provides corresponding multiclass predictions. It is also possible to fit upon a 2d array of binary label indicators:

```
>>> y = LabelBinarizer().fit_transform(y)
>>> classif.fit(X, y).predict(X)
array([[1, 0, 0],
       [1, 0, 0],
       [0, 1, 0],
       [0, 0, 0],
       [0, 0, 0]])
```

Here, the classifier is `fit()` on a 2d binary label representation of `y`, using the *LabelBinarizer*. In this case `predict()` returns a 2d array representing the corresponding multilabel predictions.

Note that the fourth and fifth instances returned all zeroes, indicating that they matched none of the three labels `fit` upon. With multilabel outputs, it is similarly possible for an instance to be assigned multiple labels:

```
>> from sklearn.preprocessing import MultiLabelBinarizer
>> y = [[0, 1], [0, 2], [1, 3], [0, 2, 3], [2, 4]]
>> y = preprocessing.MultiLabelBinarizer().fit_transform(y)
>> classif.fit(X, y).predict(X)
array([[1, 1, 0, 0, 0],
       [1, 0, 1, 0, 0],
       [0, 1, 0, 1, 0],
       [1, 0, 1, 1, 0],
       [0, 0, 1, 0, 1]])
```

In this case, the classifier is fit upon instances each assigned multiple labels. The *MultiLabelBinarizer* is used to binarize the 2d array of multilabels to `fit` upon. As a result, `predict()` returns a 2d array with multiple predicted labels for each instance.

2.2 A tutorial on statistical-learning for scientific data processing

Statistical learning

Machine learning is a technique with a growing importance, as the size of the datasets experimental sciences are facing is rapidly growing. Problems it tackles range from building a prediction function linking different observations, to classifying observations, or learning the structure in an unlabeled dataset.

This tutorial will explore *statistical learning*, the use of machine learning techniques with the goal of statistical inference: drawing conclusions on the data at hand.

Scikit-learn is a Python module integrating classic machine learning algorithms in the tightly-knit world of scientific Python packages (NumPy, SciPy, matplotlib).

2.2.1 Statistical learning: the setting and the estimator object in scikit-learn

Datasets

Scikit-learn deals with learning information from one or more datasets that are represented as 2D arrays. They can be understood as a list of multi-dimensional observations. We say that the first axis of these arrays is the **samples** axis, while the second is the **features** axis.

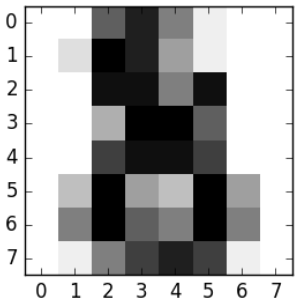
A simple example shipped with the scikit: iris dataset

```
>>> from sklearn import datasets
>>> iris = datasets.load_iris()
>>> data = iris.data
>>> data.shape
(150, 4)
```

It is made of 150 observations of irises, each described by 4 features: their sepal and petal length and width, as detailed in `iris.DESCR`.

When the data is not initially in the `(n_samples, n_features)` shape, it needs to be preprocessed in order to be used by scikit-learn.

An example of reshaping data would be the digits dataset



The digits dataset is made of 1797 8x8 images of hand-written digits

```
>>> digits = datasets.load_digits()
>>> digits.images.shape
(1797, 8, 8)
>>> import matplotlib.pyplot as plt
>>> plt.imshow(digits.images[-1], cmap=plt.cm.gray_r)
<matplotlib.image.AxesImage object at ...>
```

To use this dataset with the scikit, we transform each 8x8 image into a feature vector of length 64

```
>>> data = digits.images.reshape((digits.images.shape[0], -1))
```

Estimators objects

Fitting data: the main API implemented by scikit-learn is that of the *estimator*. An estimator is any object that learns from data; it may be a classification, regression or clustering algorithm or a *transformer* that extracts/filters useful features from raw data.

All estimator objects expose a `fit` method that takes a dataset (usually a 2-d array):

```
>>> estimator.fit(data)
```

Estimator parameters: All the parameters of an estimator can be set when it is instantiated or by modifying the corresponding attribute:

```
>>> estimator = Estimator(param1=1, param2=2)
>>> estimator.param1
1
```

Estimated parameters: When data is fitted with an estimator, parameters are estimated from the data at hand. All the estimated parameters are attributes of the estimator object ending by an underscore:

```
>>> estimator.estimated_param_
```

2.2.2 Supervised learning: predicting an output variable from high-dimensional observations

The problem solved in supervised learning

Supervised learning consists in learning the link between two datasets: the observed data `X` and an external variable `y` that we are trying to predict, usually called "target" or "labels". Most often, `y` is a 1D array of length `n_samples`.

All supervised estimators in scikit-learn implement a `fit(X, y)` method to fit the model and a `predict(X)` method that, given unlabeled observations `X`, returns the predicted labels `y`.

Vocabulary: classification and regression

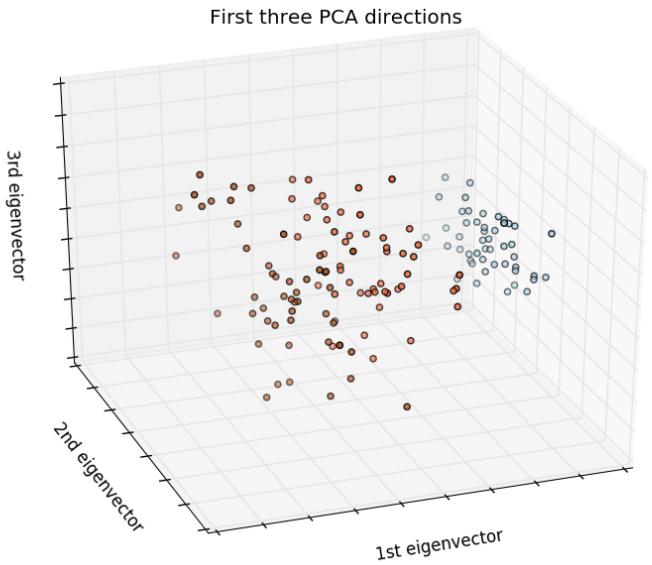
If the prediction task is to classify the observations in a set of finite labels, in other words to "name" the objects observed, the task is said to be a **classification** task. On the other hand, if the goal is to predict a continuous target variable, it is said to be a **regression** task.

When doing classification in scikit-learn, `y` is a vector of integers or strings.

Note: See the *Introduction to machine learning with scikit-learn Tutorial* for a quick run-through on the basic machine learning vocabulary used within scikit-learn.

Nearest neighbor and the curse of dimensionality

Classifying irises:



The iris dataset is a classification task consisting in identifying 3 different types of irises (Setosa, Versicolour, and Virginica) from their petal and sepal length and width:

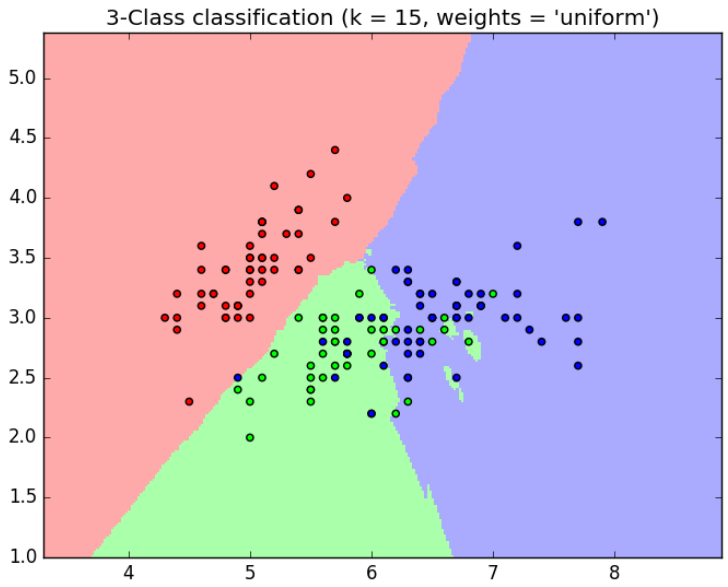
```
>>> import numpy as np
>>> from sklearn import datasets
>>> iris = datasets.load_iris()
>>> iris_X = iris.data
>>> iris_y = iris.target
>>> np.unique(iris_y)
array([0, 1, 2])
```

k-Nearest neighbors classifier

The simplest possible classifier is the nearest neighbor: given a new observation `X_test`, find in the training set (i.e. the data used to train the estimator) the observation with the closest feature vector. (Please see the *Nearest Neighbors section* of the online Scikit-learn documentation for more information about this type of classifier.)

Training set and testing set

While experimenting with any learning algorithm, it is important not to test the prediction of an estimator on the data used to fit the estimator as this would not be evaluating the performance of the estimator on **new data**. This is why datasets are often split into *train* and *test* data.



KNN (k nearest neighbors) classification example:

```
>>> # Split iris data in train and test data
>>> # A random permutation, to split the data randomly
>>> np.random.seed(0)
>>> indices = np.random.permutation(len(iris_X))
>>> iris_X_train = iris_X[indices[:-10]]
>>> iris_y_train = iris_y[indices[:-10]]
>>> iris_X_test  = iris_X[indices[-10:]]
>>> iris_y_test  = iris_y[indices[-10:]]
>>> # Create and fit a nearest-neighbor classifier
>>> from sklearn.neighbors import KNeighborsClassifier
```

```
>>> knn = KNeighborsClassifier()
>>> knn.fit(iris_X_train, iris_y_train)
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
           metric_params=None, n_jobs=1, n_neighbors=5, p=2,
           weights='uniform')
>>> knn.predict(iris_X_test)
array([1, 2, 1, 0, 0, 0, 2, 1, 2, 0])
>>> iris_y_test
array([1, 1, 1, 0, 0, 0, 2, 1, 2, 0])
```

The curse of dimensionality

For an estimator to be effective, you need the distance between neighboring points to be less than some value d, which depends on the problem. In one dimension, this requires on average $n\ 1/d$ points. In the context of the above k-NN example, if the data is described by just one feature with values ranging from 0 to 1 and with n training observations, then new data will be no further away than $1/n$. Therefore, the nearest neighbor decision rule will be efficient as soon as $1/n$ is small compared to the scale of between-class feature variations.

If the number of features is p, you now require $n\ 1/d^p$ points. Let's say that we require 10 points in one dimension: now 10^p points are required in p dimensions to pave the $[0, 1]$ space. As p becomes large, the number of training points required for a good estimator grows exponentially.

For example, if each point is just a single number (8 bytes), then an effective k-NN estimator in a paltry p 20 dimensions would require more training data than the current estimated size of the entire internet ($\pm$1000 Exabytes or so).

This is called the curse of dimensionality and is a core problem that machine learning addresses.

Linear model: from regression to sparsity

Diabetes dataset

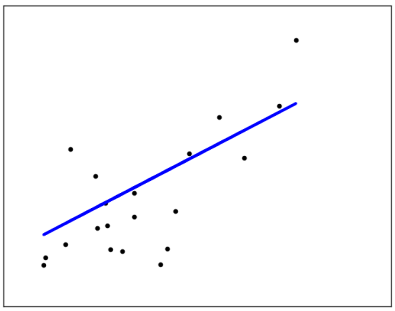
The diabetes dataset consists of 10 physiological variables (age, sex, weight, blood pressure) measure on 442 patients, and an indication of disease progression after one year:

```
>>> diabetes = datasets.load_diabetes()
>>> diabetes_X_train = diabetes.data[:-20]
>>> diabetes_X_test  = diabetes.data[-20:]
>>> diabetes_y_train = diabetes.target[:-20]
>>> diabetes_y_test  = diabetes.target[-20:]
```

The task at hand is to predict disease progression from physiological variables.

Linear regression

LinearRegression, in its simplest form, fits a linear model to the data set by adjusting a set of parameters in order to make the sum of the squared residuals of the model as small as possible.



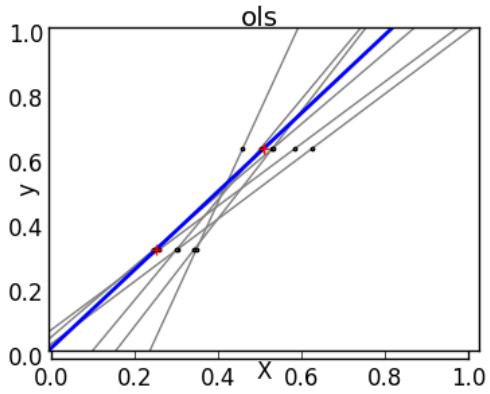
Linear models: $y = X\beta + \epsilon$

- X: data
- y: target variable
- β: Coefficients
- ϵ: Observation noise

```
>>> from sklearn import linear_model
>>> regr = linear_model.LinearRegression()
>>> regr.fit(diabetes_X_train, diabetes_y_train)
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1, normalize=False)
>>> print(regr.coef_)
[   0.30349955 -237.63931533  510.53060544  327.73698041 -814.13170937
  492.81458798  102.84845219  184.60648906  743.51961675   76.09517222]

>>> # The mean square error
>>> np.mean((regr.predict(diabetes_X_test)-diabetes_y_test)**2)
2004.56760268...

>>> # Explained variance score: 1 is perfect prediction
>>> # and 0 means that there is no linear relationship
>>> # between X and y.
>>> regr.score(diabetes_X_test, diabetes_y_test)
0.5850753022690...
```

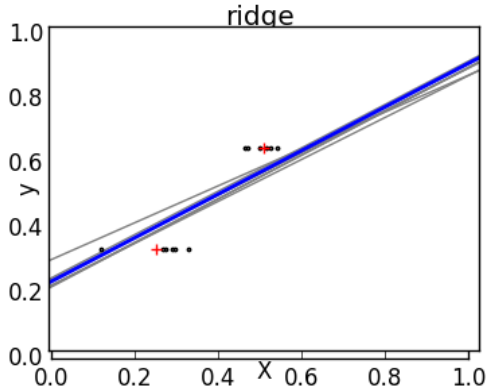
Shrinkage

If there are few data points per dimension, noise in the observations induces high variance:



```
>>> X = np.c_[ .5, 1].T
>>> y = [.5, 1]
>>> test = np.c_[ 0, 2].T
>>> regr = linear_model.LinearRegression()

>>> import matplotlib.pyplot as plt
>>> plt.figure()

>>> np.random.seed(0)
>>> for _ in range(6):
...     this_X = .1*np.random.normal(size=(2, 1)) + X
...     regr.fit(this_X, y)
...     plt.plot(test, regr.predict(test))
...     plt.scatter(this_X, y, s=3)
```

A solution in high-dimensional statistical learning is to *shrink* the regression coefficients to zero: any two randomly chosen set of observations are likely to be uncorrelated. This is called `Ridge` regression:




```
>>> regr = linear_model.Ridge(alpha=.1)

>>> plt.figure()

>>> np.random.seed(0)
>>> for _ in range(6):
...     this_X = .1*np.random.normal(size=(2, 1)) + X
...     regr.fit(this_X, y)
...     plt.plot(test, regr.predict(test))
...     plt.scatter(this_X, y, s=3)
```

This is an example of **bias/variance tradeoff**: the larger the ridge `alpha` parameter, the higher the bias and the lower the variance.

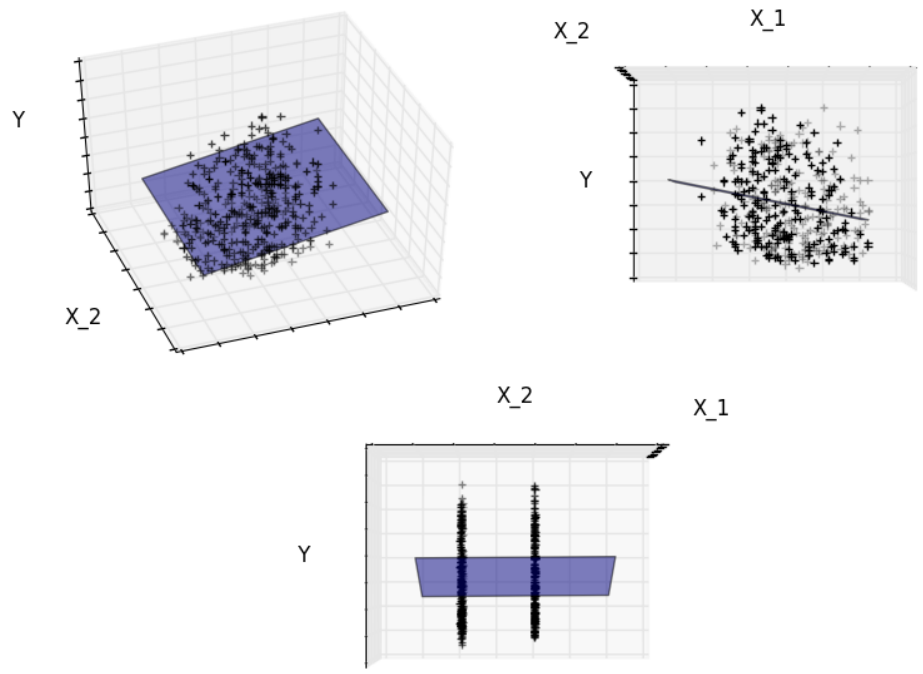
We can choose `alpha` to minimize left out error, this time using the diabetes dataset rather than our synthetic data:

```
>>> alphas = np.logspace(-4, -1, 6)
>>> from __future__ import print_function
>>> print([regr.set_params(alpha=alpha
...             ).fit(diabetes_X_train, diabetes_y_train,
...             ).score(diabetes_X_test, diabetes_y_test) for alpha in alphas])
[0.5851110683883..., 0.5852073015444..., 0.5854677540698..., 0.5855512036503..., 0.
↪5830717085554..., 0.57058999437...]
```

Note: Capturing in the fitted parameters noise that prevents the model to generalize to new data is called overfitting. The bias introduced by the ridge regression is called a regularization.

Sparsity

Fitting only features 1 and 2



Note: A representation of the full diabetes dataset would involve 11 dimensions (10 feature dimensions and one of the target variable). It is hard to develop an intuition on such representation, but it may be useful to keep in mind that it would be a fairly *empty* space.

We can see that, although feature 2 has a strong coefficient on the full model, it conveys little information on `y` when considered with feature 1.

To improve the conditioning of the problem (i.e. mitigating the *The curse of dimensionality*), it would be interesting to select only the informative features and set non-informative ones, like feature 2 to 0. Ridge regression will decrease their contribution, but not set them to zero. Another penalization approach, called *Lasso* (least absolute shrinkage and selection operator), can set some coefficients to zero. Such methods are called **sparse method** and sparsity can be seen as an application of Occam's razor: *prefer simpler models*.

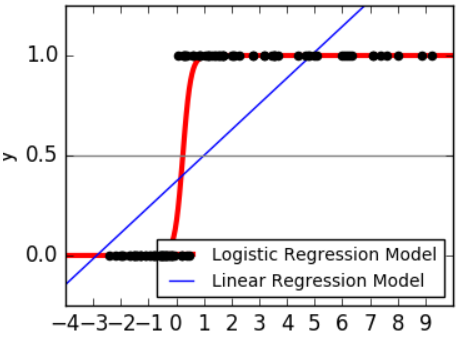
```
>>> regr = linear_model.Lasso()
>>> scores = [regr.set_params(alpha=alpha
...              ).fit(diabetes_X_train, diabetes_y_train
...              ).score(diabetes_X_test, diabetes_y_test)
...         for alpha in alphas]
>>> best_alpha = alphas[scores.index(max(scores))]
>>> regr.alpha = best_alpha
```

```
>>> regr.fit(diabetes_X_train, diabetes_y_train)
Lasso(alpha=0.025118864315095794, copy_X=True, fit_intercept=True,
   max_iter=1000, normalize=False, positive=False, precompute=False,
   random_state=None, selection='cyclic', tol=0.0001, warm_start=False)
>>> print(regr.coef_)
[   0.         -212.43764548  517.19478111  313.77959962 -160.8303982    -0.
 -187.19554705   69.38229038  508.66011217   71.84239008]
```

Different algorithms for the same problem

Different algorithms can be used to solve the same mathematical problem. For instance the `Lasso` object in scikit-learn solves the lasso regression problem using a coordinate decent method, that is efficient on large datasets. However, scikit-learn also provides the *`LassoLars`* object using the *LARS* algorithm, which is very efficient for problems in which the weight vector estimated is very sparse (i.e. problems with very few observations).

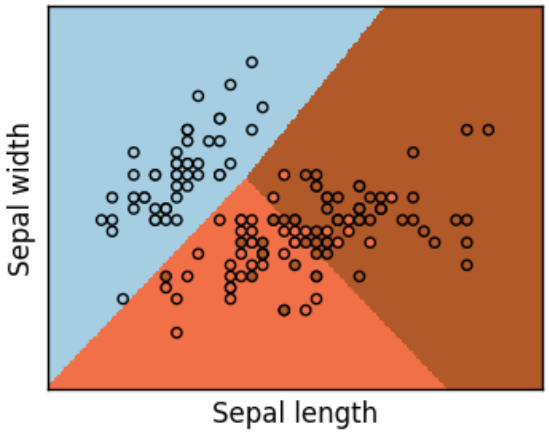
Classification



For classification, as in the labeling iris task, linear regression is not the right approach as it will give too much weight to data far from the decision frontier. A linear approach is to fit a sigmoid function or **logistic** function:

$$y = \text{sigmoid}(X\beta - \text{offset}) + \epsilon = \frac{1}{1 + \exp(-X\beta + \text{offset})} + \epsilon$$

```
>>> logistic = linear_model.LogisticRegression(C=1e5)
>>> logistic.fit(iris_X_train, iris_y_train)
LogisticRegression(C=100000.0, class_weight=None, dual=False,
          fit_intercept=True, intercept_scaling=1, max_iter=100,
          multi_class='ovr', n_jobs=1, penalty='l2', random_state=None,
          solver='liblinear', tol=0.0001, verbose=0, warm_start=False)
```



This is known as *LogisticRegression*.

Multiclass classification

If you have several classes to predict, an option often used is to fit one-versus-all classifiers and then use a voting heuristic for the final decision.

Shrinkage and sparsity with logistic regression

The `C` parameter controls the amount of regularization in the *LogisticRegression* object: a large value for `C` results in less regularization. `penalty="l2"` gives *Shrinkage* (i.e. non-sparse coefficients), while `penalty="l1"` gives *Sparsity*.

Exercise

Try classifying the digits dataset with nearest neighbors and a linear model. Leave out the last 10% and test prediction performance on these observations.

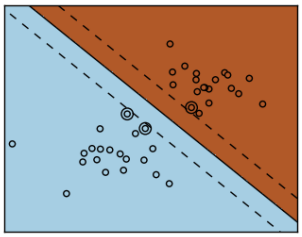
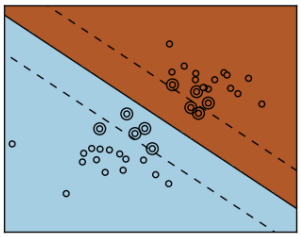
```
from sklearn import datasets, neighbors, linear_model

digits = datasets.load_digits()
X_digits = digits.data
y_digits = digits.target
```

Solution: `../../auto_examples/exercises/digits_classification_exercise.py`

Support vector machines (SVMs)

Linear SVMs

Support Vector Machines belong to the discriminant model family: they try to find a combination of samples to build a plane maximizing the margin between the two classes. Regularization is set by the `C` parameter: a small value for `C` means the margin is calculated using many or all of the observations around the separating line (more regularization); a large value for `C` means the margin is calculated on observations close to the separating line (less regularization).

Unregularized SVM	Regularized SVM (default)
	

Example:

- *Plot different SVM classifiers in the iris dataset*

SVMs can be used in regression –*SVR* (Support Vector Regression)–, or in classification –*SVC* (Support Vector Classification).

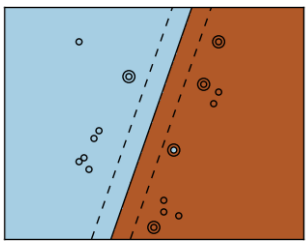
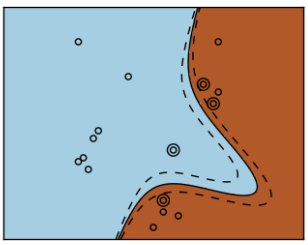
```
>>> from sklearn import svm
>>> svc = svm.SVC(kernel='linear')
>>> svc.fit(iris_X_train, iris_y_train)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
```

Warning: Normalizing data

For many estimators, including the SVMs, having datasets with unit standard deviation for each feature is important to get good prediction.

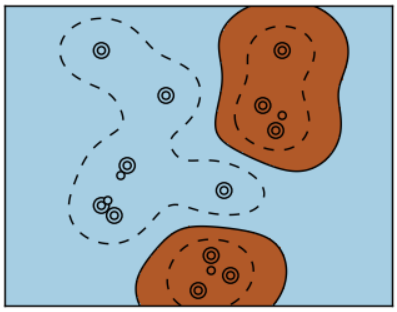
Using kernels

Classes are not always linearly separable in feature space. The solution is to build a decision function that is not linear but may be polynomial instead. This is done using the *kernel trick* that can be seen as creating a decision energy by positioning *kernels* on observations:

Linear kernel	Polynomial kernel
	

`>>> svc = svm.SVC(kernel='linear')`	`>>> svc = svm.SVC(kernel='poly',`
	`...  degree=3)`
	`>>> # degree: polynomial degree`

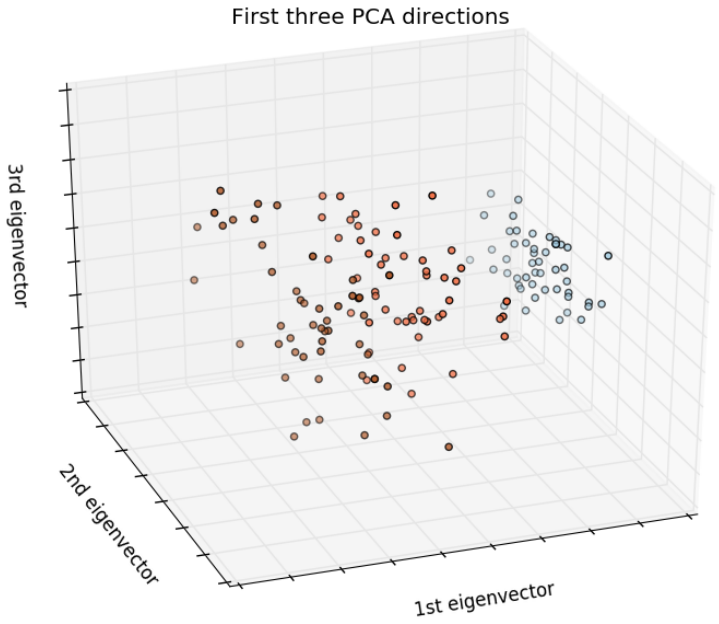
RBF kernel (Radial Basis Function)



```
>>> svc = svm.SVC(kernel='rbf')
>>> # gamma: inverse of size of
>>> # radial kernel
```

Interactive example

See the *SVM GUI* to download `svm_gui.py`; add data points of both classes with right and left button, fit the model and change parameters and data.



Exercise

Try classifying classes 1 and 2 from the iris dataset with SVMs, with the 2 first features. Leave out 10% of each class and test prediction performance on these observations.

Warning: the classes are ordered, do not leave out the last 10%, you would be testing on only one class.

Hint: You can use the `decision_function` method on a grid to get intuitions.

```
iris = datasets.load_iris()
X = iris.data
y = iris.target

X = X[y != 0, :2]
y = y[y != 0]
```

Solution: `../../auto_examples/exercises/plot_iris_exercise.py`

2.2.3 Model selection: choosing estimators and their parameters

Score, and cross-validated scores

As we have seen, every estimator exposes a `score` method that can judge the quality of the fit (or the prediction) on new data. **Bigger is better**.

```
>>> from sklearn import datasets, svm
>>> digits = datasets.load_digits()
>>> X_digits = digits.data
>>> y_digits = digits.target
>>> svc = svm.SVC(C=1, kernel='linear')
>>> svc.fit(X_digits[:-100], y_digits[:-100]).score(X_digits[-100:], y_digits[-100:])
0.97999999999999998
```

To get a better measure of prediction accuracy (which we can use as a proxy for goodness of fit of the model), we can successively split the data in *folds* that we use for training and testing:

```
>>> import numpy as np
>>> X_folds = np.array_split(X_digits, 3)
>>> y_folds = np.array_split(y_digits, 3)
>>> scores = list()
>>> for k in range(3):
...     # We use 'list' to copy, in order to 'pop' later on
...     X_train = list(X_folds)
...     X_test  = X_train.pop(k)
...     X_train = np.concatenate(X_train)
...     y_train = list(y_folds)
...     y_test  = y_train.pop(k)
...     y_train = np.concatenate(y_train)
...     scores.append(svc.fit(X_train, y_train).score(X_test, y_test))
>>> print(scores)
[0.93489148580968284, 0.95659432387312182, 0.93989983305509184]
```

This is called a *KFold* cross-validation.

Cross-validation generators

Scikit-learn has a collection of classes which can be used to generate lists of train/test indices for popular cross-validation strategies.

They expose a `split` method which accepts the input dataset to be split and yields the train/test set indices for each iteration of the chosen cross-validation strategy.

This example shows an example usage of the `split` method.

```
>>> from sklearn.model_selection import KFold, cross_val_score
>>> X = ["a", "a", "b", "c", "c", "c"]
>>> k_fold = KFold(n_splits=3)
>>> for train_indices, test_indices in k_fold.split(X):
...      print('Train: %s | test: %s' % (train_indices, test_indices))
Train: [2 3 4 5] | test: [0 1]
Train: [0 1 4 5] | test: [2 3]
Train: [0 1 2 3] | test: [4 5]
```

The cross-validation can then be performed easily:

```
>>> kfold = KFold(n_splits=3)
>>> [svc.fit(X_digits[train], y_digits[train]).score(X_digits[test], y_digits[test])
...           for train, test in k_fold.split(X_digits)]
[0.93489148580968284, 0.95659432387312182, 0.93989983305509184]
```

The cross-validation score can be directly calculated using the *cross_val_score* helper. Given an estimator, the cross-validation object and the input dataset, the *cross_val_score* splits the data repeatedly into a training and a testing set, trains the estimator using the training set and computes the scores based on the testing set for each iteration of cross-validation.

By default the estimator's `score` method is used to compute the individual scores.

Refer the *metrics module* to learn more on the available scoring methods.

```
>>> cross_val_score(svc, X_digits, y_digits, cv=k_fold, n_jobs=-1)
array([ 0.93489149,  0.95659432,  0.93989983])
```

n_jobs=-1 means that the computation will be dispatched on all the CPUs of the computer.

Alternatively, the `scoring` argument can be provided to specify an alternative scoring method.

```
>>> cross_val_score(svc, X_digits, y_digits, cv=k_fold,
...                 scoring='precision_macro')
array([ 0.93969761,  0.95911415,  0.94041254])
```

Cross-validation generators

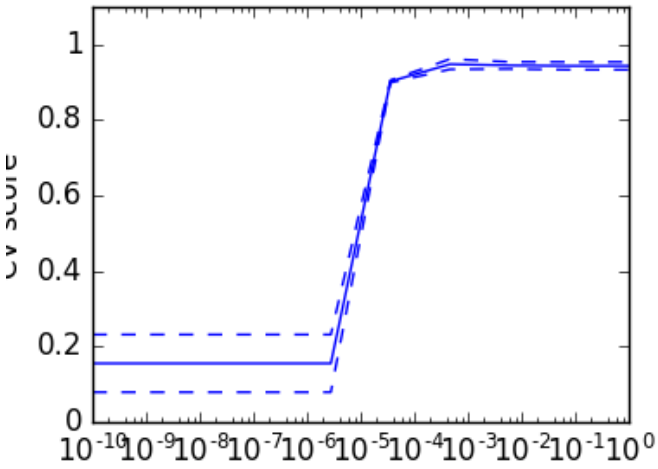
KFold **(n_splits, shuffle, random_state)**	*StratifiedKFold* **(n_iter, test_size, train_size, random_state)**	*GroupKFold* **(n_splits, shuffle, random_state)**
Splits it into K folds, trains on K-1 and then tests on the left-out.	Same as K-Fold but preserves the class distribution within each fold.	Ensures that the same group is not in both testing and training sets.

ShuffleSplit **(n_iter, test_size, train_size, random_state)**	*StratifiedShuffleSplit*	*GroupShuffleSplit*
Generates train/test indices based on random permutation.	Same as shuffle split but preserves the class distribution within each iteration.	Ensures that the same group is not in both testing and training sets.

LeaveOneGroupOut ()	*LeavePGroupsOut* **(p)**	*LeaveOneOut* ()
Takes a group array to group observations.	Leave P groups out.	Leave one observation out.

LeavePOut **(p)**	*PredefinedSplit*
Leave P observations out.	Generates train/test indices based on predefined splits.

Exercise



On the digits dataset, plot the cross-validation score of a *SVC* estimator with an linear kernel as a function of parameter `C` (use a logarithmic grid of points, from 1 to 10).

```
import numpy as np
from sklearn.model_selection import cross_val_score
from sklearn import datasets, svm

digits = datasets.load_digits()
X = digits.data
y = digits.target

svc = svm.SVC(kernel='linear')
C_s = np.logspace(-10, 0, 10)
```

Solution: *Cross-validation on Digits Dataset Exercise*

Grid-search and cross-validated estimators

Grid-search

scikit-learn provides an object that, given data, computes the score during the fit of an estimator on a parameter grid and chooses the parameters to maximize the cross-validation score. This object takes an estimator during the construction and exposes an estimator API:

```
>>> from sklearn.model_selection import GridSearchCV, cross_val_score
>>> Cs = np.logspace(-6, -1, 10)
>>> clf = GridSearchCV(estimator=svc, param_grid=dict(C=Cs),
...                    n_jobs=-1)
>>> clf.fit(X_digits[:1000], y_digits[:1000])
GridSearchCV(cv=None,...
>>> clf.best_score_
0.925...
>>> clf.best_estimator_.C
0.0077...
```

```
>>> # Prediction performance on test set is not as good as on train set
>>> clf.score(X_digits[1000:], y_digits[1000:])
0.943...
```

By default, the *GridSearchCV* uses a 3-fold cross-validation. However, if it detects that a classifier is passed, rather than a regressor, it uses a stratified 3-fold.

Nested cross-validation

```
>>> cross_val_score(clf, X_digits, y_digits)
...
array([ 0.938...,  0.963...,  0.944...])
```

Two cross-validation loops are performed in parallel: one by the *GridSearchCV* estimator to set `gamma` and the other one by `cross_val_score` to measure the prediction performance of the estimator. The resulting scores are unbiased estimates of the prediction score on new data.

Warning: You cannot nest objects with parallel computing (`n_jobs` different than 1).

Cross-validated estimators

Cross-validation to set a parameter can be done more efficiently on an algorithm-by-algorithm basis. This is why, for certain estimators, scikit-learn exposes *Cross-validation: evaluating estimator performance* estimators that set their parameter automatically by cross-validation:

```
>>> from sklearn import linear_model, datasets
>>> lasso = linear_model.LassoCV()
>>> diabetes = datasets.load_diabetes()
>>> X_diabetes = diabetes.data
>>> y_diabetes = diabetes.target
>>> lasso.fit(X_diabetes, y_diabetes)
LassoCV(alphas=None, copy_X=True, cv=None, eps=0.001, fit_intercept=True,
    max_iter=1000, n_alphas=100, n_jobs=1, normalize=False, positive=False,
    precompute='auto', random_state=None, selection='cyclic', tol=0.0001,
    verbose=False)
>>> # The estimator chose automatically its lambda:
>>> lasso.alpha_
0.01229...
```

These estimators are called similarly to their counterparts, with 'CV' appended to their name.

Exercise

On the diabetes dataset, find the optimal regularization parameter alpha.

Bonus: How much can you trust the selection of alpha?

```
from sklearn import datasets
from sklearn.linear_model import LassoCV
from sklearn.linear_model import Lasso
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score

diabetes = datasets.load_diabetes()
```

Solution: *Cross-validation on diabetes Dataset Exercise*

2.2.4 Unsupervised learning: seeking representations of the data

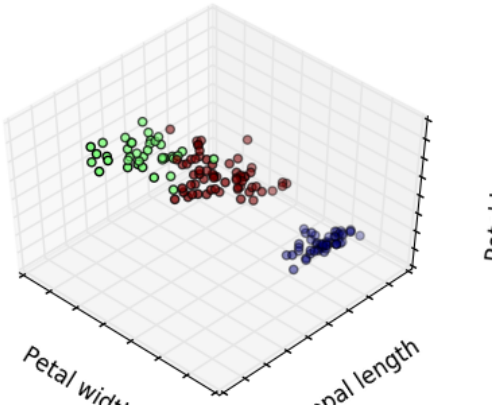
Clustering: grouping observations together

The problem solved in clustering

Given the iris dataset, if we knew that there were 3 types of iris, but did not have access to a taxonomist to label them: we could try a **clustering task**: split the observations into well-separated group called *clusters*.

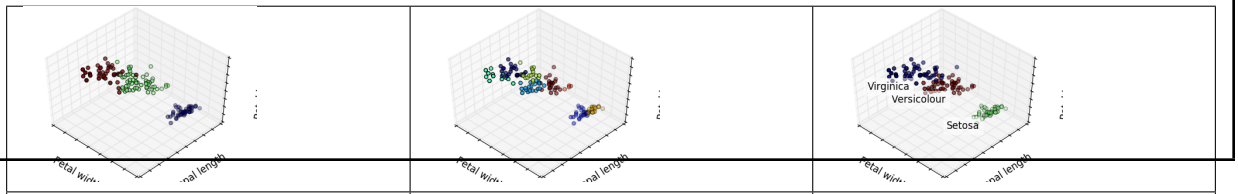
K-means clustering

Note that there exist a lot of different clustering criteria and associated algorithms. The simplest clustering algorithm is *K-means*.



```
>>> from sklearn import cluster, datasets
>>> iris = datasets.load_iris()
>>> X_iris = iris.data
>>> y_iris = iris.target

>>> k_means = cluster.KMeans(n_clusters=3)
>>> k_means.fit(X_iris)
KMeans(algorithm='auto', copy_x=True, init='k-means++', ...
>>> print(k_means.labels_[::10])
[1 1 1 1 1 0 0 0 0 0 2 2 2 2 2]
>>> print(y_iris[::10])
[0 0 0 0 0 1 1 1 1 1 2 2 2 2 2]
```

Warning: There is absolutely no guarantee of recovering a ground truth. First, choosing the right number of clusters is hard. Second, the algorithm is sensitive to initialization, and can fall into local minima, although scikit-learn employs several tricks to mitigate this issue.



Bad initialization | **8 clusters** | **Ground truth**