scikits.learn user guide

Release 0.8.1

scikits.learn developers

July 06, 2011

CONTENTS

`scikits.learn` is a Python module integrating classic machine learning algorithms in the tightly-knit world of scientific Python packages (numpy, scipy, matplotlib).
It aims to provide simple and efficient solutions to learning problems that are accessible to everybody and reusable in various contexts: **machine-learning as a versatile tool for science and engineering**.

Features

- **Solid**: *Supervised learning*: *Support Vector Machines*, *Generalized Linear Models*.
- **Work in progress**: *Unsupervised learning*: *Clustering*, *Gaussian mixture models*, manifold learning, *ICA*, *Gaussian Processes*
- **Planed**: Gaussian graphical models, matrix factorization

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Note: This document describes scikits.learn 0.8.1. For other versions and printable format, see *documentation_resources*.

CHAPTER

ONE

USER GUIDE

1.1 Installing *scikits.learn*

There are different ways to get scikits.learn installed:

- Install the version of scikits.learn provided by your *operating system distribution* . This is the quickest option for those who have operating systems that distribute scikits.learn.
- *Install an official release*. This is the best approach for users who want a stable version number and aren't concerned about running a slightly older version of scikits.learn.
- *Install the latest development version*. This is best for users who want the latest-and-greatest features and aren't afraid of running brand-new code.

1.1.1 Installing an official release

Installing from source

Installing from source requires you to have installed numpy, scipy, setuptools, python development headers and a working C++ compiler. Under debian-like systems you can get all this by executing with root privileges:

```
sudo apt-get install python-dev python-numpy python-numpy-dev python-setuptools python-numpy-dev pyth
```

Note: In Order to build the documentation and run the example code contains in this documentation you will need matplotlib:

```
sudo apt-get install python-matplotlib
```

Note: On Ubuntu LTS (10.04) the package *libatlas-dev* is called *libatlas-headers*

Easy install

This is usually the fastest way to install the latest stable release. If you have pip or easy_install, you can install or update with the command:

```
pip install -U scikits.learn
```

or:

```
easy_install -U scikits.learn
```

for easy_install. Note that you might need root privileges to run these commands.

From source package

Download the package from http://sourceforge.net/projects/scikit-learn/files , unpack the sources and cd into archive.

This packages uses distutils, which is the default way of installing python modules. The install command is:

```
python setup.py install
```

Windows installer

You can download a windows installer from downloads in the project's web page. Note that must also have installed the packages numpy and setuptools.

This package is also expected to work with python(x,y) as of 2.6.5.5.

Building on windows

To build scikits.learn on windows you will need a C/C++ compiler in addition to numpy, scipy and setuptools. At least MinGW (a port of GCC to Windows OS) and the Microsoft Visual C++ 2008 should work out of the box. To force the use of a particular compiler, write a file named `setup.cfg` in the source directory with the content:

```
[build_ext]
compiler=my_compiler

[build]
compiler=my_compiler
```

where `my_compiler` should be one of `mingw32` or `msvc`.

When the appropriate compiler has been set, and assuming Python is in your PATH (see Python FAQ for windows for more details), installation is done by executing the command:

```
python setup.py install
```

To build a precompiled package like the ones distributed at the downloads section, the command to execute is:

```
python setup.py bdist_wininst -b doc/logos/scikit-learn-logo.bmp
```

This will create an installable binary under directory `dist/`.

1.1.2 Third party distributions of scikits.learn

Some third-party distributions are now providing versions of scikits.learn integrated with their package-management systems.

These can make installation and upgrading much easier for users since the integration includes the ability to automatically install dependencies (numpy, scipy) that scikits.learn requires.

The following is a list of linux distributions that provide their own version of scikits.learn:

Debian and derivatives (Ubuntu)

The Debian package is named python-scikits-learn and can be install using the following commands with root privileges:

```
apt-get install python-scikits-learn
```

Python(x, y)

The Python(x, y) distributes scikit-learn as an additional plugin, which can be found in the Additional plugins page.

Enthought python distribution

The Enthought Python Distribution already ships the latest version.

Macports

The macport's package is named py26-scikits-learn and can be installed by typing the following command:

```
sudo port install py26-scikits-learn
```

NetBSD

scikits.learn is available via pkgsrc-wip:

http://pkgsrc.se/wip/py-scikits_learn

1.1.3 Bleeding Edge

See section *Retrieving the latest code* on how to get the development version.

1.1.4 Testing

Testing requires having the nose library. After installation, the package can be tested by executing *from outside* the source directory:

```
python -c "import scikits.learn as skl; skl.test()"
```

This should give you a lot of output (and some warnings) but eventually should finish with the a text similar to:

```
Ran 601 tests in 27.920s
OK (SKIP=2)
```

otherwise please consider posting an issue into the bug tracker or to the *mailing_lists*.

scikits.learn can also be tested without having the package installed. For this you must compile the sources inplace from the source directory:

```
python setup.py build_ext --inplace
```

Test can now be run using nosetest:

```
nosetests scikits/learn/
```

If you are running the deveopment version, this is automated in the commands *make in* and *make test*.

Warning: Because nosetest does not play well with multiprocessing on windows, this last approach is not recommended on such system.

1.2 Getting started: an introduction to machine learning with scikits.learn

Section contents

In this section, we introduce the machine learning vocabulary that we use through-out *scikits.learn* and give a simple learning example.

1.2.1 Machine learning: the problem setting

In general, a learning problem considers a set of n *samples* of data and try 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), is it 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. 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 digit recognition example, in which the aim is to assign each input vector to one of a finite number of discrete categories.
  - **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 thee dimensions for the purpose of *visualization*.

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 in two sets, one that we call a *training set* on which we learn data properties, and one that we call a *testing set*, on which we test these properties.

1.2.2 Loading an example dataset

scikits.learn comes with a few standard datasets, for instance the iris dataset, or the digits dataset:

```
>>> from scikits.learn 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, explanatory 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, *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 the *scikit.learn*.

`scikits.learn` also offers the possibility to reuse external datasets coming from the http://mlcomp.org online service that provides a repository of public datasets for various tasks (binary & multi label classification, regression, document classification, ...) along with a runtime environment to compare program performance on those datasets. Please refer to the following example for for instructions on the `mlcomp` dataset loader: *example mlcomp sparse document classification*.

1.2.3 Learning and Predicting

In the case of the digits dataset, the task is to predict the value of a hand-written digit from an image. We are given samples of each of the 10 possible classes on which we *fit* an *estimator* to be able to *predict* the labels corresponding to new data.

In *scikit.learn*, an *estimator* is just a plain Python class that implements the methods *fit(X, Y)* and *predict(T)*.

An example of estimator is the class `scikits.learn.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 and not worry about these:

```
>>> from scikits.learn import svm
>>> clf = svm.SVC()
```

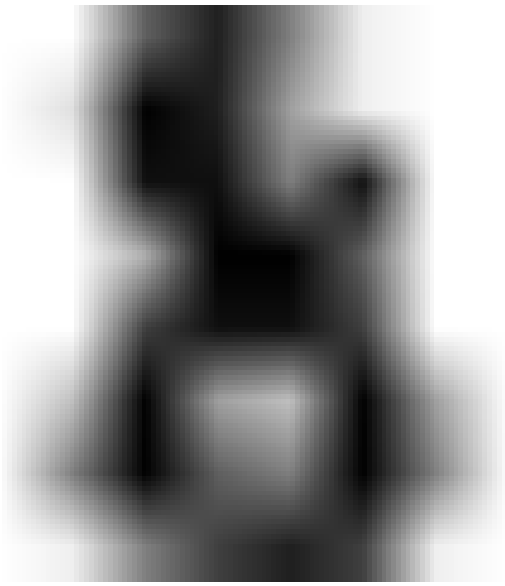
We call our estimator instance *clf* as it is a classifier. It now must be fitted to the model, that is, it must *learn* from the model. This is done by passing our training set to the `fit` method. As a training set, let us use all the images of our dataset apart from the last one:

```
>>> clf.fit(digits.data[:-1], digits.target[:-1])
SVC(kernel='rbf', C=1.0, probability=False, degree=3, coef0=0.0, tol=0.001,
  cache_size=100.0, shrinking=True, gamma=0.000556792873051)
```

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*.

1.2.4 Model persistence

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

```
>>> from scikits.learn import svm
>>> from scikits.learn import datasets
>>> clf = svm.SVC()
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
>>> clf.fit(X, y)
SVC(kernel='rbf', C=1.0, probability=False, degree=3, coef0=0.0, tol=0.001,
  cache_size=100.0, shrinking=True, gamma=0.00666666666667)
>>> import pickle
>>> s = pickle.dumps(clf)
>>> clf2 = pickle.loads(s)
>>> clf2.predict(X[0])
array([ 0.])
>>> y[0]
0
```

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

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

1.3 Supervised learning

1.3.1 Generalized Linear Models

The following are a set of methods intended for regression in which the target value is expected to be a linear combination of the input variables. In mathematical notion, if $\hat{y}$ is the predicted value.

$$\hat{y}(\beta, x) = \beta_0 + \beta_1 x_1 + ... + \beta_D x_D$$

Across the module, we designate the vector $\beta = (\beta_1, ..., \beta_D)$ as `coef_` and β_0 as `intercept_`.

To perform classification with generalized linear models, see *Logisitic regression*.

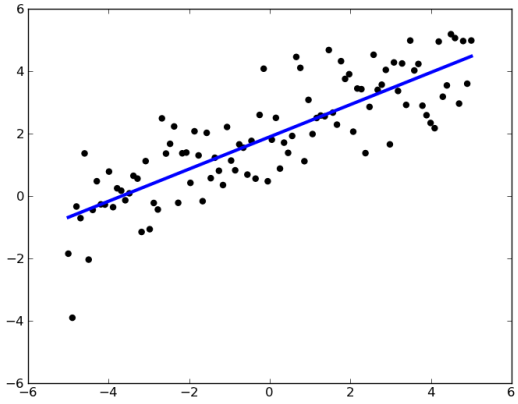
Ordinary Least Squares (OLS)

`LinearRegression` fits a linear model with coefficients $\beta = (\beta_1, ..., \beta_D)$ to minimize the residual sum of squares between the observed responses in the dataset, and the responses predicted by the linear approximation.

`LinearRegression` will take in its *fit* method arrays X, y and will store the coefficients w of the linear model in its *coef_* member.

```
>>> from scikits.learn import linear_model
>>> clf = linear_model.LinearRegression()
>>> clf.fit ([[0, 0], [1, 1], [2, 2]], [0, 1, 2])
LinearRegression(fit_intercept=True)
>>> clf.coef_
array([ 0.5,  0.5])
```

However, coefficient estimates for Ordinary Least Squares rely on the independence of the model terms. When terms are correlated and the columns of the design matrix X have an approximate linear dependence, the matrix $X(X^T X)^{-1}$ becomes close to singular and as a result, the least-squares estimate becomes highly sensitive to random errors in the



observed response, producing a large variance. This situation of *multicollinearity* can arise, for example, when data are collected without an experimental design.

Examples:

- *Ordinary Least Squares*

OLS Complexity

This method computes the least squares solution using a singular value decomposition of X. If X is a matrix of size (n, p) this method has a cost of $O(np^2)$, assuming that $n \geq p$.

Ridge Regression

`Ridge` regression addresses some of the problems of *Ordinary Least Squares (OLS)* by imposing a penalty on the size of coefficients. The ridge coefficients minimize a penalized residual sum of squares,

$$\beta^{ridge} = \underset{\beta}{argmin} \sum_{i=1} N(y_i - \beta_0 - \sum_{j=1} px_i j\beta_j)^2 + \alpha \sum_{j=1} p\beta_j^2$$

Here, $\alpha \geq 0$ is a complexity parameter that controls the amount of shrinkage: the larger the value of α, the greater the amount of shrinkage:

```
>>> from scikits.learn import linear_model
>>> clf = linear_model.Ridge (alpha = .5)
>>> clf.fit ([[0, 0], [0, 0], [1, 1]], [0, .1, 1])
Ridge(alpha=0.5, fit_intercept=True)
>>> clf.coef_
array([ 0.34545455,  0.34545455])
>>> clf.intercept_
0.13636...
```

Ridge Complexity

This method has the same order of complexity than an *Ordinary Least Squares (OLS)*.

Generalized Cross-Validation

`RidgeCV` implements ridge regression with built-in cross-validation of the alpha parameter. The object works in the same way as GridSearchCV except that it defaults to Generalized Cross-Validation (GCV), an efficient form of leave-one-out cross-validation.

```
>>> from scikits.learn import linear_model
>>> clf = linear_model.RidgeCV(alphas=[0.1, 1.0, 10.0])
>>> clf.fit ([[0, 0], [0, 0], [1, 1]], [0, .1, 1])
RidgeCV(alphas=[0.1, 1.0, 10.0], loss_func=None, cv=None, score_func=None,
    fit_intercept=True)
>>> clf.best_alpha
0.10000000000000001
```

References

- "Notes on Regularized Least Squares", Rifkin & Lippert (technical report, course slides).

Lasso

The `Lasso` is a linear model trained with L1 prior as regularizer. The objective function to minimize is:

$$0.5 * ||y - Xw||_2^2 + \alpha * ||w||_1$$

The lasso estimate thus solves the minimization of the least-squares penalty with $\alpha * ||w||_1$ added, where α is a constant and $||w||_1$ is the L1-norm of the parameter vector.

This formulation is useful in some contexts due to its tendency to prefer solutions with fewer parameter values, effectively reducing the number of variables upon which the given solution is dependent. For this reason, the Lasso and its variants are fundamental to the field of compressed sensing.

This implementation uses coordinate descent as the algorithm to fit the coefficients. See *Least Angle Regression* for another implementation.

```
>>> clf = linear_model.Lasso(alpha = 0.1)
>>> clf.fit ([[0, 0], [1, 1]], [0, 1])
Lasso(alpha=0.1, fit_intercept=True)
>>> clf.predict ([[1, 1]])
array([ 0.8])
```

The function `lasso_path` computes the coefficients along the full path of possible values.

Examples:

- *Lasso regression example*,
- *Lasso parameter estimation with path and cross-validation*

Elastic Net

`ElasticNet` is a linear model trained with L1 and L2 prior as regularizer.

The objective function to minimize is in this case

$$0.5 * ||y - Xw||_2^2 + \alpha * \rho * ||w||_1 + \alpha * (1 - \rho) * 0.5 * ||w||_2^2$$

Examples:

- *Lasso regression example*
- *Lasso and Elastic Net*

Least Angle Regression

Least-angle regression (LARS) is a regression algorithm for high-dimensional data, developed by Bradley Efron, Trevor Hastie, Iain Johnstone and Robert Tibshirani.

The advantages of LARS are:

- It is computationally just as fast as forward selection and has the same order of complexity as an ordinary least squares.
- It produces a full piecewise linear solution path, which is useful in cross-validation or similar attempts to tune the model.
- If two variables are almost equally correlated with the response, then their coefficients should increase at approximately the same rate. The algorithm thus behaves as intuition would expect, and also is more stable.
- It is easily modified to produce solutions for other estimators, like the Lasso.
- It is effective in contexts where p >> n (i.e., when the number of dimensions is significantly greater than the number of points)

The disadvantages of the LARS method include:

- Because LARS is based upon an iterative refitting of the residuals, it would appear to be especially sensitive to the effects of noise. This problem is discussed in detail by Weisberg in the discussion section of the Efron et al. (2004) Annals of Statistics article.

The LARS model can be used using estimator `LARS`, or its low-level implementation `lars_path`.

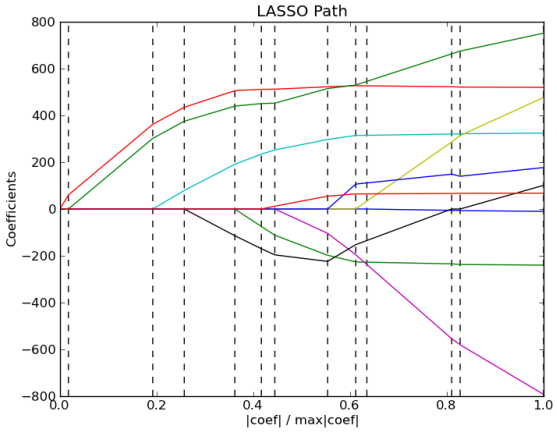
LARS Lasso

`LassoLARS` is a lasso model implemented using the LARS algorithm, and unlike the implementation based on coordinate_descent, this yields the exact solution, which is piecewise linear as a function of the norm of its coefficients.

```
>>> from scikits.learn import linear_model
>>> clf = linear_model.LassoLARS(alpha=.1)
>>> clf.fit ([[0, 0], [1, 1]], [0, 1])
LassoLARS(alpha=0.1, verbose=False, fit_intercept=True)
>>> clf.coef_
array([ 0.30710678,  0.        ])
```

Examples:

- *Lasso path using LARS*



The LARS algorithm provides the full path of the coefficients along the regularization parameter almost for free, thus a common operation consist of retrieving the path with function `lars_path`

Mathematical formulation

The algorithm is similar to forward stepwise regression, but instead of including variables at each step, the estimated parameters are increased in a direction equiangular to each one's correlations with the residual.

Instead of giving a vector result, the LARS solution consists of a curve denoting the solution for each value of the L1 norm of the parameter vector. The full coeffients path is stored in the array `coef_path_`, which has size (n_features, max_features+1). The first column is always zero.

References:

- Original Algorithm is detailed in the paper Least Angle Regression by Hastie et al.

Bayesian Regression

Bayesian regression techniques can be used to include regularization parameters in the estimation procedure. This can be done by introducing some prior knowledge over the parameters. For example, penalization by weighted ℓ_2 norm is equivalent to setting Gaussian priors on the weights.

The advantages of *Bayesian Regression* are:

- It adapts to the data at hand.
- It can be used to include regularization parameters in the estimation procedure.

The disadvantages of *Bayesian Regression* include:

- Inference of the model can be time consuming.

Bayesian Ridge Regression

`BayesianRidge` tries to avoid the overfit issue of *Ordinary Least Squares (OLS)*, by adding the following prior on β:

$$p(\beta|\lambda) = \mathcal{N}(\beta|0, \lambda^{-1}\mathbf{I_p})$$

The resulting model is called *Bayesian Ridge Regression*, it is similar to the classical `Ridge`. λ is an *hyper-parameter* and the prior over β performs a shrinkage or regularization, by constraining the values of the weights to be small. Indeed, with a large value of λ, the Gaussian is narrowed around 0 which does not allow large values of β, and with low value of λ, the Gaussian is very flattened which allows values of β. Here, we use a *non-informative* prior for λ. The parameters are estimated by maximizing the *marginal log likelihood*. There is also a Gamma prior for λ and α:

$$g(\alpha|\alpha_1, \alpha_2) = \frac{\alpha_2^{\alpha_1}}{\Gamma(\alpha_1)}\alpha^{\alpha_1 - 1}e^{-\alpha_2\alpha}$$

$$g(\lambda|\lambda_1, \lambda_2) = \frac{\lambda_2^{\lambda_1}}{\Gamma(\lambda_1)}\lambda^{\lambda_1 - 1}e^{-\lambda_2\lambda}$$

By default $\alpha_1 = \alpha_2 = \lambda_1 = \lambda_2 = 1.e^{-6}$**, *i.e.*** very slightly informative priors.

Bayesian Ridge Regression is used for regression:

```
>>> from scikits.learn import linear_model
>>> X = [[0., 0.], [1., 1.], [2., 2.], [3., 3.]]
>>> Y = [0., 1., 2., 3.]
>>> clf = linear_model.BayesianRidge()
>>> clf.fit (X, Y)
BayesianRidge(n_iter=300, verbose=False, lambda_1=1e-06, lambda_2=1e-06,
       fit_intercept=True, eps=0.001, alpha_2=1e-06, alpha_1=1e-06,
       compute_score=False)
```

After being fitted, the model can then be used to predict new values:

```
>>> clf.predict ([[1, 0.]])
array([ 0.50000013])
```

The weights β of the model can be access:

```
>>> clf.coef_
array([ 0.49999993,  0.49999993])
```

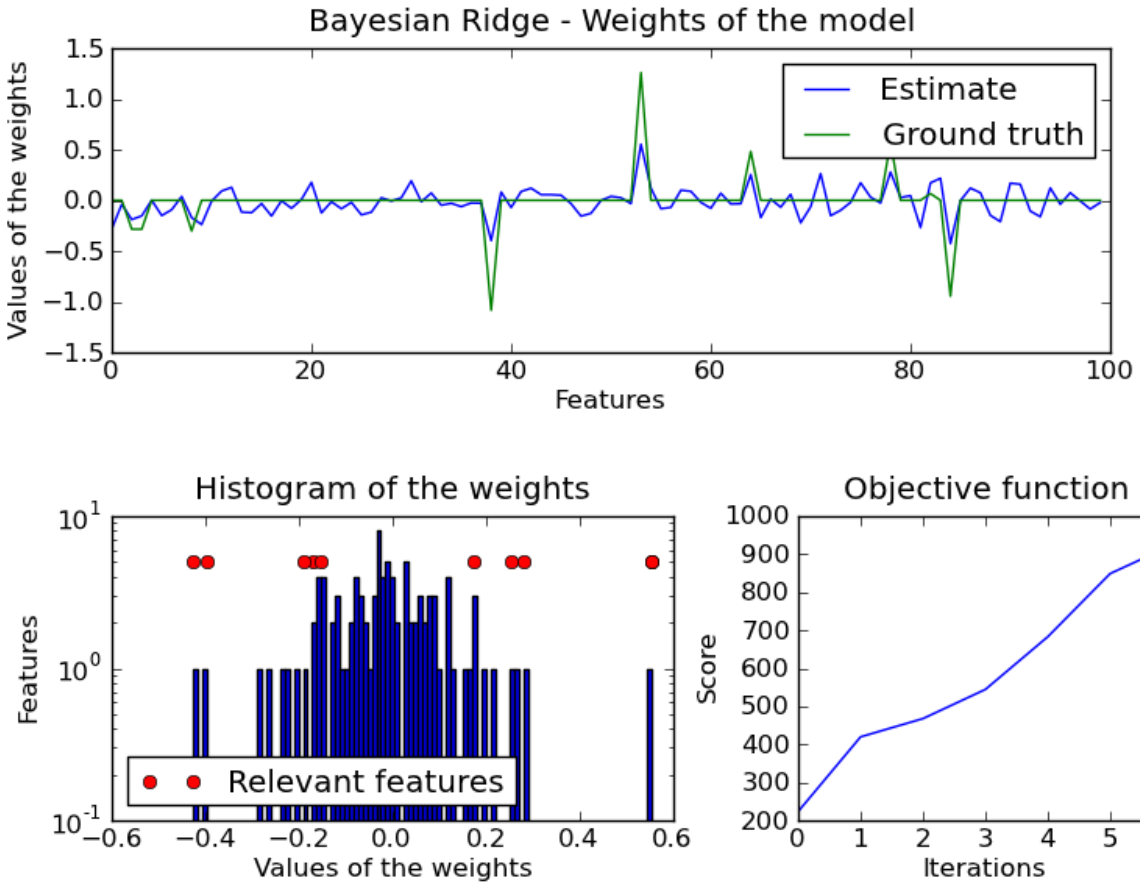
Due to the Bayesian framework, the weights found are slightly different to the ones found by *Ordinary Least Squares (OLS)*. However, *Bayesian Ridge Regression* is more robust to ill-posed problem.

Examples:

- *Bayesian Ridge Regression*

References

- More details can be found in the article Bayesian Interpolation by MacKay, David J. C.


Bayesian Ridge - Weights of the model
Values of the weights
Features
Estimate
Ground truth
Histogram of the weights
Features
Values of the weights
Relevant features
Objective function
Score
Iterations

Automatic Relevance Determination - ARD

`ARDRegression` adds a more sophisticated prior β, where we assume that each weight β_i is drawn in a Gaussian distribution, centered on zero and with a precision λ_i:

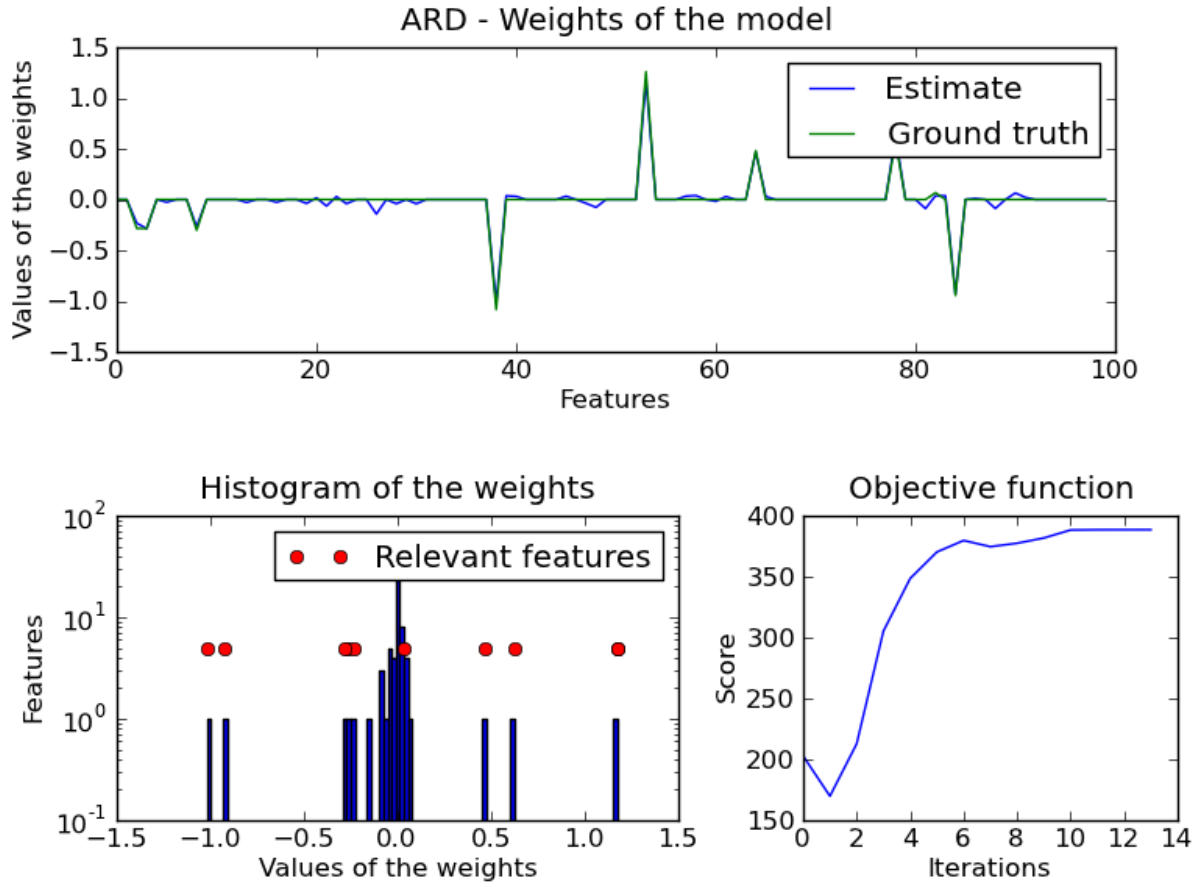
$$p(\beta|\lambda) = \mathcal{N}(\beta|0, A^{-1})$$

with $diag\ (A) = \lambda = \{\lambda_1, ..., \lambda_p\}$. There is also a Gamma prior for λ and α:

$$g(\alpha|\alpha_1, \alpha_2) = \frac{\alpha_2^{\alpha_1}}{\Gamma(\alpha_1)} \alpha^{\alpha_1 - 1} e^{-\alpha_2 \alpha}$$

$$g(\lambda|\lambda_1, \lambda_2) = \frac{\lambda_2^{\lambda_1}}{\Gamma(\lambda_1)} \lambda^{\lambda_1 - 1} e^{-\lambda_2 \lambda}$$

By default $\alpha_1 = \alpha_2 = \lambda_1 = \lambda_2 = 1.e-6$**, *i.e.*** very slightly informative priors.



Examples:

- *Automatic Relevance Determination Regression (ARD)*

Mathematical formulation

A prior is introduced as a distribution $p(\theta)$ over the parameters. This distribution is set before processing the data. The parameters of a prior distribution are called *hyper-parameters*. This description is based on the Bayes theorem :

$$p(\theta|\{X,y\}) = \frac{p(\{X,y\}|\theta)p(\theta)}{p(\{X,y\})}$$

With :

- $p(X,y|\theta)$ the likelihood : it expresses how probable it is to observe X, y given θ.
- $p(X,y)$ the marginal probability of the data : it can be considered as a normalizing constant, and is computed by integrating $p(X,y|\theta)$ with respect to θ.
- $p(\theta)$ the prior over the parameters : it expresses the knowledge that we can have about θ before processing the data.
- $p(\theta|X,y)$ the conditional probability (or posterior probability) : it expresses the uncertainty in θ after observing the data.

All the following regressions are based on the following Gaussian assumption:

$$p(y|X,w,\alpha) = \mathcal{N}(y|Xw,\alpha)$$

where α is the precision of the noise.

References

- Original Algorithm is detailed in the book *Bayesian learning for neural networks* by Radford M. Neal

Logisitic regression

If the task at hand is to do choose which class a sample belongs to given a finite (hopefuly small) set of choices, the learning problem is a classification, rather than regression. Linear models can be used for such a decision, but it is best to use what is called a logistic regression, that doesn't try to minimize the sum of square residuals, as in regression, but rather a "hit or miss" cost.

The `LogisticRegression` class can be used to do L1 or L2 penalized logistic regression. L1 penalization yields sparse predicting weights. For L1 penalization `scikits.learn.svm.l1_min_c` allows to calculate the lower bound for C in order to get a non "null" (all feature weights to zero) model.

Examples:

- *Logistic Regression*
- *Path with L1- Logistic Regression*

Stochastic Gradient Descent - SGD

Stochastic gradient descent is a simple yet very efficient approach to fit linear models. It is particulary useful when the number of samples (and the number of features) is very large.

The classes `SGDClassifier` and `SGDRegressor` provide functionality to fit linear models for classification and regression using different (convex) loss functions and different penalties.

References

- *Stochastic Gradient Descent*

1.3.2 Support Vector Machines

Support vector machines (SVMs) are a set of supervised learning methods used for *classification*, *regression* and *outliers detection*.

The advantages of Support Vector Machines are:

- Effective in high dimensional spaces.
- Still effective in cases where number of dimensions is greater than the number of samples.
- Uses a subset of training points in the decision function (called support vectors), so it is also memory efficient.
- Versatile: different *Kernel functions* can be specified for the decision function. Common kernels are provided, but it is also possible to specify custom kernels.

The disadvantages of Support Vector Machines include:

- If the number of features is much greater than the number of samples, the method is likely to give poor performances.
- SVMs do not directly provide probability estimates, these are calculated using five-fold cross-validation, and thus performance can suffer.

Note: Avoiding data copy

If the data passed to certain methods is not C-ordered and contiguous, it will be copied before calling the underlying C implementation. You can check whether a give numpy array is C-contiguous by inspecting its *flags* dictionnary.

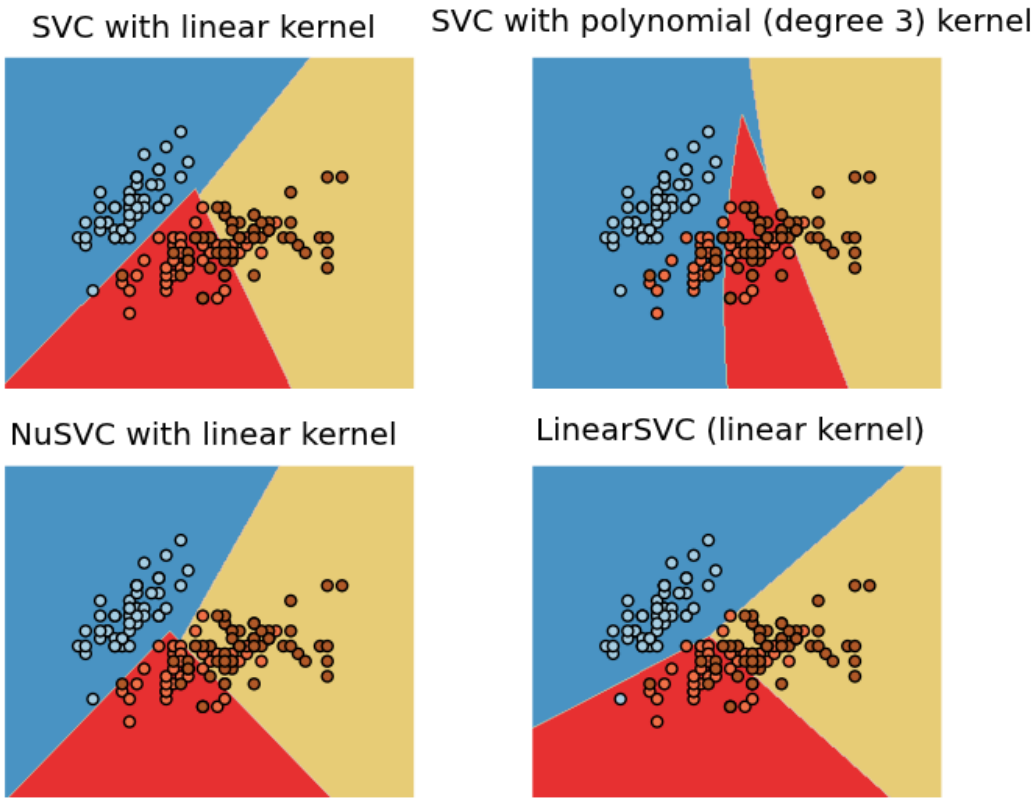
Classification

`SVC`, `NuSVC` and `LinearSVC` are classes capable of performing multi-class classification on a dataset.

`SVC` and `NuSVC` are similar methods, but accept slightly different sets of parameters and have different mathematical formulations (see section *Mathematical formulation*). On the other hand, `LinearSVC` is another implementation of Support Vector Classification for the case of a linear kernel. Note that `LinearSVC` does not accept keyword 'kernel', as this is assumed to be linear. It also lacks some of the members of `SVC` and `NuSVC`, like support_.

As other classifiers, `SVC`, `NuSVC` and `LinearSVC` take as input two arrays: an array X of size [n_samples, n_features] holding the training samples, and an array Y of integer values, size [n_samples], holding the class labels for the training samples:

```
>>> from scikits.learn import svm
>>> X = [[0, 0], [1, 1]]
>>> Y = [0, 1]
>>> clf = svm.SVC()
>>> clf.fit(X, Y)
SVC(kernel='rbf', C=1.0, probability=False, degree=3, coef0=0.0, tol=0.001,
  cache_size=100.0, shrinking=True, gamma=0.5)
```


SVC with linear kernel
SVC with polynomial (degree 3) kernel
NuSVC with linear kernel
LinearSVC (linear kernel)

After being fitted, the model can then be used to predict new values:

```
>>> clf.predict([[2., 2.]])
array([ 1.])
```

SVMs decision function depends on some subset of the training data, called the support vectors. Some properties of these support vectors can be found in members *support_vectors_*, *support_* and *n_support*:

```
>>> # get support vectors
>>> clf.support_vectors_
array([[ 0.,  0.],
       [ 1.,  1.]])
>>> # get indices of support vectors
>>> clf.support_
array([0, 1]...)
>>> # get number of support vectors for each class
>>> clf.n_support_
array([1, 1]...)
```

Multi-class classification

`SVC` and `NuSVC` implement the "one-against-one" approach (Knerr et al., 1990) for multi- class classification. If n_class is the number of classes, then n_class * (n_class - 1)/2 classifiers are constructed and each one trains data from two classes.

```
>>> X = [[0], [1], [2], [3]]
>>> Y = [0, 1, 2, 3]
>>> clf = svm.SVC()
>>> clf.fit(X, Y)
SVC(kernel='rbf', C=1.0, probability=False, degree=3, coef0=0.0, tol=0.001,
  cache_size=100.0, shrinking=True, gamma=0.25)
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes: 4*3/2 = 6
6
```

On the other hand, `LinearSVC` implements "one-vs-the-rest" multi-class strategy, thus training n_class models. If there are only two classes, only one model is trained.

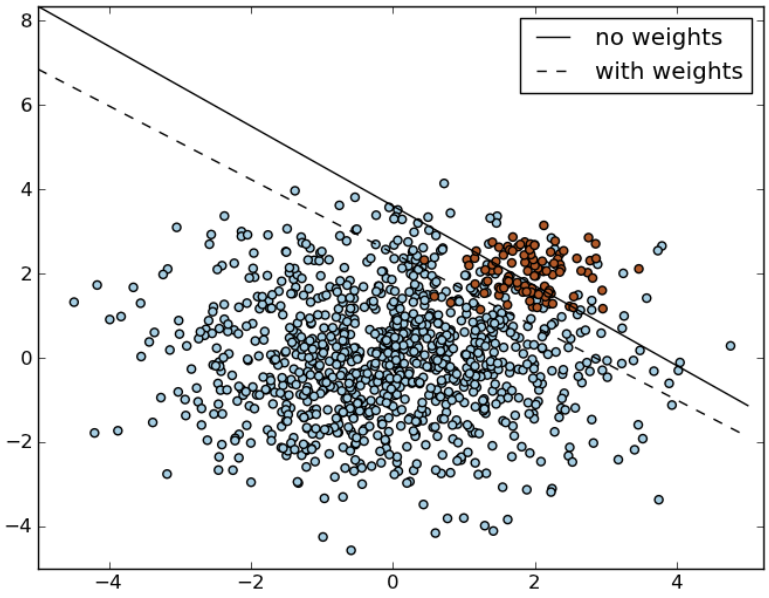
```
>>> lin_clf = svm.LinearSVC()
>>> lin_clf.fit(X, Y)
LinearSVC(loss='l2', C=1.0, dual=True, fit_intercept=True, penalty='l2',
     multi_class=False, tol=0.0001, intercept_scaling=1)
>>> dec = lin_clf.decision_function([[1]])
>>> dec.shape[1]
4
```

See *Mathematical formulation* for a complete description of the decision function.

Unbalanced problems

In problems where it is desired to give more importance to certain classes or certain individual samples keywords `class_weight` and `sample_weight` can be used.

`SVC` (but not `NuSVC`) implement a keyword `class_weight` in the fit method. It's a dictionary of the form `{class_label : value}`, where value is a floating point number > 0 that sets the parameter C of class `class_label` to C * value.



`SVC`, `NuSVC`, `SVR`, `NuSVR` and `OneClassSVM` implement also weights for individual samples in method `fit` through keyword sample_weight.

Examples:

- *Plot different SVM classifiers in the iris dataset*,
- *SVM: Maximum margin separating hyperplane*,
- *SVM: Separating hyperplane for unbalanced classes*
- *SVM-Anova: SVM with univariate feature selection*,
- *Non-linear SVM*
- *SVM: Weighted samples*,

Regression

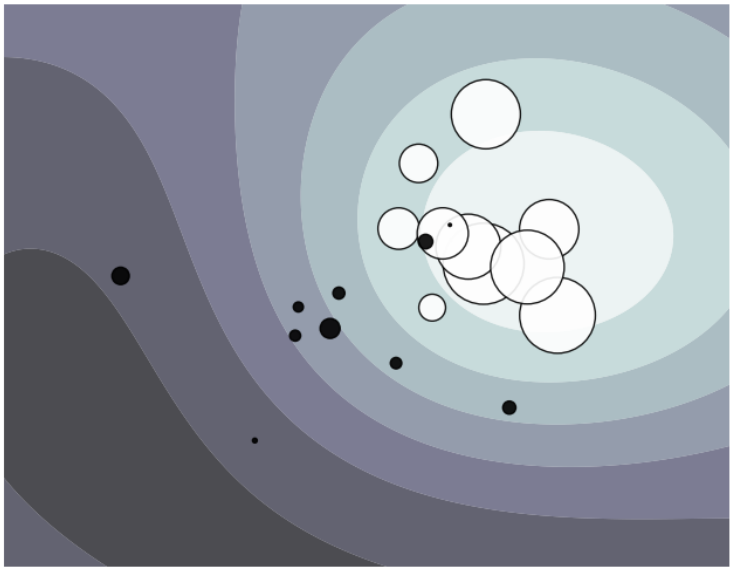
The method of Support Vector Classification can be extended to solve regression problems. This method is called Support Vector Regression.

The model produced by support vector classification (as described above) depends only on a subset of the training data, because the cost function for building the model does not care about training points that lie beyond the margin. Analogously, the model produced by Support Vector Regression depends only on a subset of the training data, because the cost function for building the model ignores any training data close to the model prediction.

There are two flavors of Support Vector Regression: `SVR` and `NuSVR`.

As with classification classes, the fit method will take as argument vectors X, y, only that in this case y is expected to have floating point values instead of integer values.

```
>>> from scikits.learn import svm
>>> X = [[0, 0], [2, 2]]
>>> y = [0.5, 2.5]
```



```
>>> clf = svm.SVR()
>>> clf.fit(X, y)
SVR(kernel='rbf', C=1.0, probability=False, degree=3, epsilon=0.1,
  shrinking=True, tol=0.001, cache_size=100.0, coef0=0.0, nu=0.5,
  gamma=0.5)
>>> clf.predict([[1, 1]])
array([ 1.5])
```

Examples:

- *Support Vector Regression (SVR) using linear and non-linear kernels*

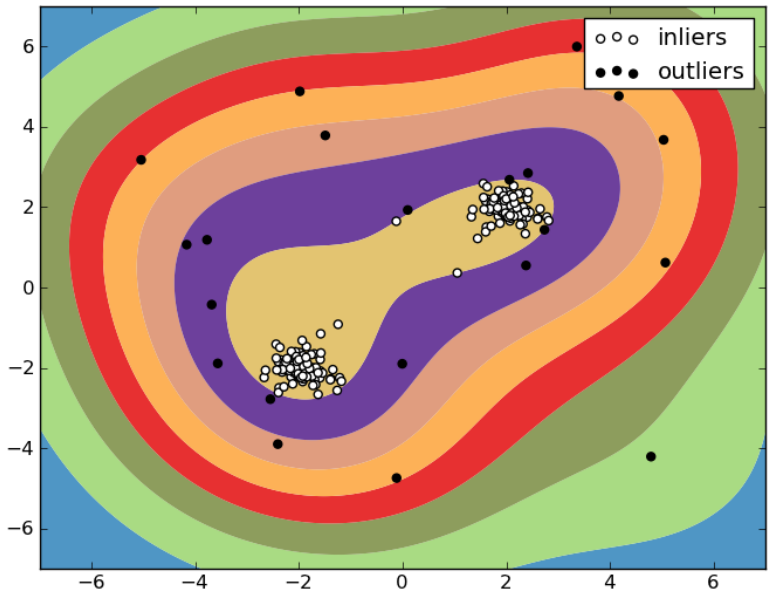
Density estimation, outliers detection

One-class SVM is used for outliers detection, that is, given a set of samples, it will detect the soft boundary of that set so as to classify new points as belonging to that set or not. The class that implements this is called `OneClassSVM`

In this case, as it is a type of unsupervised learning, the fit method will only take as input an array X, as there are no class labels.

Examples:

- *One-class SVM with non-linear kernel (RBF)*
- *Species distribution modeling*



Support Vector machines for sparse data

There is support for sparse data given in any matrix in a format supported by scipy.sparse. Classes have the same name, just prefixed by the *sparse* namespace, and take the same arguments, with the exception of training and test data, which is expected to be in a matrix format defined in scipy.sparse.

For maximum efficiency, use the CSR matrix format as defined in scipy.sparse.csr_matrix.

Implemented classes are `SVC`, `NuSVC`, `SVR`, `NuSVR`, `OneClassSVM`, `LinearSVC`.

Complexity

Support Vector Machines are powerful tools, but their compute and storage requirements increase rapidly with the number of training vectors. The core of an SVM is a quadratic programming problem (QP), separating support vectors from the rest of the training data. The QP solver used by this libsvm-based implementation scales between $O(n_{features} \times n_{samples}^2)$ and $O(n_{features} \times n_{samples}^3)$ depending on how efficiently the libsvm cache is used in practice (dataset dependent). If the data is very sparse $n_{features}$ should be replaced by the average number of non-zero features in a sample vector.

Also note that for the linear case, the algorithm used in `LinearSVC` by the liblinear implementation is much more efficient than its libsvm-based `SVC` counterpart and can scale almost linearly to millions of samples and/or features.

Tips on Practical Use

- Support Vector Machine algorithms are not scale invariant, so it is highly recommended to scale your data. For example, scale each attribute on the input vector X to [0,1] or [-1,+1], or standardize it to have mean 0 and variance 1. Note that the *same* scaling must be applied to the test vector to obtain meaningful results. See The CookBook for some examples on scaling.
- Parameter nu in NuSVC/OneClassSVM/NuSVR approximates the fraction of training errors and support vectors.

- In SVC, if data for classification are unbalanced (e.g. many positive and few negative), set class_weight='auto' and/or try different penalty parameters C.
- Specify larger cache size (keyword cache) for huge problems.
- The underlying `LinearSVC` implementation uses a random number generator to select features when fitting the model. It is thus not uncommon, to have slightly different results for the same input data. If that happens, try with a smaller tol parameter.
- Using L1 penalization as provided by LinearSVC(loss='l2', penalty='l1', dual=False) yields a sparse solution, i.e. only a subset of feature weights is different from zero and contribute to the decision function. Increasing C yields a more complex model (more feature are selected). The C value that yields a "null" model (all weights equal to zero) can be calculated using `l1_min_c`.

Kernel functions

The *kernel function* can be any of the following:

- linear: $< x_i, x'_j >$.
- polynomial: $(\gamma < x, x' > +r)^d$. d is specified by keyword *degree*.
- rbf ($exp(-\gamma|x - x'|^2), \gamma > 0$). γ is specified by keyword gamma.
- sigmoid ($tanh(< x_i, x_j > +r)$).

Different kernels are specified by keyword kernel at initialization:

```
>>> linear_svc = svm.SVC(kernel='linear')
>>> linear_svc.kernel
'linear'
>>> rbf_svc = svm.SVC(kernel='rbf')
>>> rbf_svc.kernel
'rbf'
```

Custom Kernels

You can define your own kernels by either giving the kernel as a python function or by precomputing the Gram matrix.

Classifiers with custom kernels behave the same way as any other classifiers, except that:

- Field *support_vectors_* is now empty, only indices of support vectors are stored in *support_*
- A reference (and not a copy) of the first argument in the fit() method is stored for future reference. If that array changes between the use of fit() and predict() you will have unexpected results.

Using python functions as kernels You can also use your own defined kernels by passing a function to the keyword *kernel* in the constructor.

Your kernel must take as arguments two matrices and return a third matrix.

The following code defines a linear kernel and creates a classifier instance that will use that kernel:

```
>>> import numpy as np
>>> from scikits.learn import svm
>>> def my_kernel(x, y):
...     return np.dot(x, y.T)
...
>>> clf = svm.SVC(kernel=my_kernel)
```

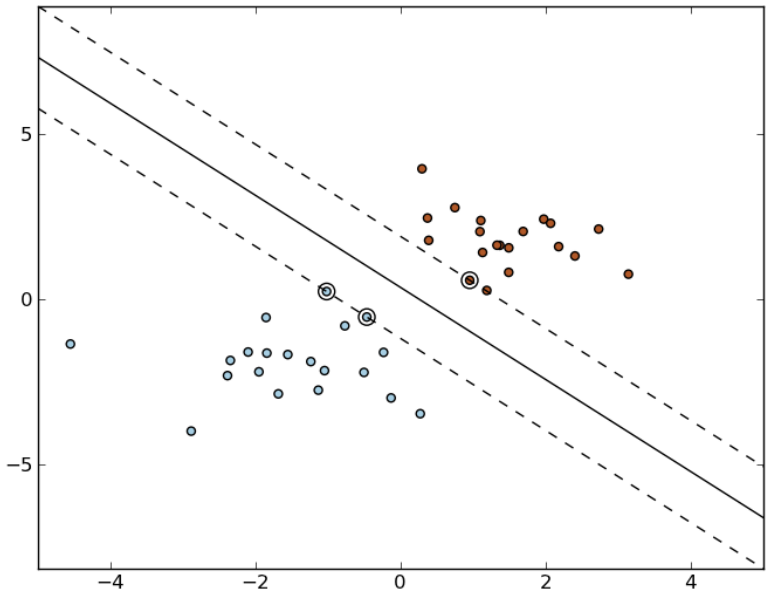
Using the Gram matrix Set kernel='precomputed' and pass the Gram matrix instead of X in the fit method.

Examples:

- *SVM with custom kernel*.

Mathematical formulation

A support vector machine constructs a hyper-plane or set of hyper-planes in a high or infinite dimensional space, which can be used for classification, regression or other tasks. Intuitively, a good separation is achieved by the hyper-plane that has the largest distance to the nearest training data points of any class (so-called functional margin), since in general the larger the margin the lower the generalization error of the classifier.



SVC

Given training vectors $x_i \in R^n$, i=1,..., l, in two classes, and a vector $y \in R^l$ such that $y_i \in 1, -1$, SVC solves the following primal problem:

$$\min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1,l} \zeta_i$$

$$\text{subject to } y_i(w^T \phi(x_i) + b) \geq 1 - \zeta_i,$$
$$\zeta_i \geq 0, i = 1, ..., l$$

Its dual is

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - e^T\alpha$$
$$\text{subject to } y^T\alpha = 0$$
$$0 \leq \alpha_i \leq C, i = 1, ..., l$$

where e is the vector of all ones, C > 0 is the upper bound, Q is an l by l positive semidefinite matrix, $Q_ij \equiv K(x_i, x_j)$ and $\phi(x_i)^T\phi(x)$ is the kernel. Here training vectors are mapped into a higher (maybe infinite) dimensional space by the function ϕ

The decision function is:

$$sgn(\sum_{i=1}^{l} y_i\alpha_i K(x_i, x) + \rho)$$

This parameters can be accessed through the members *dual_coef_* which holds the product $y_i\alpha_i$, *support_vectors_* which holds the support vectors, and *intercept_* which holds the independent term $-\rho$:

References:

- "Automatic Capacity Tuning of Very Large VC-dimension Classifiers" I Guyon, B Boser, V Vapnik - Advances in neural information processing 1993,
- "Support-vector networks" C. Cortes, V. Vapnik, Machine Leaming, 20, 273-297 (1995)

NuSVC

We introduce a new parameter ν which controls the number of support vectors and training errors. The parameter $\nu \in (0, 1]$ is an upper bound on the fraction of training errors and a lower bound of the fraction of support vectors.

Implementation details

Internally, we use libsvm and liblinear to handle all computations. These libraries are wrapped using C and Cython.

References:

For a description of the implementation and details of the algorithms used, please refer to

- LIBSVM: a library for Support Vector Machines
- LIBLINEAR – A Library for Large Linear Classification

1.3.3 Stochastic Gradient Descent

Stochastic Gradient Descent (SGD) is a simple yet very efficient approach to discriminative learning of linear classifiers under convex loss functions such as (linear) Support Vector Machines and Logistic Regression. Even though SGD has been around in the machine learning community for a long time, it has received a considerable amount of attention just recently in the context of large-scale learning.

SGD has been successfully applied to large-scale and sparse machine learning problems often encountered in text classification and natural language processing. Given that the data is sparse, the classifiers in this module easily scale to problems with more than 10^5 training examples and more than 10^5 features.

The advantages of Stochastic Gradient Descent are:

- Efficiency.
- Ease of implementation (lots of opportunities for code tuning).

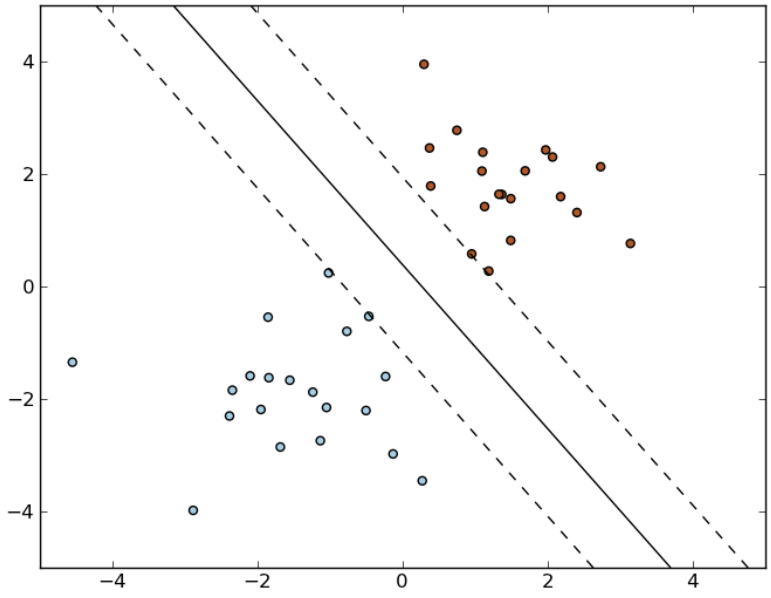
The disadvantages of Stochastic Gradient Descent include:

- SGD requires a number of hyperparameters such as the regularization parameter and the number of iterations.
- SGD is sensitive to feature scaling.

Classification

Warning: Make sure you permute (shuffle) your training data before fitting the model or use *shuffle=True* to shuffle after each iterations.

The class `SGDClassifier` implements a plain stochastic gradient descent learning routine which supports different loss functions and penalties for classification.



As other classifiers, SGD has to be fitted with two arrays: an array X of size [n_samples, n_features] holding the training samples, and an array Y of size [n_samples] holding the target values (class labels) for the training samples:

```
>>> from scikits.learn.linear_model import SGDClassifier
>>> X = [[0., 0.], [1., 1.]]
>>> y = [0, 1]
>>> clf = SGDClassifier(loss="hinge", penalty="l2")
>>> clf.fit(X, y)
SGDClassifier(loss='hinge', n_jobs=1, shuffle=False, verbose=0, n_iter=5,
       learning_rate='optimal', fit_intercept=True, penalty='l2',
       power_t=0.5, seed=0, eta0=0.0, rho=1.0, alpha=0.0001)
```

After being fitted, the model can then be used to predict new values:

```
>>> clf.predict([[2., 2.]])
array([ 1.])
```

SGD fits a linear model to the training data. The member *coef_* holds the model parameters:

```
>>> clf.coef_
array([[ 9.90090187,  9.90090187]])
```

Member *intercept_* holds the intercept (aka offset or bias):

```
>>> clf.intercept_
array(-9.990...)
```

Whether or not the model should use an intercept, i.e. a biased hyperplane, is controlled by the parameter *fit_intercept*.

To get the signed distance to the hyperplane use *decision_function*:

```
>>> clf.decision_function([[2., 2.]])
array([ 29.61357756])
```

The concrete loss function can be set via the *loss* parameter. `SGDClassifier` supports the following loss functions:

- *loss="hinge"*: (soft-margin) linear Support Vector Machine.
- *loss="modified_huber"*: smoothed hinge loss.
- *loss="log"*: Logistic Regression

The first two loss functions are lazy, they only update the model parameters if an example violates the margin constraint, which makes training very efficient. Log loss, on the other hand, provides probability estimates.

In the case of binary classification and *loss="log"* you get a probability estimate P(y=C|x) using *predict_proba*, where *C* is the largest class label:

```
>>> clf = SGDClassifier(loss="log").fit(X, y)
>>> clf.predict_proba([[1., 1.]])
array([ 0.99999949])
```

The concrete penalty can be set via the *penalty* parameter. *SGD* supports the following penalties:

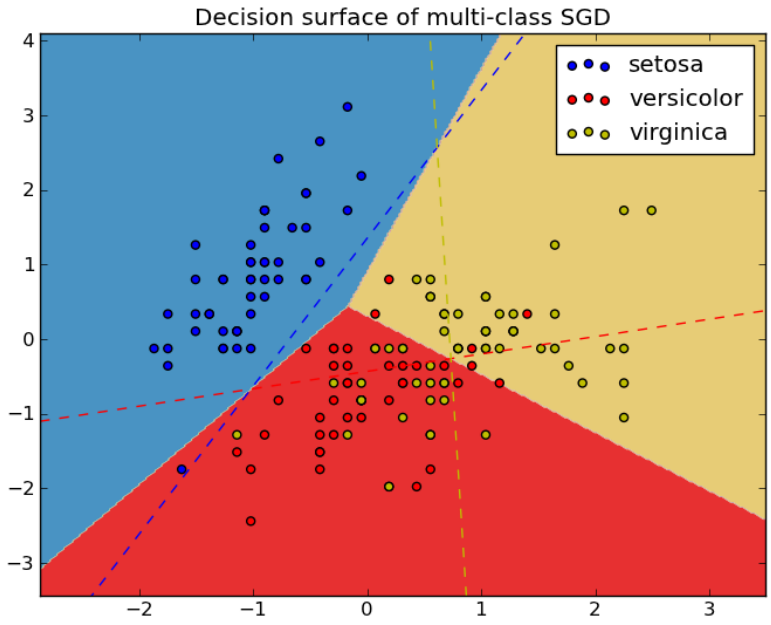
- *penalty="l2"*: L2 norm penalty on *coef_*.
- *penalty="l1"*: L1 norm penalty on *coef_*.
- *penalty="elasticnet"*: Convex combination of L2 and L1; *rho * L2 + (1 - rho) * L1*.

The default setting is *penalty="l2"*. The L1 penalty leads to sparse solutions, driving most coefficients to zero. The Elastic Net solves some deficiencies of the L1 penalty in the presence of highly correlated attributes. The parameter *rho* has to be specified by the user.

`SGDClassifier` supports multi-class classification by combining multiple binary classifiers in a "one versus all" (OVA) scheme. For each of the *K* classes, a binary classifier is learned that discriminates between that and all other *K-1* classes. At testing time, we compute the confidence score (i.e. the signed distances to the hyperplane) for each classifier and choose the class with the highest confidence. The Figure below illustrates the OVA approach on the iris dataset. The dashed lines represent the three OVA classifiers; the background colors show the decision surface induced by the three classifiers.

In the case of multi-class classification *coef_* is a two-dimensionaly array of shape [n_classes, n_features] and *intercept_* is a one dimensional array of shape [n_classes]. The i-th row of *coef_* holds the weight vector of the OVA classifier for the i-th class; classes are indexed in ascending order (see attribute *classes*).

`SGDClassifier` supports both weighted classes and weighted instances via the fit parameters *class_weight* and *sample_weight*. See the examples below and the doc string of `SGDClassifier.fit` for further information.



Examples:

- *SGD: Maximum margin separating hyperplane*,
- *Plot multi-class SGD on the iris dataset*
- *SGD: Separating hyperplane with weighted classes*
- *SGD: Weighted samples*

Regression

The class `SGDRegressor` implements a plain stochastic gradient descent learning routine which supports different loss functions and penalties to fit linear regression models. `SGDRegressor` is well suited for regression problems with a large number of training samples (> 10.000), for other problems we recommend `Ridge`, `Lasso`, or `ElasticNet`.

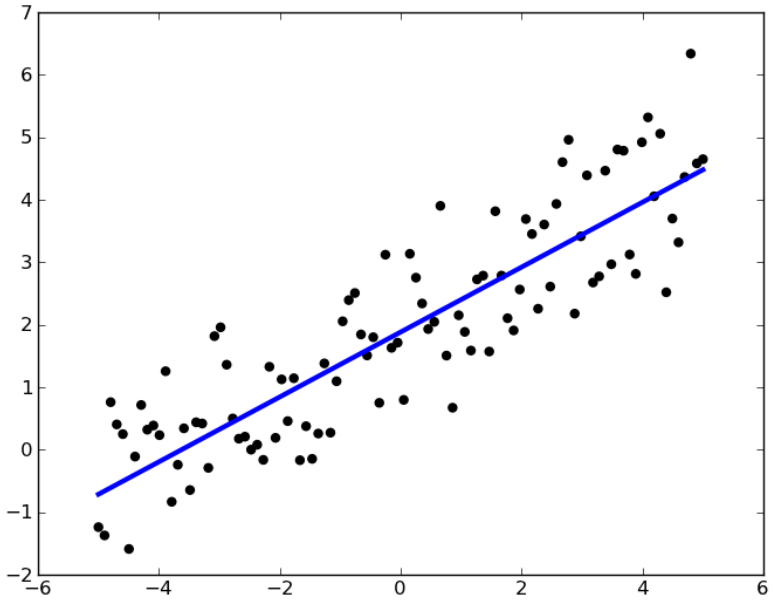
The concrete loss function can be set via the *loss* parameter. `SGDRegressor` supports the following loss functions:

- *loss="squared_loss"*: Ordinary least squares.
- *loss="huber"*: Huber loss for robust regression.

The Huber loss function is an epsilon insensitive loss function for robust regression. The width of the insensitive region has to be specified via the parameter *epsilon*.

Examples:

- *Ordinary Least Squares with SGD*,



Stochastic Gradient Descent for sparse data

Note: The sparse implementation produces slightly different results than the dense implementation due to a shrunk learning rate for the intercept.

There is support for sparse data given in any matrix in a format supported by scipy.sparse. Classes have the same name, just prefixed by the *sparse* namespace, and take the same arguments, with the exception of training and test data, which is expected to be in a matrix format defined in scipy.sparse.

For maximum efficiency, use the CSR matrix format as defined in scipy.sparse.csr_matrix.

Implemented classes are `SGDClassifier` and `SGDRegressor`. During training both classes maintain a dense representation of the model parameters. After training has completed you can obtain a sparse representation of the model parameters via the attribute *sparse_coef_*.

Examples:

- *Classification of text documents using sparse features*

Complexity

The major advantage of SGD is its efficiency, which is basically linear in the number of training examples. If X is a matrix of size (n, p) training has a cost of $O(kn\bar{p})$, where k is the number of iterations (epochs) and $\bar{p}$ is the average number of non-zero attributes per sample.

Recent theoretical results, however, show that the runtime to get some desired optimization accuracy does not increase as the training set size increases.

Tips on Practical Use

- Stochastic Gradient Descent is sensitive to feature scaling, so it is highly recommended to scale your data. For example, scale each attribute on the input vector X to [0,1] or [-1,+1], or standardize it to have mean 0 and variance 1. Note that the *same* scaling must be applied to the test vector to obtain meaningful results. This can be easily done using `Scaler`:

```
from scikits.learn.preprocessing import Scaler
scaler = Scaler()
scaler.fit(X_train)  # Don't cheat - fit only on training data
scaler.transform(X_train)
scaler.transform(X_test)  # apply same transformation to test data
```

  If your attributes have an intrinsic scale (e.g. word frequencies or indicator features) scaling is not needed.

- Finding a reasonable regularization term α is best done using `GridSearchCV`, usually in the range *10.0**-np.arange(1,7)*.
- Empirically, we found that SGD converges after observing approx. 10^6 training samples. Thus, a reasonable first guess for the number of iterations is *n_iter = np.ceil(10**6 / n)*, where *n* is the size of the training set.
- If you apply SGD to features extracted using PCA we found that it is often wise to scale the feature values by some constant *c* such that the average L2 norm of the training data equals one.

References:

- "Efficient BackProp" Y. LeCun, L. Bottou, G. Orr, K. Müller - In Neural Networks: Tricks of the Trade 1998.

Mathematical formulation

Given a set of training examples $(x_1, y_1), \ldots, (x_n, y_n)$ where $x_i \in \mathbf{R}^n$ and $y_i \in \{-1, 1\}$, our goal is to learn a linear scoring function $f(x) = w^T x + b$ with model parameters $w \in \mathbf{R}^m$ and intercept $b \in \mathbf{R}$. In order to make predictions, we simply look at the sign of $f(x)$. A common choice to find the model parameters is by minimizing the regularized training error given by

$$E(w,b) = \sum_{i=1}^{n} L(y_i, f(x_i)) + \alpha R(w)$$

where L is a loss function that measures model (mis)fit and R is a regularization term (aka penalty) that penalizes model complexity; $\alpha > 0$ is a non-negative hyperparameter.

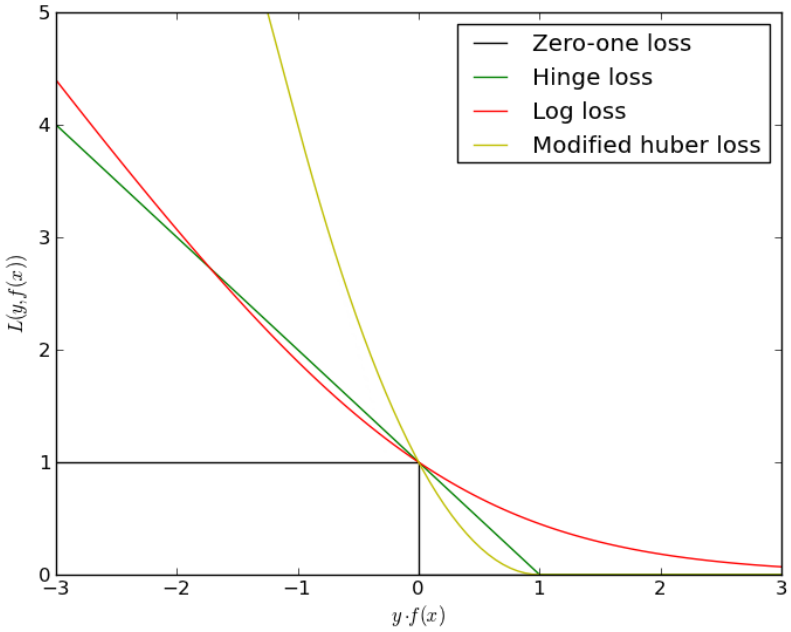
Different choices for L entail different classifiers such as

- Hinge: (soft-margin) Support Vector Machines.
- Log: Logistic Regression.
- Least-Squares: Ridge Regression.

All of the above loss functions can be regarded as an upper bound on the misclassification error (Zero-one loss) as shown in the Figure below.

Popular choices for the regularization term R include:

- L2 norm: $R(w) := \frac{1}{2} \sum_{i=1}^{n} w_i^2$,
- L1 norm: $R(w) := \sum_{i=1}^{n} |w_i|$, which leads to sparse solutions.



- Elastic Net: $R(w) := \rho \frac{1}{2} \sum_{i=1}^{n} w_i^2 + (1-\rho) \sum_{i=1}^{n} |w_i|$, a convex combination of L2 and L1.

The Figure below shows the contours of the different regularization terms in the parameter space when $R(w) = 1$.

SGD

Stochastic gradient descent is an optimization method for unconstrained optimization problems. In contrast to (batch) gradient descent, SGD approximates the true gradient of $E(w, b)$ by considering a single training example at a time.

The class `SGDClassifier` implements a first-order SGD learning routine. The algorithm iterates over the training examples and for each example updates the model parameters according to the update rule given by

$$w \leftarrow w - \eta(\alpha \frac{\partial R(w)}{\partial w} + \frac{\partial L(w^T x_i + b, y_i)}{\partial w})$$

where η is the learning rate which controls the step-size in the parameter space. The intercept b is updated similarly but without regularization.

The learning rate η can be either constant or gradually decaying. For classification, the default learning rate schedule (*learning_rate='optimal'*) is given by

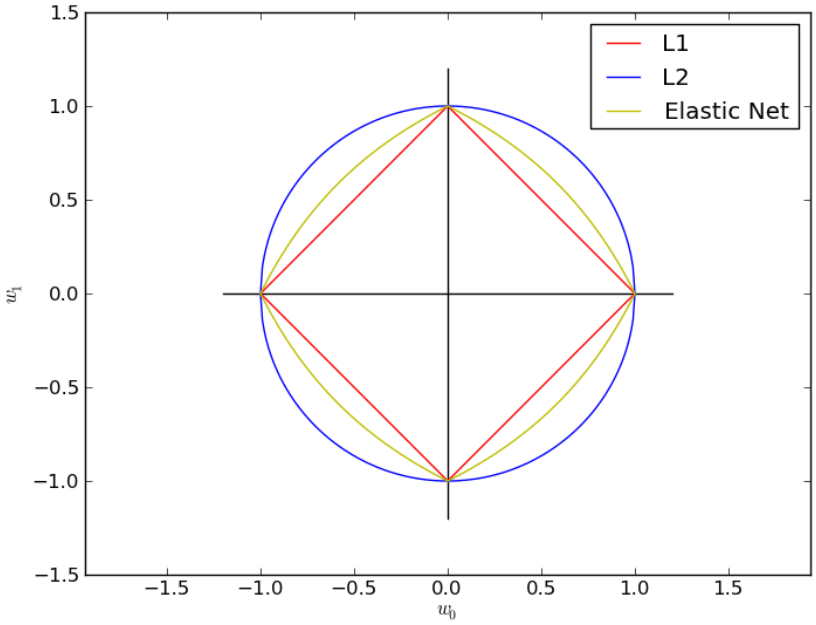
$$\eta^{(t)} = \frac{1.0}{t + t0}$$

where $t0$ is the time step (there are a total of *n_samples*epochs* time steps), $t0$ is choosen automatically assuming that the norm of the training samples is approx. 1. For regression, the default learning rate schedule, inverse scaling (*learning_rate='invscaling'*), is given by

$$\eta^{(t)} = \frac{eta_0}{t^{power\_t}}$$

where eta_0 and $power\_t$ are hyperparameters choosen by the user. For a constant learning rate use *learning_rate='constant'* and use *eta0* to specify the learning rate.

The model parameters can be accessed through the members coef_ and intercept_:



- Member coef_ holds the weights w
- Member intercept_ holds b

References:

- "Solving large scale linear prediction problems using stochastic gradient descent algorithms" T. Zhang - In Proceedings of ICML '04.
- "Regularization and variable selection via the elastic net" H. Zou, T. Hastie - Journal of the Royal Statistical Society Series B, 67 (2), 301-320.

Implementation details

The implementation of SGD is influenced by the Stochastic Gradient SVM of Léon Bottou. Similar to SvmSGD, the weight vector is represented as the product of a scalar and a vector which allows an efficient weight update in the case of L2 regularization. In the case of sparse feature vectors, the intercept is updated with a smaller learning rate (multiplied by 0.01) to account for the fact that it is updated more frequently. Training examples are picked up sequentially and the learning rate is lowered after each observed example. We adopted the learning rate schedule from Shalev-Shwartz et al. 2007. For multi-class classification, a "one versus all" approach is used. We use the truncated gradient algorithm proposed by Tsuruoka et al. 2009 for L1 regularization (and the Elastic Net). The code is written in Cython.

References:

- "Stochastic Gradient Descent" L. Bottou - Website, 2010.
- "Pegasos: Primal estimated sub-gradient solver for svm" S. Shalev-Shwartz, Y. Singer, N. Srebro - In Proceedings of ICML '07.
- "Stochastic gradient descent training for l1-regularized log-linear models with cumulative penalty" Y. Tsuruoka, J. Tsujii, S. Ananiadou - In Proceedings of the AFNLP/ACL '09.

1.3.4 Nearest Neighbors

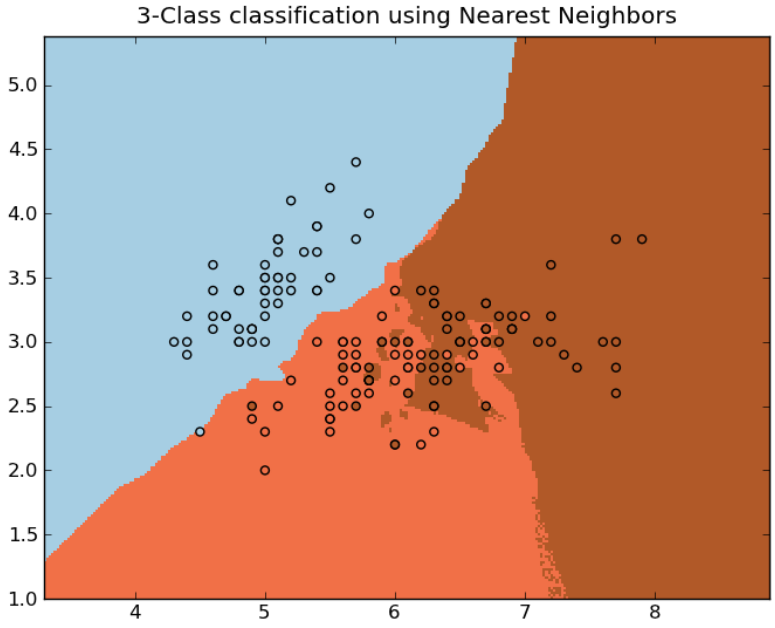
The principle behind nearest neighbor methods is to find the k training points closest in euclidean distance to x0, and then classify using a majority vote among the k neighbors.

Despite its simplicity, nearest neighbors has been successful in a large number of classification problems, including handwritten digits or satellite image scenes. It is ofter successful in situation where the decision boundary is very irregular.

Classification

The `NeighborsClassifier` implements the nearest-neighbors classification method using a vote heuristic: the class most present in the k nearest neighbors of a point is assigned to this point.

It is possible to use different nearest neighbor search algorithms by using the keyword `algorithm`. Possible values are `'auto'`, `'ball_tree'`, `'brute'` and `'brute_inplace'`. `'ball_tree'` will create an instance of `BallTree` to conduct the search, which is usually very efficient in low-dimensional spaces. In higher dimension, a brute-force approach is prefered thus parameters `'brute'` and `'brute_inplace'` can be used . Both conduct a brute-force search, the difference being that `'brute_inplace'` does not perform any precomputations, and thus is better suited for low-memory settings. Finally, `'auto'` is a simple heuristic that will guess the best approach based on the current dataset.

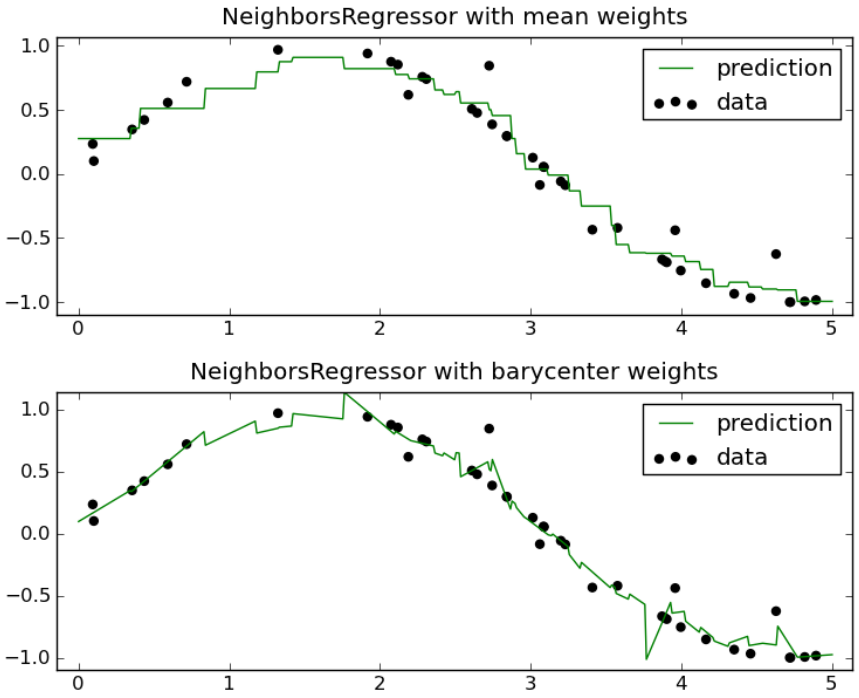


Examples:

- *Nearest Neighbors*: an example of classification using nearest neighbor.

Regression

The `NeighborsRegressor` estimator implements a nearest-neighbors regression method by weighting the targets of the k-neighbors. Two different weighting strategies are implemented: `barycenter` and `mean`. `barycenter` will apply the weights that best reconstruct the point from its neighbors while `mean` will apply constant weights to each point. This plot shows the behavior of both classifier for a simple regression task.



Examples:

- *k-Nearest Neighbors regression*: an example of regression using nearest neighbor.

Efficient implementation: the ball tree

Behind the scenes, nearest neighbor search is done by the object `BallTree`. This algorithm makes it possible to rapidly look up the nearest neighbors in low-dimensional spaces.

This class provides an interface to an optimized BallTree implementation to rapidly look up the nearest neighbors of any point. Ball Trees are particularly useful for low-dimensional data and scales better than traditional tree searches (e.g. KD-Trees) as the number of dimensions grow. However, on high-dimensional spaces (dim > 50), brute force will eventually take on and become more efficient on such spaces.

Compared to a KDTree, the cost is a slightly longer construction time, though for repeated queries, this added construction time quickly becomes insignificant. A Ball Tree reduces the number of candidate points for a neighbor search

through use of the triangle inequality:

$$|x + y| \leq |x| + |y|$$

Each node of the `BallTree` defines a centroid, C, and a radius r such that each point in the node lies within the hypersphere of radius r, centered at C. With this setup, a single distance calculation between a test point and the centroid is sufficient to determine a lower bound on the distance to all points within the node. Carefully taking advantage of this property leads to determining neighbors in O[log(N)] time, as opposed to O[N] time for a brute-force search.

A pure C implementation of brute-force search is also provided in function `knn_brute`.

References:

- "Five balltree construction algorithms", Omohundro, S.M., International Computer Science Institute Technical Report

1.3.5 Feature selection

Univariate feature selection

Univariate feature selection works by selecting the best features based on univariate statistical tests. It can seen as a preprocessing step to an estimator. The *scikit.learn* exposes feature selection routines a objects that implement the *transform* method. The k-best features can be selected based on:

`scikits.learn.feature_selection.univariate_selection.`**`SelectKBest`**(*score_func*, *k=10*)

Filter : Select the k lowest p-values

or by setting a percentile of features to keep using

`scikits.learn.feature_selection.univariate_selection.`**`SelectPercentile`**(*score_func*, *percentile=10*)

Filter : Select the best percentile of the p_values

or using common statistical quantities:

`scikits.learn.feature_selection.univariate_selection.`**`SelectFpr`**(*score_func*, *alpha=0.05*)

Filter : Select the pvalues below alpha

`scikits.learn.feature_selection.univariate_selection.`**`SelectFdr`**(*score_func*, *alpha=0.05*)

Filter : Select the p-values corresponding to an estimated false discovery rate of alpha. This uses the Benjamini-Hochberg procedure

`scikits.learn.feature_selection.univariate_selection.`**`SelectFwe`**(*score_func*, *alpha=0.05*)

Filter : Select the p-values corresponding to a corrected p-value of alpha

These objects take as input a scoring function that returns univariate p-values.

Examples:

Univariate Feature Selection

Feature scoring functions

Warning: Beware not to use a regression scoring function with a classification problem.

For classification

scikits.learn.feature_selection.univariate_selection.**f_classif**(*X*, *y*)

Compute the Anova F-value for the provided sample

Parameters **X** : array of shape (n_samples, n_features)

the set of regressors sthat will tested sequentially

y : array of shape(n_samples)

the data matrix

Returns **F** : array of shape (m),

the set of F values

pval : array of shape(m),

the set of p-values

For regression

scikits.learn.feature_selection.univariate_selection.**f_regression**(*X*, *y*, *center=True*)

Quick linear model for testing the effect of a single regressor, sequentially for many regressors This is done in 3 steps: 1. the regressor of interest and the data are orthogonalized wrt constant regressors 2. the cross correlation between data and regressors is computed 3. it is converted to an F score then to a p-value

Parameters **X** : array of shape (n_samples, n_features)

the set of regressors sthat will tested sequentially

y : array of shape(n_samples)

the data matrix

center : True, bool,

If true, X and y are centered

Returns **F** : array of shape (m),

the set of F values

pval : array of shape(m)

the set of p-values

1.3.6 Gaussian Processes

Gaussian Processes for Machine Learning (GPML) is a generic supervised learning method primarily designed to solve *regression* problems. It has also been extended to *probabilistic classification*, but in the present implementation, this is only a post-processing of the *regression* exercise.

The advantages of Gaussian Processes for Machine Learning are:

- The prediction interpolates the observations (at least for regular correlation models).

- The prediction is probabilistic (Gaussian) so that one can compute empirical confidence intervals and exceedence probabilities that might be used to refit (online fitting, adaptive fitting) the prediction in some region of interest.
- Versatile: different *linear regression models* and *correlation models* can be specified. Common models are provided, but it is also possible to specify custom models provided they are stationary.

The disadvantages of Gaussian Processes for Machine Learning include:

- It is not sparse. It uses the whole samples/features information to perform the prediction.
- It loses efficiency in high dimensional spaces – namely when the number of features exceeds a few dozens. It might indeed give poor performance and it loses computational efficiency.
- Classification is only a post-processing, meaning that one first need to solve a regression problem by providing the complete scalar float precision output y of the experiment one attempt to model.

Thanks to the Gaussian property of the prediction, it has been given varied applications: e.g. for global optimization, probabilistic classification.

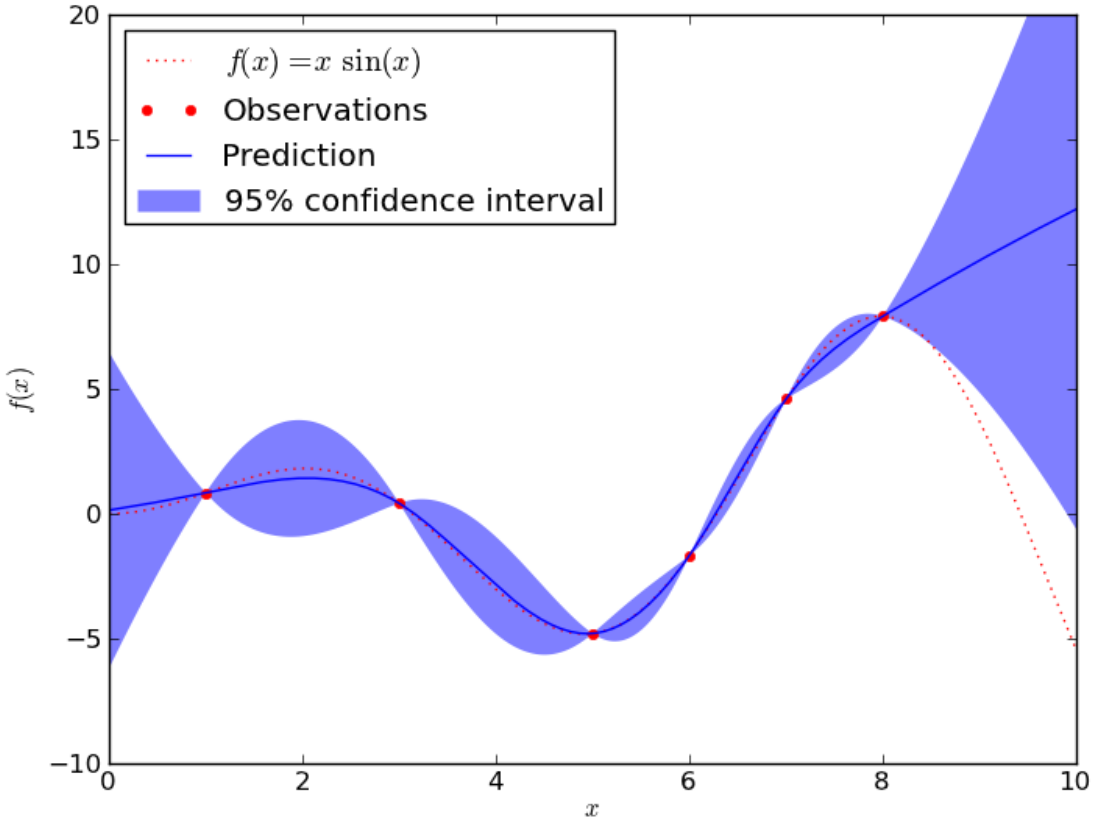
An introductory regression example

Say we want to surrogate the function $g(x) = x\sin(x)$. To do so, the function is evaluated onto a design of experiments. Then, we define a GaussianProcess model whose regression and correlation models might be specified using additional kwargs, and ask for the model to be fitted to the data. Depending on the number of parameters provided at instanciation, the fitting procedure may recourse to maximum likelihood estimation for the parameters or alternatively it uses the given parameters.

```
>>> import numpy as np
>>> from scikits.learn import gaussian_process
>>> def f(x):
...     return x * np.sin(x)
>>> X = np.atleast_2d([1., 3., 5., 6., 7., 8.]).T
>>> y = f(X).ravel()
>>> x = np.atleast_2d(np.linspace(0, 10, 1000)).T
>>> gp = gaussian_process.GaussianProcess(theta0=1e-2, thetaL=1e-4, thetaU=1e-1)
>>> gp.fit(X, y)
GaussianProcess(normalize=True, theta0=array([[ 0.01]]),
        optimizer='fmin_cobyla', verbose=False, storage_mode='full',
        nugget=2.2204460492503131e-15, thetaU=array([[ 0.1]]),
        regr=<function constant at 0x...>, random_start=1,
        corr=<function squared_exponential at 0x...>, beta0=None,
        thetaL=array([[ 0.0001]]))
>>> y_pred, sigma2_pred = gp.predict(x, eval_MSE=True)
```

Other examples

- *Gaussian Processes classification example: exploiting the probabilistic output*
- *example_gaussian_process_plot_gp_diabetes_dataset.py*


$f(x) = x\ \sin(x)$
Observations
Prediction
95% confidence interval
20
15
10
5
0
−5
−10
0
2
4
6
8
10
$f(x)$
x

Mathematical formulation

The initial assumption

Suppose one wants to model the output of a computer experiment, say a mathematical function:

$$\begin{aligned} g : &\mathbb{R}^{n_{\text{features}}} \to \mathbb{R} \\ &X \mapsto y = g(X) \end{aligned}$$

GPML starts with the assumption that this function is *a* conditional sample path of *a* Gaussian process G which is additionally assumed to read as follows:

$$G(X) = f(X)^T\beta + Z(X)$$

where $f(X)^T\beta$ is a linear regression model and $Z(X)$ is a zero-mean Gaussian process with a fully stationary covariance function:

$$C(X, X') = \sigma^2 R(|X - X'|)$$

σ^2 being its variance and R being the correlation function which solely depends on the absolute relative distance between each sample, possibly featurewise (this is the stationarity assumption).

From this basic formulation, note that GPML is nothing but an extension of a basic least squares linear regression problem:

$$g(X) \approx f(X)^T\beta$$

Except we additionaly assume some spatial coherence (correlation) between the samples dictated by the correlation function. Indeed, ordinary least squares assumes the correlation model $R(|X - X'|)$ is one when $X = X'$ and zero otherwise : a *dirac* correlation model – sometimes referred to as a *nugget* correlation model in the kriging literature.

The best linear unbiased prediction (BLUP)

We now derive the *best linear unbiased prediction* of the sample path g conditioned on the observations:

$$\hat{G}(X) = G(X|y_1 = g(X_1), ..., y_{n_{\text{samples}}} = g(X_{n_{\text{samples}}}))$$

It is derived from its *given properties*:

- It is linear (a linear combination of the observations)

$$\hat{G}(X) \equiv a(X)^T y$$

- It is unbiased

$$\mathbb{E}[G(X) - \hat{G}(X)] = 0$$

- It is the best (in the Mean Squared Error sense)

$$\hat{G}(X)^* = \arg\min_{\hat{G}(X)} \mathbb{E}[(G(X) - \hat{G}(X))^2]$$

So that the optimal weight vector $a(X)$ is solution of the following equality constrained optimization problem:

$$\begin{aligned} a(X)^* = \arg\min_{a(X)} &\mathbb{E}[(G(X) - a(X)^T y)^2] \\ &\text{s.t. } \mathbb{E}[G(X) - a(X)^T y] = 0 \end{aligned}$$

Rewriting this constrained optimization problem in the form of a Lagrangian and looking further for the first order optimality conditions to be satisfied, one ends up with a closed form expression for the sought predictor – see references for the complete proof.

In the end, the BLUP is shown to be a Gaussian random variate with mean:

$$\mu_{\hat{Y}}(X) = f(X)^T \hat{\beta} + r(X)^T \gamma$$

and variance:

$$\sigma^2_{\hat{Y}}(X) = \sigma^2_Y \left(1 - r(X)^T R^{-1} r(X) + u(X)^T \left(F^T R^{-1} F\right)^{-1} u(X)\right)$$

where we have introduced:

- the correlation matrix whose terms are defined wrt the autocorrelation function and its built-in parameters θ:

$$R_{i\,j} = R(|X_i - X_j|, \theta),\ i,\ j = 1, ..., m$$

- the vector of cross-correlations between the point where the prediction is made and the points in the DOE:

$$r_i = R(|X - X_i|, \theta),\ i = 1, ..., m$$

- the regression matrix (eg the Vandermonde matrix if f is a polynomial basis):

$$F_{i\,j} = f_i(X_j),\ i = 1, ..., p,\ j = 1, ..., m$$

- the generalized least square regression weights:

$$\hat{\beta} = \left(F^T R^{-1} F\right)^{-1} F^T R^{-1} Y$$

- and the vectors:

$$\gamma = R^{-1}(Y - F\,\hat{\beta})$$
$$u(X) = F^T R^{-1} r(X) - f(X)$$

It is important to notice that the probabilistic response of a Gaussian Process predictor is fully analytic and mostly relies on basic linear algebra operations. More precisely the mean prediction is the sum of two simple linear combinations (dot products), and the variance requires two matrix inversions, but the correlation matrix can be decomposed only once using a Cholesky decomposition algorithm.

The empirical best linear unbiased predictor (EBLUP)

Until now, both the autocorrelation and regression models were assumed given. In practice however they are never known in advance so that one has to make (motivated) empirical choices for these models *Correlation Models*.

Provided these choices are made, one should estimate the remaining unknown parameters involved in the BLUP. To do so, one uses the set of provided observations in conjunction with some inference technique. The present implementation, which is based on the DACE's Matlab toolbox uses the *maximum likelihood estimation* technique – see DACE manual in references for the complete equations. This maximum likelihood estimation problem is turned into a global optimization problem onto the autocorrelation parameters. In the present implementation, this global optimization is solved by means of the fmin_cobyla optimization function from scipy.optimize. In the case of anisotropy however, we provide an implementation of Welch's componentwise optimization algorithm – see references.

For a more comprehensive description of the theoretical aspects of Gaussian Processes for Machine Learning, please refer to the references below:

References:

- DACE, A Matlab Kriging Toolbox S Lophaven, HB Nielsen, J Sondergaard 2002
- Screening, predicting, and computer experiments WJ Welch, RJ Buck, J Sacks, HP Wynn, TJ Mitchell, and MD Morris Technometrics 34(1) 15–25, 1992
- Gaussian Processes for Machine Learning CE Rasmussen, CKI Williams MIT Press, 2006 (Ed. T Dietrich)
- The design and analysis of computer experiments TJ Santner, BJ Williams, W Notz Springer, 2003

Correlation Models

Common correlation models matches some famous SVM's kernels because they are mostly built on equivalent assumptions. They must fulfill Mercer's conditions and should additionaly remain stationary. Note however, that the choice of the correlation model should be made in agreement with the known properties of the original experiment from which the observations come. For instance:

- If the original experiment is known to be infinitely differentiable (smooth), then one should use the *squared-exponential correlation model*.
- If it's not, then one should rather use the *exponential correlation model*.
- Note also that there exists a correlation model that takes the degree of derivability as input: this is the Matern correlation model, but it's not implemented here (TODO).

For a more detailed discussion on the selection of appropriate correlation models, see the book by Rasmussen & Williams in references.

Regression Models

Common linear regression models involve zero- (constant), first- and second-order polynomials. But one may specify its own in the form of a Python function that takes the features X as input and that returns a vector containing the values of the functional set. The only constraint is that the number of functions must not exceed the number of available observations so that the underlying regression problem is not *underdetermined*.

Implementation details

The present implementation is based on a translation of the DACE Matlab toolbox.

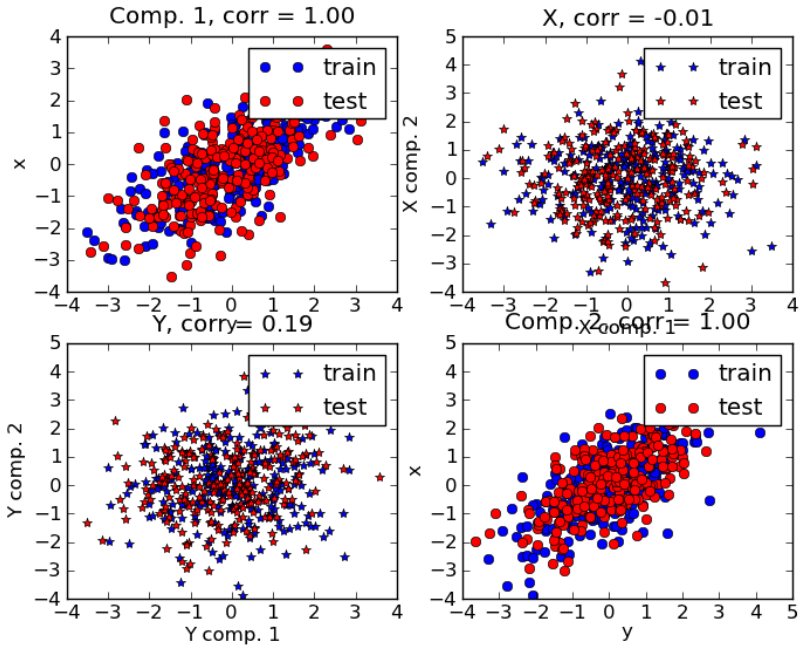
References:

- DACE, A Matlab Kriging Toolbox S Lophaven, HB Nielsen, J Sondergaard 2002,

1.3.7 Partial Least Squares

Partial least squares (PLS) models are useful to find linear relations between two multivariate datasets: in PLS the *X* and *Y* arguments of the *fit* method are 2D arrays.

PLS finds the fundamental relations between two matrices (X and Y): it is a latent variable approach to modeling the covariance structures in these two spaces. A PLS model will try to find the multidimensional direction in the X space that explains the maximum multidimensional variance direction in the Y space. PLS-regression is particularly



suited when the matrix of predictors has more variables than observations, and when there is multicollinearity among X values. By contrast, standard regression will fail in these cases.

Classes included in this module are `PLSRegression` `PLSCanonical`, `CCA` and `PLSSVD`

Reference:

- JA Wegelin A survey of Partial Least Squares (PLS) methods, with emphasis on the two-block case

Examples:

- *PLS Partial Least Squares*

1.3.8 Naive Bayes

Naive Bayes algorithms are a set of supervised learning methods based on applying Baye's theorem with strong (naive) independence assumptions.

The advantage of Naive Bayes approaches are:

- It requires a small amount of training data to estimate the parameters necessary for classification.
- In spite of their naive design and apparently over-simplified assumptions, naive Bayes classifiers have worked quite well in many complex real-world situations.
- The decoupling of the class conditional feature distributions means that each distribution can be independently estimated as a one dimensional distribution. This in turn helps to alleviate problems stemming from the curse of dimensionality.

Gaussian Naive Bayes

`GNB` implements the Gaussian Naive Bayes algorithm for classification.

Examples:

- *Gaussian Naive Bayes*,

1.4 Unsupervised learning

1.4.1 Gaussian mixture models

scikits.learn.mixture is a package which enables to create Mixture Models (diagonal, spherical, tied and full covariance matrices supported), to sample them, and to estimate them from data using Expectation Maximization algorithm. It can also draw confidence ellipsoides for multivariate models, and compute the Bayesian Information Criterion to assess the number of clusters in the data.

For the moment, only Gaussian Mixture Models (GMM) are implemented. These are a class of probabilistic models describing the data as drawn from a mixture of Gaussian probability distributions. The challenge that is GMM tackles is to learn the parameters of these Gaussians from the data.

GMM classifier

The `GMM` object implements a `GMM.fit` method to learn a Gaussian Mixture Models from train data. Given test data, it can assign to each sample the class of the Gaussian it mostly probably belong to using the `GMM.predict` method.

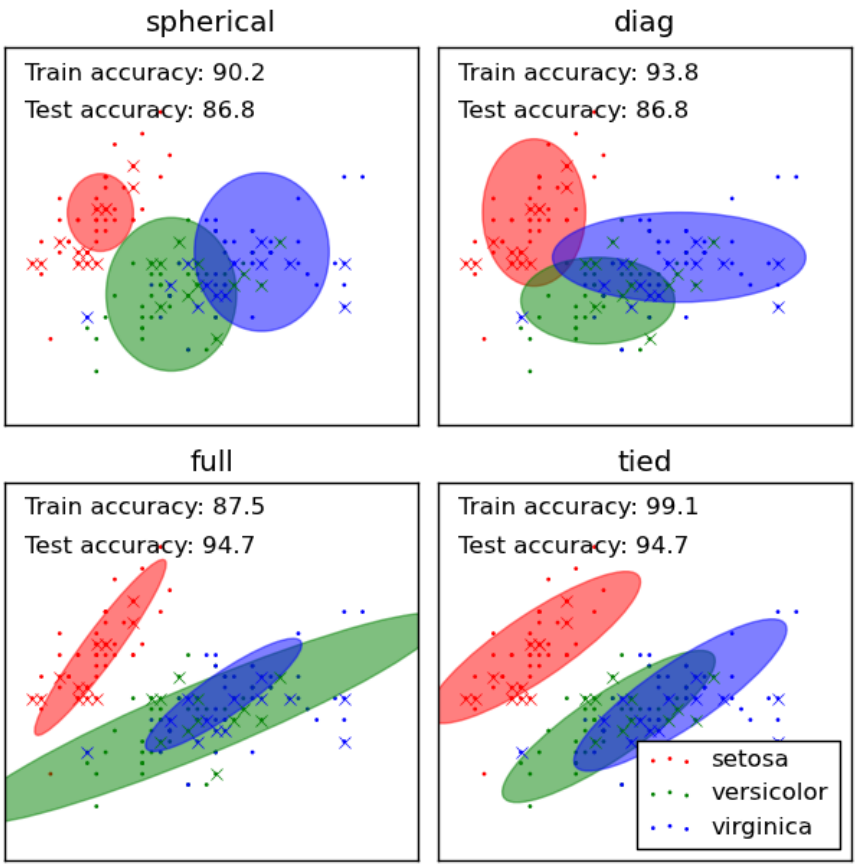
Examples:

- See *GMM classification* for an example of using a GMM as a classifier on the iris dataset.
- See *Gaussian Mixture Model Ellipsoids* for an example on plotting the confidence ellipsoids.
- See *Density Estimation for a mixture of Gaussians* for an example on plotting the density estimation.

1.4.2 Clustering

Clustering of unlabeled data can be performed with the module `scikits.learn.cluster`.

Each clustering algorithm comes in two variants: a class, that implements the *fit* method to learn the clusters on train data, and a function, that, given train data, returns an array of integer labels corresponding to the different clusters. For the class, the labels over the training data can be found in the *labels_* attribute.



Input data

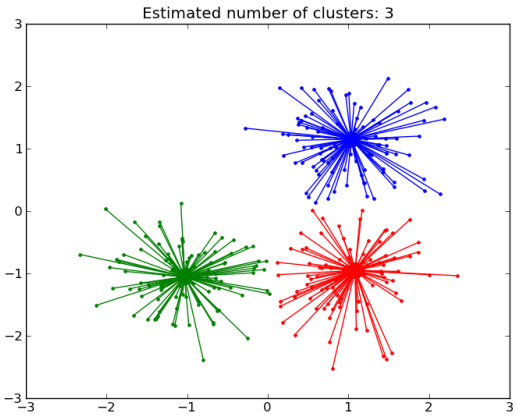
One important thing to note is that the algorithms implemented in this module take different kinds of matrix as input. On one hand, `MeanShift` and `KMeans` take data matrices of shape [n_samples, n_features]. These can be obtained from the classes in the `scikits.learn.feature_extraction` module. On the other hand, `AffinityPropagation` and `SpectralClustering` take similarity matrices of shape [n_samples, n_samples]. These can be obtained from the functions in the `scikits.learn.metrics.pairwise` module. In other words, `MeanShift` and `KMeans` work with points in a vector space, whereas `AffinityPropagation` and `SpectralClustering` can work with arbitrary objects, as long as a similarity measure exists for such objects.

K-means

The `KMeans` algorithm clusters data by trying to separate samples in n groups of equal variance, minimizing a criterion known as the 'inertia' of the groups. This algorithm requires the number of cluster to be specified. It scales well to large number of samples, however its results may be dependent on an initialisation.

Affinity propagation

`AffinityPropagation` clusters data by diffusion in the similarity matrix. This algorithm automatically sets its numbers of cluster. It will have difficulties scaling to thousands of samples.

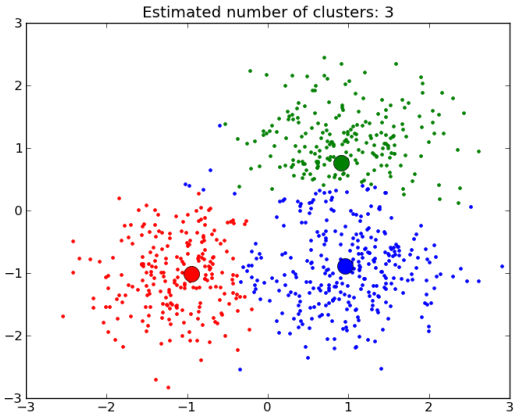


Examples:

- *Demo of affinity propagation clustering algorithm*: Affinity Propagation on a synthetic 2D datasets with 3 classes.
- *Finding structure in the stock market* Affinity Propagation on Financial time series to find groups of companies

Mean Shift

`MeanShift` clusters data by estimating *blobs* in a smooth density of points matrix. This algorithm automatically sets its numbers of cluster. It will have difficulties scaling to thousands of samples.



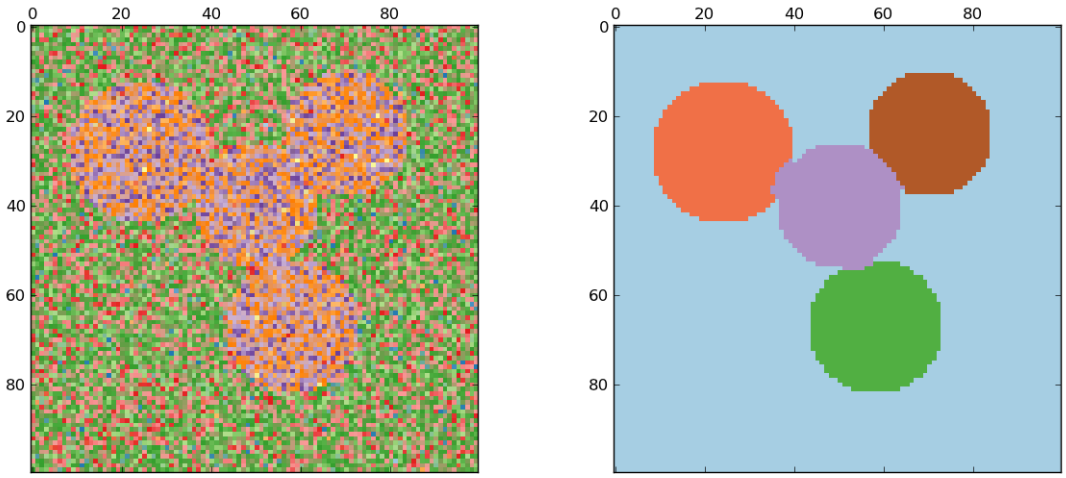
Examples:

- *A demo of the mean-shift clustering algorithm*: Mean Shift clustering on a synthetic 2D datasets with 3 classes.

Spectral clustering

`SpectralClustering` does a low-dimension embedding of the affinity matrix between samples, followed by a KMeans in the low dimensional space. It is especially efficient if the affinity matrix is sparse and the pyamg module is installed. SpectralClustering requires the number of clusters to be specified. It works well for a small number of clusters but is not advised when using many clusters.

For two clusters, it solves a convex relaxation of the normalised cuts problem on the similarity graph: cutting the graph in two so that the weight of the edges cut is small compared to the weights in of edges inside each cluster. This criteria is especially interesting when working on images: graph vertices are pixels, and edges of the similarity graph are a function of the gradient of the image.



Examples:

- *Spectral clustering for image segmentation*: Segmenting objects from a noisy background using spectral clustering.
- *Segmenting the picture of Lena in regions*: Spectral clustering to split the image of lena in regions.

References:

- "A Tutorial on Spectral Clustering" Ulrike von Luxburg, 2007
- "Normalized cuts and image segmentation" Jianbo Shi, Jitendra Malik, 2000
- "A Random Walks View of Spectral Segmentation" Marina Meila, Jianbo Shi, 2001
- "On Spectral Clustering: Analysis and an algorithm" Andrew Y. Ng, Michael I. Jordan, Yair Weiss, 2001

Hierarchical clustering

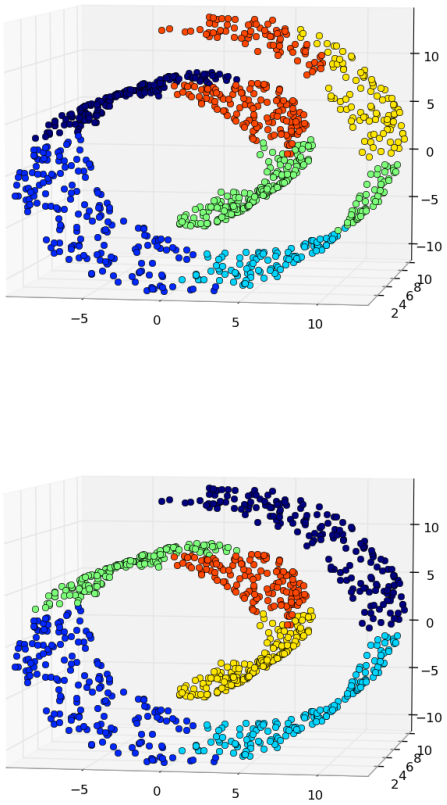
Hierarchical clustering is a general family of clustering algorithms that build nested clusters by merging them successively. This hierarchy of clusters represented as a tree (or dendrogram). The root of the tree is the unique cluster that gathers all the samples, the leaves being the clusters with only one sample. See the Wikipedia page for more details.

The `Ward` object performs a hierarchical clustering based on the Ward algorithm, that is a variance-minimizing approach. At each step, it minimizes the sum of squared differences within all clusters (inertia criterion).

This algorithm can scale to large number of samples when it is used jointly with an connectivity matrix, but can be computationally expensive when no connectivity constraints are added between samples: it considers at each step all the possible merges.

Adding connectivity constraints

An interesting aspect of the `Ward` object is that connectivity constraints can be added to this algorithm (only adjacent clusters can be merged together), through an connectivity matrix that defines for each sample the neighboring samples following a given structure of the data. For instance, in the swiss-roll example below, the connectivity constraints forbid the merging of points that are not adjacent on the swiss roll, and thus avoid forming clusters that extend across overlapping folds of the roll.



The connectivity constraints are imposed via an connectivity matrix: a scipy sparse matrix that has elements only at the intersection of a row and a column with indices of the dataset that should be connected. This matrix can be constructed from apriori information, for instance if you whish to cluster web pages, but only merging pages with a link pointing from one to another. It can also be learned from the data, for instance using `scikits.learn.neighbors.kneighbors_graph` to restrict merging to nearest neighbors as in the *swiss roll* example, or using `scikits.learn.feature_extraction.image.grid_to_graph` to enable only merging of neighboring pixels on an image, as in the *Lena* example.

Examples:

- *A demo of structured Ward hierarchical clustering on Lena image*: Ward clustering to split the image of lena in regions.
- *Hierarchical clustering: structured vs unstructured ward*: Example of Ward algorithm on a swiss-roll, comparison of structured approaches versus unstructured approaches.
- *Feature agglomeration vs. univariate selection*: Example of dimensionality reduction with feature agglomeration based on Ward hierarchical clustering.

1.4.3 Decomposing signals in components (matrix factorization problems)

Principal component analysis (PCA)

Exact PCA and probabilistic interpretation

PCA is used to decompose a multivariate dataset in a set of successive orthogonal components that explain a maximum amount of the variance. In the scikit-learn, `PCA` is implemented as a *transformer* object that learns n components in its *fit* method, and can be used on new data to project it on these components.

The optional parameter *whiten=True* parameter make it possible to project the data onto the singular space while scaling each component to unit variance. This is often useful if the models down-stream make strong assumptions on the isotropy of the signal: this is for example the case for Support Vector Machines with the RBF kernel and the K-Means clustering algorithm. However in that case the inverse transform is no longer exact since some information is lost while forward transforming.

In addition, the `ProbabilisticPCA` object provides a probabilistic interpretation of the PCA that can give a likelihood of data based on the amount of variance it explains. As such it implements a *score* method that can be used in cross-validation.

Below is an example of the iris dataset, which is comprised of 4 features, projected on the 2 dimensions that explain most variance:

Examples:

- *PCA 2D projection of Iris dataset*

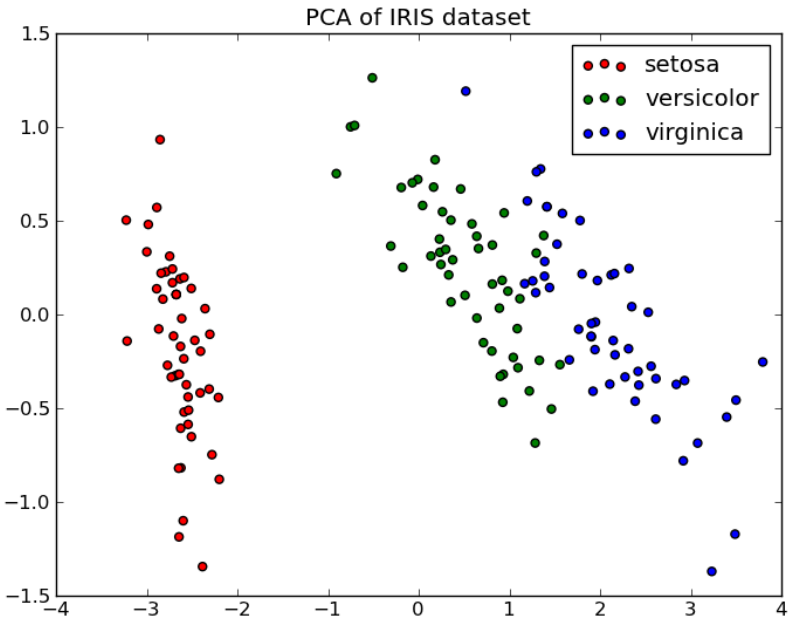
Approximate PCA

Often we are interested in projecting the data onto a lower dimensional space that preserves most of the variance by dropping the singular vector of components associated with lower singular values.

For instance for face recognition, if we work with 64x64 gray level pixel pictures the dimensionality of the data is 4096 and it is slow to train a RBF Support Vector Machine on such wide data. Furthermore we know that intrinsic dimensionality of the data is much lower than 4096 since all faces pictures look alike. The samples lie on a manifold of much lower dimension (say around 200 for instance). The PCA algorithm can be used to linearly transform the data while both reducing the dimensionality and preserve most of the explained variance at the same time.

The class `RandomizedPCA` is very useful in that case: since we are going to drop most of the singular vectors it is much more efficient to limit the computation to an approximated estimate of the singular vectors we will keep to actually perform the transform.

`RandomizedPCA` can hence be used as a drop in replacement for `PCA` minor the exception that we need to give it the size of the lower dimensional space *n_components* as mandatory input parameter.



If we note $n_{max} = max(n_{samples}, n_{features})$ and $n_{min} = min(n_{samples}, n_{features})$, the time complexity of `RandomizedPCA` is $O(n_{max}^2 \cdot n_{components})$ instead of $O(n_{max}^2 \cdot n_{min})$ for the exact method implemented in `PCA`.

The memory footprint of `RandomizedPCA` is also proportional to $2 \cdot n_{max} \cdot n_{components}$ instead of $n_{max} \cdot n_{min}$ for the exact method.

Furthermore `RandomizedPCA` is able to work with *scipy.sparse* matrices as input which make it suitable for reducing the dimensionality of features extracted from text documents for instance.

Note: the implementation of *inverse_transform* in `RandomizedPCA` is not the exact inverse transform of *transform* even when *whiten=False* (default).

Examples:

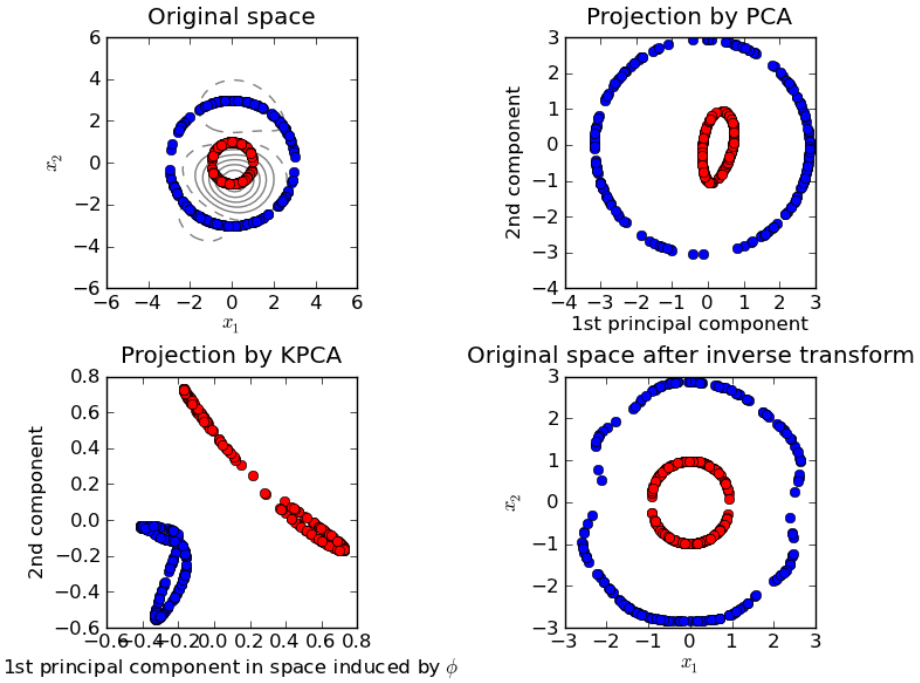
- *Faces recognition example using eigenfaces and SVMs*

References:

- "Finding structure with randomness: Stochastic algorithms for constructing approximate matrix decompositions" Halko, et al., 2009

Kernel PCA

`KernelPCA` is an extension of PCA which achieves non-linear dimensionality reduction through the use of kernels. It has many applications including denoising, compression and structured prediction (kernel dependency estimation). `KernelPCA` supports both *transform* and *inverse_transform*.

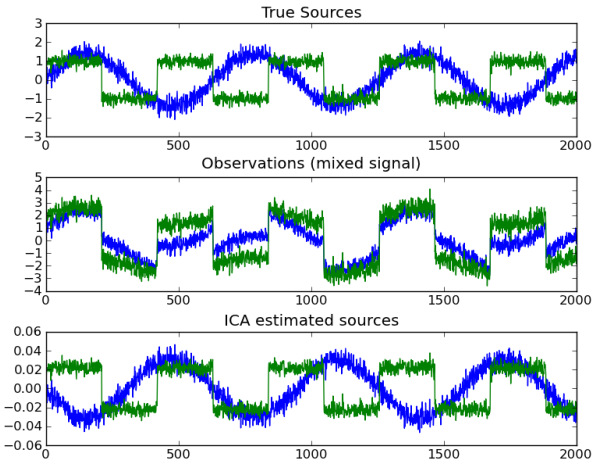


Examples:

- *Kernel PCA*

Independent component analysis (ICA)

ICA finds components that are maximally independent. It is classically used to separate mixed signals (a problem know as *blind source separation*), as in the example below:



Examples:

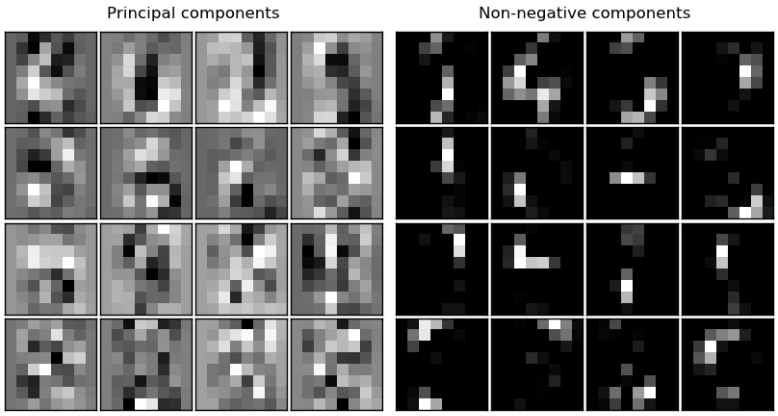
- *Blind source separation using FastICA*
- *FastICA on 2D point clouds*

Non-negative matrix factorization (NMF)

`NMF` is an alternative approach to decomposition that assumes that the data and the components are non-negative. `NMF` can be plugged in instead of `PCA` or its variants, in the cases where the data matrix does not contain negative values.

Unlike `PCA`, the representation of a vector is obtained in an additive fashion, by superimposing the components, without substracting. Such additive models are efficient for representing images and text.

It has been observed in [Hoyer, 04] that, when carefully constrained, `NMF` can produce a parts-based representation of the dataset, resulting in interpretable models. The following example displays 16 sparse components found by `NMF` on the digits dataset.



The `init` attribute determines the initialization method applied, which has a great impact on the performance of the method. `NMF` implements the method Nonnegative Double Singular Value Decomposition. NNDSVD is based on two SVD processes, one approximating the data matrix, the other approximating positive sections of the resulting partial SVD factors utilizing an algebraic property of unit rank matrices. The basic NNDSVD algorithm is better fit for sparse factorization. Its variants NNDSVDa (in which all zeros are set equal to the mean of all elements of the data), and NNDSVDar (in which the zeros are set to random perturbations less than the mean of the data divided by 100) are recommended in the dense case.

`NMF` can also be initialized with random non-negative matrices, by passing an integer seed or a *RandomState* to `init`.

In `NMF`, sparseness can be enforced by setting the attribute `sparseness` to *data* or *components*. Sparse components lead to localized features, and sparse data leads to a more efficient representation of the data.

Examples:

- *NMF for digits feature extraction*

References:

- "Learning the parts of objects by non-negative matrix factorization" D. Lee, S. Seung, 1999
- "Non-negative Matrix Factorization with Sparseness Constraints" P. Hoyer, 2004
- "Projected gradient methods for non-negative matrix factorization" C.-J. Lin, 2007
- "SVD based initialization: A head start for nonnegative matrix factorization" C. Boutsidis, E. Gallopoulos, 2008

1.4.4 Covariance estimation

Many statistical problems require at some point the estimation of a population's covariance matrix, which can be seen as an estimation of data set scatter plot shape. Most of the time, such an estimation has to be done on a sample whose properties (size, structure, homogeneity) has a large influence on the estimation's quality. The *scikits.learn.covariance* package aims at providing tools affording an accurate estimation of a population's covariance matrix under various settings.

The package does not include robust tools yet, so we assume that the data sets do not contain any outlying data. We also assume thah the observations are independant and identically distributed.

Empirical covariance

The covariance matrix of a data set is known to be well approximated with the classical *Maximum Likelihood Estimator* (or *empirical covariance*), provided the number of observations is large enough compared to the number of features (the variables describing the observations). More precisely, the Maximum Likelihood Estimator of a sample is an unbiased estimator of the corresponding population covariance matrix.

The empirical covariance matrix of a sample can be computed using the `empirical_covariance` function of the package, or by fitting an `EmpiricalCovariance` object to the data sample with the `EmpiricalCovariance.fit` method. Be careful that depending whether the data are centered or not, the result will be different, so one may want to use the *assume_centered* parameter accurately.

Examples:

- See *Ledoit-Wolf vs Covariance simple estimation* for an example on how to fit an `EmpiricalCovariance` object to data.

Shrunk Covariance

Basic shrinkage

Despite it is an unbiased estimator of the covariance matrix, the Maximum Likelihood Estimator is not a good estimator of the eigenvalues of the covariance matrix, so the precision matrix obtained from its inversion is not accurate. Sometimes, it even occurs that the empirical covariance matrix cannot be inverted for numerical reasons. To avoid such an inversion problem, a transformation of the empirical covariance matrix has been introduced: the *shrinkage*. It consists in reducing the ratio between the smallest and the largest eigenvalue of the empirical covariance matrix. This can be done by simply shifting every eigenvalue according to a given offset, which is equivalent of finding the l2-Penalized Maximum Likelihood Estimator of the covariance matrix, or by reducing the highest eigenvalue while increasing the smallest with the help of a convex transformation : $\Sigma_{\text{shrunk}} = (1-\alpha)\hat{\Sigma} + \alpha\frac{\text{Tr}\hat{\Sigma}}{p}\text{Id}$. The latter approach has been implemented in scikit-learn.

A convex transformation (with a user-defined shrinkage coefficient) can be directly applied to a pre-computed covariance with the `shrunk_covariance` method. Also, a shrunk estimator of the covariance can be fitted to data with a `ShrunkCovariance` object and its `ShrunkCovariance.fit` method. Again, depending whether the data are centered or not, the result will be different, so one may want to use the *assume_centered* parameter accurately.

Examples:

- See *Ledoit-Wolf vs Covariance simple estimation* for an example on how to fit a `ShrunkCovariance` object to data.

Ledoit-Wolf shrinkage

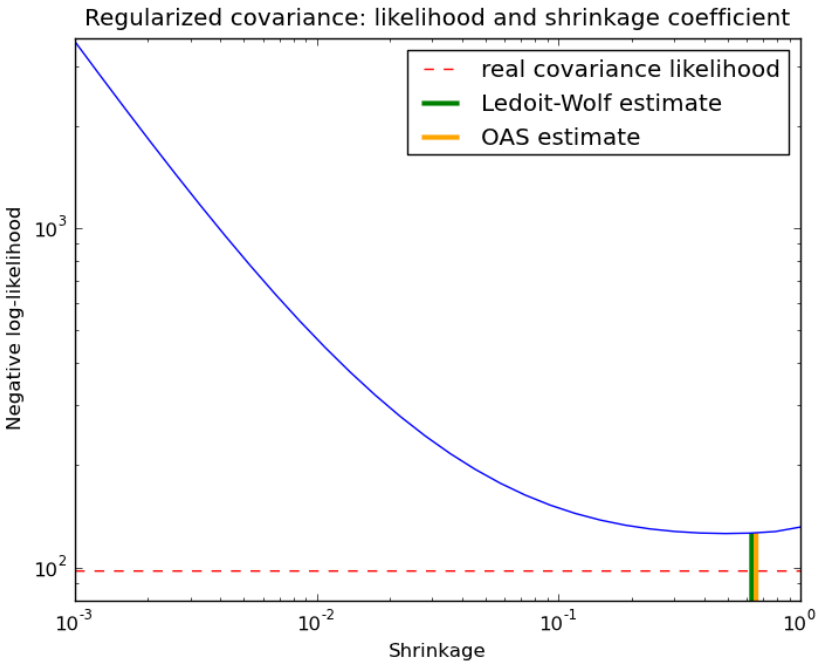
In their 2004 paper [1], O. Ledoit and M. Wolf propose a formula so as to compute the optimal shrinkage coefficient α that minimizes the Mean Squared Error between the estimated and the real covariance matrix in terms of Frobenius norm.

The Ledoit-Wolf estimator of the covariance matrix can be computed on a sample with the `ledoit_wolf` function of the *scikits.learn.covariance* package, or it can be otherwise obtained by fitting a `LedoitWolf` object to the same sample.

[1] "A Well-Conditioned Estimator for Large-Dimensional Covariance Matrices", Ledoit and Wolf, Journal of Multivariate Analysis, Volume 88, Issue 2, February 2004, pages 365-411.

Examples:

- See *Ledoit-Wolf vs Covariance simple estimation* for an example on how to fit a `LedoitWolf` object to data and for visualizing the performances of the Ledoit-Wolf estimator in terms of likelihood.



Oracle Approximating Shrinkage

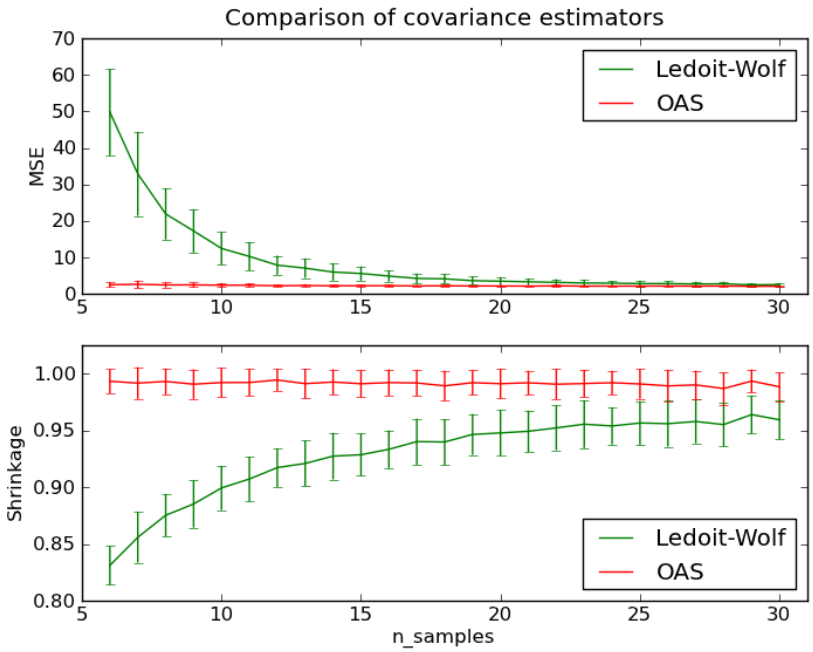
Under the assumption that the data are Gaussian distributed, Chen et al. [2] derived a formula aimed at choosing a shrinkage coefficient that yields a smaller Mean Squared Error than the one given by Ledoit and Wolf's formula. The resulting estimator is known as the Oracle Shrinkage Approximating estimator of the covariance.

The OAS estimator of the covariance matrix can be computed on a sample with the `oas` function of the *scikits.learn.covariance* package, or it can be otherwise obtained by fitting an `OAS` object to the same sample. The formula we used to implement the OAS does not correspond to the one given in the article. It has been taken from the matlab programm available from the authors webpage (https://tbayes.eecs.umich.edu/yilun/covestimation).

[2] "Shrinkage Algorithms for MMSE Covariance Estimation" Chen et al., IEEE Trans. on Sign. Proc., Volume 58, Issue 10, October 2010.

Examples:

- See *Ledoit-Wolf vs Covariance simple estimation* for an example on how to fit an `OAS` object to data.
- See *Ledoit-Wolf vs OAS estimation* to visualize the Mean Squared Error difference between a `LedoitWolf` and an `OAS` estimator of the covariance.



1.5 Model Selection

1.5.1 Cross-Validation

Learning the parameters of a prediction function and testing it on the same data yields a methodological bias. To avoid over-fitting, we have to define two different sets : a *learning set* X^l, y^l which is used for learning the prediction function (also called *training set*), and a *test set* X^t, y^t which is used for testing the prediction function. However, by defining these two sets, we drastically reduce the number of samples which can be used for learning the model, and the results can depend on a particular couple of *learning set* and *test set*.

A solution is to split the whole data in different learning set and test set, and to return the averaged value of the prediction scores obtained with the different sets. Such a procedure is called *cross-validation*. This approach can be computationally expensive, but does not waste too much data (as it is the case when fixing an arbitrary test set), which is a major advantage in problem such as inverse inference where the number of samples is very small.

Examples

Receiver operating characteristic (ROC) with cross validation, *Parameter estimation using grid search with a nested cross-validation*, *example_rfe_with_cross_validation.py*,

Leave-One-Out - LOO

`LeaveOneOut` The *Leave-One-Out* (or LOO) is a simple cross-validation. Each learning set is created by taking all the samples except one, the test set being the sample left out. Thus, for *n* samples, we have *n* different learning sets and *n* different tests set. This cross-validation procedure does not waste much data as only one sample is removed from the learning set.

```
>>> import numpy as np
>>> from scikits.learn.cross_val import LeaveOneOut
>>> X = np.array([[0., 0.], [1., 1.], [-1., -1.], [2., 2.]])
>>> Y = np.array([0, 1, 0, 1])
>>> loo = LeaveOneOut(len(Y))
>>> print loo
scikits.learn.cross_val.LeaveOneOut(n=4)
>>> for train, test in loo: print train, test
[False  True  True  True] [ True False False False]
[ True False  True  True] [False  True False False]
[ True  True False  True] [False False  True False]
[ True  True  True False] [False False False  True]
```

Each fold is constituted by two arrays: the first one is related to the *training set*, and the second one to the *test set*. Thus, one can create the training/test sets using:

```
>>> X_train, X_test, y_train, y_test = X[train], X[test], Y[train], Y[test]
```

If X or Y are *scipy.sparse* matrices, train and test need to be integer indices. It can be obtained by setting the parameter indices to True when creating the cross-validation procedure.

```
>>> import numpy as np
>>> from scikits.learn.cross_val import LeaveOneOut
>>> X = np.array([[0., 0.], [1., 1.], [-1., -1.], [2., 2.]])
>>> Y = np.array([0, 1, 0, 1])
>>> loo = LeaveOneOut(len(Y), indices=True)
>>> print loo
scikits.learn.cross_val.LeaveOneOut(n=4)
>>> for train, test in loo: print train, test
[1 2 3] [0]
[0 2 3] [1]
[0 1 3] [2]
[0 1 2] [3]
```

Leave-P-Out - LPO

`LeavePOut` *Leave-P-Out* is very similar to *Leave-One-Out*, as it creates all the possible training/test sets by removing *P* samples from the complete set.

Example of Leave-2-Out:

```
>>> from scikits.learn.cross_val import LeavePOut
>>> X = [[0., 0.], [1., 1.], [-1., -1.], [2., 2.]]
>>> Y = [0, 1, 0, 1]
>>> loo = LeavePOut(len(Y), 2)
>>> print loo
scikits.learn.cross_val.LeavePOut(n=4, p=2)
>>> for train, test in loo: print train,test
[False False  True  True] [ True  True False False]
[False  True False  True] [ True False  True False]
[False  True  True False] [ True False False  True]
[ True False False  True] [False  True  True False]
[ True False  True False] [False  True False  True]
[ True  True False False] [False False  True  True]
```

All the possible folds are created, and again, one can create the training/test sets using:

```
>>> import numpy as np
>>> X = np.asanyarray(X)
>>> Y = np.asanyarray(Y)
>>> X_train, X_test, y_train, y_test = X[train], X[test], Y[train], Y[test]
```

K-fold

`KFold`

The *K-fold* divides all the samples in *K* groups of samples, called folds (if $K = n$, we retrieve the *LOO*), of equal sizes (if possible). The prediction function is learned using *K - 1* folds, and the fold left out is used for test.

Example of 2-fold:

```
>>> from scikits.learn.cross_val import KFold
>>> X = [[0., 0.], [1., 1.], [-1., -1.], [2., 2.]]
>>> Y = [0, 1, 0, 1]
>>> loo = KFold(len(Y), 2)
>>> print loo
scikits.learn.cross_val.KFold(n=4, k=2)
>>> for train, test in loo: print train,test
[False False  True  True] [ True  True False False]
[ True  True False False] [False False  True  True]
```

Stratified K-Fold

`StratifiedKFold`

The *Stratified K-Fold* is a variation of *K-fold*, which returns stratified folds, *i.e* which creates folds by preserving the same percentage for each class as in the complete set.

Example of stratified 2-fold:

```
>>> from scikits.learn.cross_val import StratifiedKFold
>>> X = [[0., 0.], [1., 1.], [-1., -1.], [2., 2.], [3., 3.], [4., 4.], [0., 1.]]
>>> Y = [0, 0, 0, 1, 1, 1, 0]
>>> skf = StratifiedKFold(Y, 2)
>>> print skf
scikits.learn.cross_val.StratifiedKFold(labels=[0 0 0 1 1 1 0], k=2)
>>> for train, test in skf: print train, test
```

```
[False  True False False  True False  True] [ True False  True  True False  True False]
[ True False  True  True False  True False] [False  True False False  True False  True]
```

Leave-One-Label-Out - LOLO

`LeaveOneLabelOut`

The *Leave-One-Label-Out* (LOLO) is a cross-validation scheme which removes the samples according to a specific label. Each training set is thus constituted by all the samples except the ones related to a specific label.

For example, in the cases of multiple experiments, *LOLO* can be used to create a cross-validation based on the different experiments: we create a training set using the samples of all the experiments except one.

```
>>> from scikits.learn.cross_val import LeaveOneLabelOut
>>> X = [[0., 0.], [1., 1.], [-1., -1.], [2., 2.]]
>>> Y = [0, 1, 0, 1]
>>> labels = [1, 1, 2, 2]
>>> loo = LeaveOneLabelOut(labels)
>>> print loo
scikits.learn.cross_val.LeaveOneLabelOut(labels=[1, 1, 2, 2])
>>> for train, test in loo: print train,test
[False False  True  True] [ True  True False False]
[ True  True False False] [False False  True  True]
```

Leave-P-Label-Out

`LeavePLabelOut`

Leave-P-Label-Out is similar as *Leave-One-Label-Out*, but removes samples related to *P* labels for each training/test set.

Example of Leave-2-Label Out:

```
>>> from scikits.learn.cross_val import LeavePLabelOut
>>> X = [[0., 0.], [1., 1.], [-1., -1.], [2., 2.], [3., 3.], [4., 4.]]
>>> Y = [0, 1, 0, 1, 0, 1]
>>> labels = [1, 1, 2, 2, 3, 3]
>>> loo = LeavePLabelOut(labels, 2)
>>> print loo
scikits.learn.cross_val.LeavePLabelOut(labels=[1, 1, 2, 2, 3, 3], p=2)
>>> for train, test in loo: print train,test
[False False False False  True  True] [ True  True  True  True False False]
[False False  True  True False False] [ True  True False False  True  True]
[ True  True False False False False] [False False  True  True  True  True]
```

1.5.2 Grid Search

Grid Search is used to optimize the parameters of a model (e.g. Support Vector Classifier, Lasso, etc.) using cross-validation.

Main class is `GridSearchCV`.

Examples

See *Parameter estimation using grid search with a nested cross-validation* for an example of Grid Search computation on the digits dataset.

See *Sample pipeline for text feature extraction and evaluation* for an example of Grid Search coupling parameters from a text documents feature extractor (n-gram count vectorizer and TF-IDF transformer) with a classifier (here a linear SVM trained with SGD with either elastic net or L2 penalty).

Notes

Computations can be run in parallel if your OS supports it, by using the keyword n_jobs=-1, see function signature for more details.

1.6 Dataset loading utilities

The `scikits.learn.datasets` package embeds some small toy datasets as introduced in the "Getting Started" section.

To evaluate the impact of the scale of the dataset (`n_features` and `n_samples`) while controlling the statistical properties of the data (typically the correlation and informativeness of the features), it is also possible to generate synthetic data data

This package also features helpers to fetch larger datasets commonly used by the machine learning community to benchmark algorithm on data that comes from the 'real world'.

1.6.1 Datasets shipped with the scikit learn

The scikit learn comes with a few standard datasets:

`load_iris`()	load the iris dataset and returns it.
`load_diabetes`()	Load the diabetes dataset and returns it.
`load_digits`([n_class])	load the digits dataset and returns it.
`load_linnerud`()	Load the linnerud dataset and returns it.

1.6.2 Dataset generators

TODO

1.6.3 The Labeled Faces in the Wild face recognition dataset

This dataset is a collection of JPEG pictures of famous people collected over the internet, all details are available on the official website:

http://vis-www.cs.umass.edu/lfw/

Each picture is centered on a single face. The typical task is called Face Verification: given a pair of two pictures, a binary classifier must predict whether the two images are from the same person.

An alternative task, Face Recognition or Face Identification is: given the picture of the face of an unknown person, identify the name of the person by refering to a gallery of previously seen pictures of identified persons.

Both Face Verification and Face Recognition are tasks that are typically performed on the output of a model trained to perform Face Detection. The most popular model for Face Detection is called Viola-Johns and is implemented in the OpenCV library. The LFW faces were extracted by this face detector from various online websites.

Usage

`scikit-learn` provides two loaders that will automatically download, cache, parse the metadata files, decode the jpeg and convert the interesting slices into memmaped numpy arrays. This dataset size if more than 200 MB. The first load typically takes more than a couple of minutes to fully decode the relevant part of the JPEG files into numpy arrays. If the dataset has been loaded once, the following times the loading times less than 200ms by using a memmaped version memoized on the disk in the `~/scikit_learn_data/lfw_home/` folder using `joblib`.

The first loader is used for the Face Identification task: a multi-class classification task (hence supervised learning):

```
>>> from scikits.learn.datasets import fetch_lfw_people
>>> lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)

>>> for name in lfw_people.target_names:
...     print name
...
Ariel Sharon
Colin Powell
Donald Rumsfeld
George W Bush
Gerhard Schroeder
Hugo Chavez
Tony Blair
```

The default slice is a rectangular shape around the face, removing most of the background:

```
>>> lfw_people.data.dtype
dtype('float32')

>>> lfw_people.data.shape
(1288, 50, 37)
```

Each of the `1140` faces is assigned to a single person id in the `target` array:

```
>>> lfw_people.target.shape
(1288,)

>>> list(lfw_people.target[:10])
[5, 6, 3, 1, 0, 1, 3, 4, 3, 0]
```

The second loader is typically used for the face verification task: each sample is a pair of two picture belonging or not to the same person:

```
>>> from scikits.learn.datasets import fetch_lfw_pairs
>>> lfw_pairs_train = fetch_lfw_pairs(subset='train')

>>> list(lfw_pairs_train.target_names)
['Different persons', 'Same person']

>>> lfw_pairs_train.data.shape
(2200, 2, 62, 47)

>>> lfw_pairs_train.target.shape
(2200,)
```

Both for the `fetch_lfw_people` and `fetch_lfw_pairs` function it is possible to get an additional dimension with the RGB color channels by passing `color=True`, in that case the shape will be `(2200, 2, 62, 47, 3)`.

The `fetch_lfw_pairs` datasets is subdived in 3 subsets: the development `train` set, the development `test` set and an evaluation `10_folds` set meant to compute performance metrics using a 10-folds cross validation scheme.

References:

- Labeled Faces in the Wild: A Database for Studying Face Recognition in Unconstrained Environments. Gary B. Huang, Manu Ramesh, Tamara Berg, and Erik Learned-Miller. University of Massachusetts, Amherst, Technical Report 07-49, October, 2007.

Examples

Faces recognition example using eigenfaces and SVMs

1.6.4 The 20 newsgroups text dataset

The 20 newsgroups dataset comprises around 18000 newsgroups posts on 20 topics splitted in two subsets: one for training (or development) and the other one for testing (or for performance evaluation). The split between the train and test set is based upon a messages posted before and after a specific date.

Usage

The `scikits.learn.datasets.fetch_20newsgroups` function is a data fetching / caching functions that downloads the data archive from the original 20 newsgroups website, extracts the archive contents in the `~/scikit_learn_data/20news_home` folder and calls the `scikits.learn.datasets.load_filenames` on either the training or testing set folder:

```
>>> from scikits.learn.datasets import fetch_20newsgroups
>>> newsgroups_train = fetch_20newsgroups(subset='train')

>>> from pprint import pprint
>>> pprint(list(newsgroups_train.target_names))
['alt.atheism',
 'comp.graphics',
 'comp.os.ms-windows.misc',
 'comp.sys.ibm.pc.hardware',
 'comp.sys.mac.hardware',
 'comp.windows.x',
 'misc.forsale',
 'rec.autos',
 'rec.motorcycles',
 'rec.sport.baseball',
 'rec.sport.hockey',
 'sci.crypt',
 'sci.electronics',
 'sci.med',
 'sci.space',
 'soc.religion.christian',
 'talk.politics.guns',
 'talk.politics.mideast',
```

```
 'talk.politics.misc',
 'talk.religion.misc']
```

The real data lies in the `filenames` and `target` attributes. The target attribute is the integer index of the category:

```
>>> newsgroups_train.filenames.shape
(11314,)
>>> newsgroups_train.target.shape
(11314,)
>>> newsgroups_train.target[:10]
array([12,  6,  9,  8,  6,  7,  9,  2, 13, 19])
```

It is possible to load only a sub-selection of the categories by passing the list of the categories to load to the `fetch_20newsgroups` function:

```
>>> cats = ['alt.atheism', 'sci.space']
>>> newsgroups_train = fetch_20newsgroups(subset='train', categories=cats)

>>> list(newsgroups_train.target_names)
['alt.atheism', 'sci.space']
>>> newsgroups_train.filenames.shape
(1073,)
>>> newsgroups_train.target.shape
(1073,)
>>> newsgroups_train.target[:10]
array([1, 1, 1, 0, 1, 0, 0, 1, 1, 1])
```

In order to feed predictive or clustering models with the text data, one first need to turn the text into vectors of numerical values suitable for statistical analysis. This can be achieved with the utilities of the `scikits.learn.feature_extraction.text` as demonstrated in the following example that extract TF-IDF vectors of unigram tokens:

```
>>> from scikits.learn.feature_extraction.text import Vectorizer
>>> documents = [open(f).read() for f in newsgroups_train.filenames]
>>> vectorizer = Vectorizer()
>>> vectors = vectorizer.fit_transform(documents)
>>> vectors.shape
(1073, 21108)
```

The extracted TF-IDF vectors are very sparse with an average of 118 non zero components by sample in a more than 20000 dimensional space (less than 1% non zero features):

```
>>> vectors.nnz / vectors.shape[0]
118
```

Examples

Sample pipeline for text feature extraction and evaluation

Classification of text documents using sparse features

1.7 Class reference

1.7.1 Support Vector Machines

Support Vector Machine algorithms.

svm.SVC([C, kernel, degree, gamma, coef0, ...])	C-Support Vector Classification.
svm.LinearSVC([penalty, loss, dual, tol, C, ...])	Linear Support Vector Classification.
svm.NuSVC([nu, kernel, degree, gamma, ...])	Nu-Support Vector Classification.
svm.SVR([kernel, degree, gamma, coef0, ...])	epsilon-Support Vector Regression.
svm.NuSVR([nu, C, kernel, degree, gamma, ...])	Nu Support Vector Regression.
svm.OneClassSVM([kernel, degree, gamma, ...])	Unsupervised Outliers Detection.

svm.l1_min_c(X, y[, loss, fit_intercept, ...])	Return the maximum value for C that yields a model with coefficients

For sparse data

Support Vector Machine algorithms for sparse matrices.

This module should have the same API as scikits.learn.svm, except that matrices are expected to be in some sparse format supported by scipy.sparse.

Note: Some fields, like *dual_coef_* are not sparse matrices strictly speaking. However, they are converted to a sparse matrix for consistency and efficiency when multiplying to other sparse matrices.

svm.sparse.SVC([C, kernel, degree, gamma, ...])	SVC for sparse matrices (csr).
svm.sparse.NuSVC([nu, kernel, degree, ...])	NuSVC for sparse matrices (csr).
svm.sparse.SVR([kernel, degree, gamma, ...])	SVR for sparse matrices (csr)
svm.sparse.NuSVR([nu, C, kernel, degree, ...])	NuSVR for sparse matrices (csr)
svm.sparse.OneClassSVM([kernel, degree, ...])	NuSVR for sparse matrices (csr)
svm.sparse.LinearSVC([penalty, loss, dual, ...])	Linear Support Vector Classification, Sparse Version

Low-level methods

svm.libsvm.fit	Train the model using libsvm (low-level method)
svm.libsvm.decision_function	Predict margin (libsvm name for this is predict_values)
svm.libsvm.predict	Predict target values of X given a model (low-level method)
svm.libsvm.predict_proba	Predict probabilities svm_model stores all parameters needed to predict a given value.
svm.libsvm.cross_validation	Binding of the cross-validation routine (low-level routine)

1.7.2 Generalized Linear Models

scikits.learn.linear_model is a module to fit genelarized linear models. It includes Ridge regression, Bayesian Regression, Lasso and Elastic Net estimators computed with Least Angle Regression and coordinate descent.

It also implements Stochastic Gradient Descent related algorithms.

linear_model.LinearRegression([fit_intercept])	Ordinary least squares Linear Regression.
linear_model.Ridge([alpha, fit_intercept])	Ridge regression.
linear_model.RidgeCV([alphas, ...])	Ridge regression with built-in cross-validation.
linear_model.Lasso([alpha, fit_intercept])	Linear Model trained with L1 prior as regularizer (aka the Lasso)
linear_model.LassoCV([eps, n_alphas, ...])	Lasso linear model with iterative fitting along a regularization path
linear_model.ElasticNet([alpha, rho, ...])	Linear Model trained with L1 and L2 prior as regularizer
linear_model.ElasticNetCV([rho, eps, ...])	Elastic Net model with iterative fitting along a regularization path
linear_model.LARS([fit_intercept, verbose])	Least Angle Regression model a.k.a. LAR
linear_model.LassoLARS([alpha, ...])	Lasso model fit with Least Angle Regression a.k.a. LARS
linear_model.LogisticRegression([penalty, ...])	Logistic Regression.
linear_model.SGDClassifier([loss, penalty, ...])	Linear model fitted by minimizing a regularized empirical loss with SGD.
linear_model.SGDRegressor([loss, penalty, ...])	Linear model fitted by minimizing a regularized empirical loss with SGD
linear_model.BayesianRidge([n_iter, eps, ...])	Bayesian ridge regression
linear_model.ARDRegression([n_iter, eps, ...])	Bayesian ARD regression.

linear_model.lasso_path(X, y, **fit_params)	Compute Lasso path with coordinate descent
linear_model.lars_path(X, y[, Xy, Gram, ...])	Compute Least Angle Regression and LASSO path

For sparse data

scikits.learn.linear_model.sparse is the sparse counterpart of scikits.learn.linear_model.

linear_model.sparse.Lasso([alpha, fit_intercept])	Linear Model trained with L1 prior as regularizer
linear_model.sparse.ElasticNet([alpha, rho, ...])	Linear Model trained with L1 and L2 prior as regularizer
linear_model.sparse.SGDClassifier([loss, ...])	Linear model fitted by minimizing a regularized empirical loss with SGD
linear_model.sparse.SGDRegressor([loss, ...])	Linear model fitted by minimizing a regularized empirical loss with SGD

1.7.3 Naive Bayes

Naives Bayes classifiers.

naive_bayes.GNB	Gaussian Naive Bayes (GNB)

1.7.4 Nearest Neighbors

Nearest Neighbor related algorithms

neighbors.NeighborsClassifier([n_neighbors, ...])	Classifier implementing k-Nearest Neighbor Algorithm.
neighbors.NeighborsRegressor([n_neighbors, ...])	Regression based on k-Nearest Neighbor Algorithm
ball_tree.BallTree	

neighbors.kneighbors_graph(X, n_neighbors[, ...])	Computes the (weighted) graph of k-Neighbors for points in X

1.7.5 Gaussian Mixture Models

Gaussian Mixture Models

mixture.GMM([n_states, cvtype])	Gaussian Mixture Model

1.7.6 Hidden Markov Models

hmm.GaussianHMM([n_states, cvtype, ...])	Hidden Markov Model with Gaussian emissions
hmm.MultinomialHMM([n_states, startprob, ...])	Hidden Markov Model with multinomial (discrete) emissions
hmm.GMMHMM([n_states, n_mix, startprob, ...])	Hidden Markov Model with Gaussin mixture emissions

1.7.7 Clustering

Clustering algorithms

cluster.KMeans([k, init, n_init, max_iter, ...])	K-Means clustering
cluster.MeanShift([bandwidth])	MeanShift clustering
cluster.SpectralClustering([k, mode, ...])	Apply k-means to a projection to the normalized laplacian
cluster.AffinityPropagation([damping, ...])	Perform Affinity Propagation Clustering of data
cluster.Ward([n_clusters, memory, ...])	Ward hierarchical clustering: constructs a tree and cuts it.

1.7.8 Metrics

Metrics module with score functions, performance metrics and pairwise metrics or distances computation

metrics.euclidean_distances(X, Y[, ...])	Considering the rows of X (and Y=X) as vectors, compute the
metrics.confusion_matrix(y_true, y_pred[, ...])	Compute confusion matrix to evaluate the accuracy of a classification
metrics.roc_curve(y_true, y_score)	compute Receiver operating characteristic (ROC)
metrics.auc(x, y)	Compute Area Under the Curve (AUC) using the trapezoidal rule
metrics.precision_score(y_true, y_pred[, ...])	Compute the precision
metrics.recall_score(y_true, y_pred[, pos_label])	Compute the recall
metrics.fbeta_score(y_true, y_pred, beta[, ...])	Compute fbeta score
metrics.f1_score(y_true, y_pred[, pos_label])	Compute f1 score
metrics.precision_recall_fscore_support(...)	Compute precisions, recalls, f-measures and support for each class
metrics.classification_report(y_true, y_pred)	Build a text report showing the main classification metrics
metrics.precision_recall_curve(y_true, ...)	Compute precision-recall pairs for different probability thresholds
metrics.r2_score(y_true, y_pred)	R^2 (coefficient of determination) regression score function
metrics.zero_one_score(y_true, y_pred)	Zero-One classification score
metrics.zero_one(y_true, y_pred)	Zero-One classification loss
metrics.mean_square_error(y_true, y_pred)	Mean square error regression loss

Pairwise metrics

Utilities to evaluate pairwise distances or metrics between 2 sets of points.

metrics.pairwise.euclidean_distances(X, Y[, ...])	Considering the rows of X (and Y=X) as vectors, compute the
metrics.pairwise.linear_kernel(X, Y)	Compute the linear kernel between X and Y.
metrics.pairwise.polynomial_kernel(X, Y[, ...])	Compute the polynomial kernel between X and Y.
metrics.pairwise.rbf_kernel(X, Y[, sigma])	Compute the rbf (gaussian) kernel between X and Y.

1.7.9 Covariance Estimators

Covariance estimators

scikits.learn.covariance is a module to fit to estimate robustly the covariance of features given a set of points. The precision matrix defined as the inverse of the covariance is also estimated. Covariance estimation is closely related to the theory of Gaussian Graphical Models.

covariance.Covariance	
covariance.ShrunkCovariance([...])	Covariance estimator with shrinkage
covariance.LedoitWolf([store_precision])	LedoitWolf Estimator

covariance.ledoit_wolf(X[, assume_centered])	Estimates the shrunk Ledoit-Wolf covariance matrix.
covariance.shrunk_covariance(emp_cov[, ...])	Calculates a covariance matrix shrunk on the diagonal
covariance.oas(X[, assume_centered])	Estimate covariance with the Oracle Approximating Shrinkage algorithm.

1.7.10 Signal Decomposition

Matrix decomposition algorithms

decomposition.PCA([n_components, copy, whiten])	Principal component analysis (PCA)
decomposition.ProbabilisticPCA([...])	Additional layer on top of PCA that adds a probabilistic evaluation
decomposition.RandomizedPCA(n_components[, ...])	Principal component analysis (PCA) using randomized SVD
decomposition.KernelPCA([n_components, ...])	Kernel Principal component analysis (KPCA)
decomposition.FastICA([n_components, ...])	FastICA; a fast algorithm for Independent Component Analysis
decomposition.NMF([n_components, init, ...])	Non-Negative matrix factorization by Projected Gradient (NMF)

decomposition.fastica(X[, n_components, ...])	Perform Fast Independent Component Analysis.

1.7.11 Linear Discriminant Analysis

lda.LDA([n_components, priors])	Linear Discriminant Analysis (LDA)

1.7.12 Cross Validation

Utilities for cross validation and performance evaluation

cross_val.LeaveOneOut(n[, indices])	Leave-One-Out cross validation iterator
cross_val.LeavePOut(n, p[, indices])	Leave-P-Out cross validation iterator
cross_val.KFold(n, k[, indices])	K-Folds cross validation iterator
cross_val.StratifiedKFold(y, k[, indices])	Stratified K-Folds cross validation iterator
cross_val.LeaveOneLabelOut(labels[, indices])	Leave-One-Label_Out cross-validation iterator
cross_val.LeavePLabelOut(labels, p[, indices])	Leave-P-Label_Out cross-validation iterator

1.7.13 Grid Search

Tune the parameters of an estimator by cross-validation

grid_search.GridSearchCV(estimator, param_grid)	Grid search on the parameters of a classifier

1.7.14 Feature Selection

Feature slection module for python

feature_selection.rfe.RFE([estimator, ...])	Feature ranking with Recursive feature elimination
feature_selection.rfe.RFECV([estimator, ...])	Feature ranking with Recursive feature elimination and cross validation

1.7.15 Feature Extraction

Package for modules that deal with feature extraction from raw data

From images

Utilities to extract features from images.

feature_extraction.image.img_to_graph(img[, ...])	Graph of the pixel-to-pixel gradient connections
feature_extraction.image.grid_to_graph(n_x, n_y)	Graph of the pixel-to-pixel connections

From text

Utilities to build dense feature vectors from text documents

feature_extraction.text.RomanPreprocessor()	Fast preprocessor suitable for roman languages ..
feature_extraction.text.WordNGramAnalyzer([...])	Simple analyzer: transform a text document into a sequence of word tokens
feature_extraction.text.CharNGramAnalyzer([...])	Compute character n-grams features of a text document
feature_extraction.text.CountVectorizer([...])	Convert a collection of raw documents to a matrix of token counts
feature_extraction.text.TfidfTransformer([...])	Transform a count matrix to a TF or TF-IDF representation
feature_extraction.text.Vectorizer([...])	Convert a collection of raw documents to a matrix

1.7.16 Pipeline

Pipeline: chain transforms and estimators to build a composite estimator.

pipeline.Pipeline(steps)	Pipeline of transforms with a final estimator

1.7.17 Partial Least Squares

Partial Least Square

pls.PLSRegression([n_components, scale, ...])	PLS regression (Also known PLS2 or PLS in case of one dimensional
pls.PLSCanonical([n_components, scale, ...])	PLS canonical. PLSCanonical inherits from PLS with mode="A" and
pls.CCA([n_components, scale, algorithm, ...])	CCA Canonical Correlation Analysis. CCA inherits from PLS with
pls.PLSSVD([n_components, scale, copy])	Partial Least Square SVD

CHAPTER

TWO

EXAMPLE GALLERY

2.1 Examples

2.1.1 General examples

General-purpose and introductory examples for the scikit.

Classification of text documents using sparse features

This is an example showing how the scikit-learn can be used to classify documents by topics using a bag-of-words approach. This example uses a scipy.sparse matrix to store the features instead of standard numpy arrays.

The dataset used in this example is the 20 newsgroups dataset which will be automatically downloaded and then cached.

You can adjust the number of categories by giving there name to the dataset loader or setting them to None to get the 20 of them.

This example demos various linear classifiers with different training strategies.

To run this example use:

```
% python examples/document_classification_20newsgroups.py [options]
```

Options are:

--report	Print a detailed classification report.
--confusion-matrix	Print the confusion matrix.

Python source code: `document_classification_20newsgroups.py`

```
print __doc__

# Author: Peter Prettenhofer <peter.prettenhofer@gmail.com>
#         Olivier Grisel <olivier.grisel@ensta.org>
#         Mathieu Blondel <mathieu@mblondel.org>
# License: Simplified BSD

from time import time
import logging
import os
import sys
```

```
from scikits.learn.datasets import fetch_20newsgroups
from scikits.learn.feature_extraction.text import Vectorizer
from scikits.learn.linear_model import RidgeClassifier
from scikits.learn.svm.sparse import LinearSVC
from scikits.learn.linear_model.sparse import SGDClassifier
from scikits.learn import metrics


# Display progress logs on stdout
logging.basicConfig(level=logging.INFO,
                    format='%(asctime)s %(levelname)s %(message)s')


# parse commandline arguments
argv = sys.argv[1:]
if "--report" in argv:
    print_report = True
else:
    print_report = False
if "--confusion-matrix" in argv:
    print_cm = True
else:
    print_cm = False

###############################################################################
# Load some categories from the training set
categories = [
    'alt.atheism',
    'talk.religion.misc',
    'comp.graphics',
    'sci.space',
]
# Uncomment the following to do the analysis on all the categories
#categories = None

print "Loading 20 newsgroups dataset for categories:"
print categories

data_train = fetch_20newsgroups(subset='train', categories=categories,
                                shuffle=True, random_state=42)

data_test = fetch_20newsgroups(subset='test', categories=categories,
                               shuffle=True, random_state=42)

print "%d documents (training set)" % len(data_train.filenames)
print "%d documents (testing set)" % len(data_test.filenames)
print "%d categories" % len(data_train.target_names)
print

# split a training set and a test set
filenames_train, filenames_test = data_train.filenames, data_test.filenames
y_train, y_test = data_train.target, data_test.target

print "Extracting features from the training dataset using a sparse vectorizer"
t0 = time()
vectorizer = Vectorizer()
X_train = vectorizer.fit_transform((open(f).read() for f in filenames_train))
print "done in %fs" % (time() - t0)
```

```
print "n_samples: %d, n_features: %d" % X_train.shape
print

print "Extracting features from the test dataset using the same vectorizer"
t0 = time()
X_test = vectorizer.transform((open(f).read() for f in filenames_test))
print "done in %fs" % (time() - t0)
print "n_samples: %d, n_features: %d" % X_test.shape
print


###############################################################################
# Benchmark classifiers
def benchmark(clf):
    print 80 * '_'
    print "Training: "
    print clf
    t0 = time()
    clf.fit(X_train, y_train)
    train_time = time() - t0
    print "train time: %0.3fs" % train_time

    t0 = time()
    pred = clf.predict(X_test)
    test_time = time() - t0
    print "test time:  %0.3fs" % test_time

    score = metrics.f1_score(y_test, pred)
    print "f1-score:   %0.3f" % score

    nnz = clf.coef_.nonzero()[0].shape[0]
    print "non-zero coef: %d" % nnz
    print

    if print_report:
        print "classification report:"
        print metrics.classification_report(y_test, pred,
                                            target_names=categories)

    if print_cm:
        print "confusion matrix:"
        print metrics.confusion_matrix(y_test, pred)

    print
    return score, train_time, test_time

for clf, name in ((RidgeClassifier(), "Ridge Classifier"),):
    print 80*'='
    print name
    results = benchmark(clf)

for penalty in ["l2", "l1"]:
    print 80 * '='
    print "%s penalty" % penalty.upper()
    # Train Liblinear model
    liblinear_results = benchmark(LinearSVC(loss='l2', penalty=penalty, C=1000,
                                            dual=False, tol=1e-3))
```

```
    # Train SGD model
    sgd_results = benchmark(SGDClassifier(alpha=.0001, n_iter=50,
                                          penalty=penalty))

# Train SGD with Elastic Net penalty
print 80 * '='
print "Elastic-Net penalty"
sgd_results = benchmark(SGDClassifier(alpha=.0001, n_iter=50,
                                      penalty="elasticnet"))
```

Pipeline Anova SVM

Simple usage of Pipeline that runs successively a univariate feature selection with anova and then a C-SVM of the selected features.

Python source code: `feature_selection_pipeline.py`

```
print __doc__

from scikits.learn import svm
from scikits.learn.datasets import samples_generator
from scikits.learn.feature_selection import SelectKBest, f_regression
from scikits.learn.pipeline import Pipeline

# import some data to play with
X, y = samples_generator.test_dataset_classif(k=5)

# ANOVA SVM-C
# 1) anova filter, take 5 best ranked features
anova_filter = SelectKBest(f_regression, k=5)
# 2) svm
clf = svm.SVC(kernel='linear')

anova_svm = Pipeline([('anova', anova_filter), ('svm', clf)])
anova_svm.fit(X, y)
anova_svm.predict(X)
```

Parameter estimation using grid search with a nested cross-validation

The classifier is optimized by "nested" cross-validation using the GridSearchCV object.

The performance of the selected parameters is evaluated using cross-validation (different than the nested cross-validation that is used to select the best classifier).

Python source code: `grid_search_digits.py`

```
print __doc__

from pprint import pprint
import numpy as np

from scikits.learn import datasets
from scikits.learn.cross_val import StratifiedKFold
from scikits.learn.grid_search import GridSearchCV
from scikits.learn.metrics import classification_report
from scikits.learn.metrics import precision_score
from scikits.learn.metrics import recall_score
```

```
from scikits.learn.svm import SVC

##############################################################################
# Loading the Digits dataset
digits = datasets.load_digits()

# To apply an classifier on this data, we need to flatten the image, to
# turn the data in a (samples, feature) matrix:
n_samples = len(digits.images)
X = digits.images.reshape((n_samples, -1))
y = digits.target

# split the dataset in two equal part respecting label proportions
train, test = iter(StratifiedKFold(y, 2)).next()

##############################################################################
# Set the parameters by cross-validation
tuned_parameters = [{'kernel': ['rbf'], 'gamma': [1e-3, 1e-4],
                     'C': [1, 10, 100, 1000]},
                    {'kernel': ['linear'], 'C': [1, 10, 100, 1000]}]

scores = [
    ('precision', precision_score),
    ('recall', recall_score),
]

for score_name, score_func in scores:
    clf = GridSearchCV(SVC(C=1), tuned_parameters, score_func=score_func)
    clf.fit(X[train], y[train], cv=StratifiedKFold(y[train], 5))
    y_true, y_pred = y[test], clf.predict(X[test])

    print "Classification report for the best estimator: "
    print clf.best_estimator
    print "Tuned for '%s' with optimal value: %0.3f" % (
        score_name, score_func(y_true, y_pred))
    print classification_report(y_true, y_pred)
    print "Grid scores:"
    pprint(clf.grid_scores_)
    print

# Note the problem is too easy: the hyperparameter plateau is too flat and the
# output model is the same for precision and recall with ties in quality
```

Sample pipeline for text feature extraction and evaluation

The dataset used in this example is the 20 newsgroups dataset which will be automatically downloaded and then cached and reused for the document classification example.

You can adjust the number of categories by giving there name to the dataset loader or setting them to None to get the 20 of them.

Here is a sample output of a run on a quad-core machine:

```
Loading 20 newsgroups dataset for categories:
['alt.atheism', 'talk.religion.misc']
1427 documents
2 categories
```

```
Performing grid search...
pipeline: ['vect', 'tfidf', 'clf']
parameters:
{'clf__alpha': (1.0000000000000001e-05, 9.9999999999999995e-07),
 'clf__n_iter': (10, 50, 80),
 'clf__penalty': ('l2', 'elasticnet'),
 'tfidf__use_idf': (True, False),
 'vect__analyzer__max_n': (1, 2),
 'vect__max_df': (0.5, 0.75, 1.0),
 'vect__max_features': (None, 5000, 10000, 50000)}
done in 1737.030s

Best score: 0.940
Best parameters set:
    clf__alpha: 9.9999999999999995e-07
    clf__n_iter: 50
    clf__penalty: 'elasticnet'
    tfidf__use_idf: True
    vect__analyzer__max_n: 2
    vect__max_df: 0.75
    vect__max_features: 50000
```

Python source code: `grid_search_text_feature_extraction.py`

```
print __doc__

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# License: Simplified BSD

from pprint import pprint
from time import time
import os
import logging

from scikits.learn.datasets import fetch_20newsgroups
from scikits.learn.feature_extraction.text import CountVectorizer
from scikits.learn.feature_extraction.text import TfidfTransformer
from scikits.learn.linear_model.sparse import SGDClassifier
from scikits.learn.grid_search import GridSearchCV
from scikits.learn.pipeline import Pipeline

# Display progress logs on stdout
logging.basicConfig(level=logging.INFO,
                    format='%(asctime)s %(levelname)s %(message)s')


###############################################################################
# Load some categories from the training set
categories = [
    'alt.atheism',
    'talk.religion.misc',
]
# Uncomment the following to do the analysis on all the categories
#categories = None

print "Loading 20 newsgroups dataset for categories:"
```

```
print categories

data = fetch_20newsgroups(subset='train', categories=categories)
print "%d documents" % len(data.filenames)
print "%d categories" % len(data.target_names)
print

###############################################################################
# define a pipeline combining a text feature extractor with a simple
# classifier
pipeline = Pipeline([
    ('vect', CountVectorizer()),
    ('tfidf', TfidfTransformer()),
    ('clf', SGDClassifier()),
])

parameters = {
# uncommenting more parameters will give better exploring power but will
# increase processing time in a combinatorial way
    'vect__max_df': (0.5, 0.75, 1.0),
#    'vect__max_features': (None, 5000, 10000, 50000),
    'vect__analyzer__max_n': (1, 2), # words or bigrams
#    'tfidf__use_idf': (True, False),
    'clf__alpha': (0.00001, 0.000001),
    'clf__penalty': ('l2', 'elasticnet'),
#    'clf__n_iter': (10, 50, 80),
}

# find the best parameters for both the feature extraction and the
# classifier
grid_search = GridSearchCV(pipeline, parameters, n_jobs=-1)

# cross-validation doesn't work if the length of the data is not known,
# hence use lists instead of iterators
text_docs = [file(f).read() for f in data.filenames]

print "Performing grid search..."
print "pipeline:", [name for name, _ in pipeline.steps]
print "parameters:"
pprint(parameters)
t0 = time()
grid_search.fit(text_docs, data.target)
print "done in %0.3fs" % (time() - t0)
print

print "Best score: %0.3f" % grid_search.best_score
print "Best parameters set:"
best_parameters = grid_search.best_estimator._get_params()
for param_name in sorted(parameters.keys()):
    print "\t%s: %r" % (param_name, best_parameters[param_name])
```

Logistic Regression

with l1 and l2 penalty

Python source code: `logistic_l1_l2_coef.py`

```
print __doc__

# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

import numpy as np

from scikits.learn.linear_model import LogisticRegression
from scikits.learn import datasets

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

# Set regularization parameter
C = 0.1

classifier_l1_LR = LogisticRegression(C=C, penalty='l1')
classifier_l2_LR = LogisticRegression(C=C, penalty='l2')
classifier_l1_LR.fit(X, y)
classifier_l2_LR.fit(X, y)

hyperplane_coefficients_l1_LR = classifier_l1_LR.coef_[:]
hyperplane_coefficients_l2_LR = classifier_l2_LR.coef_[:]

# hyperplane_coefficients_l1_LR contains zeros due to the
# L1 sparsity inducing norm

pct_non_zeros_l1_LR = np.mean(hyperplane_coefficients_l1_LR != 0) * 100
pct_non_zeros_l2_LR = np.mean(hyperplane_coefficients_l2_LR != 0) * 100

print "Percentage of non zeros coefficients (L1) : %f" % pct_non_zeros_l1_LR
print "Percentage of non zeros coefficients (L2) : %f" % pct_non_zeros_l2_LR
```

Classification of text documents: using a MLComp dataset

This is an example showing how the scikit-learn can be used to classify documents by topics using a bag-of-words approach. This example uses a scipy.sparse matrix to store the features instead of standard numpy arrays.

The dataset used in this example is the 20 newsgroups dataset and should be downloaded from the http://mlcomp.org (free registration required):

> http://mlcomp.org/datasets/379

Once downloaded unzip the arhive somewhere on your filesystem. For instance in:

```
% mkdir -p ~/data/mlcomp
% cd  ~/data/mlcomp
% unzip /path/to/dataset-379-20news-18828_XXXXX.zip
```

You should get a folder `~/data/mlcomp/379` with a file named `metadata` and subfolders `raw`, `train` and `test` holding the text documents organized by newsgroups.

Then set the `MLCOMP_DATASETS_HOME` environment variable pointing to the root folder holding the uncompressed archive:

```
% export MLCOMP_DATASETS_HOME="~/data/mlcomp"
```

Then you are ready to run this example using your favorite python shell:

```
% ipython examples/mlcomp_sparse_document_classification.py
```

Python source code: mlcomp_sparse_document_classification.py

```
print __doc__

# Author: Olivier Grisel <olivier.grisel@ensta.org>
# License: Simplified BSD

from time import time
import sys
import os
import numpy as np
import scipy.sparse as sp
import pylab as pl

from scikits.learn.datasets import load_mlcomp
from scikits.learn.feature_extraction.text import Vectorizer
from scikits.learn.linear_model.sparse import SGDClassifier
from scikits.learn.metrics import confusion_matrix
from scikits.learn.metrics import classification_report

if 'MLCOMP_DATASETS_HOME' not in os.environ:
    print "Please follow those instructions to get started:"
    sys.exit(0)

# Load the training set
print "Loading 20 newsgroups training set... "
news_train = load_mlcomp('20news-18828', 'train')
print news_train.DESCR
print "%d documents" % len(news_train.filenames)
print "%d categories" % len(news_train.target_names)

print "Extracting features from the dataset using a sparse vectorizer"
t0 = time()
vectorizer = Vectorizer()
X_train = vectorizer.fit_transform((open(f).read()
                                    for f in news_train.filenames))
print "done in %fs" % (time() - t0)
print "n_samples: %d, n_features: %d" % X_train.shape
assert sp.issparse(X_train)
y_train = news_train.target

print "Training a linear classifier..."
parameters = {
    'loss': 'hinge',
    'penalty': 'l2',
    'n_iter': 50,
    'alpha': 0.00001,
    'fit_intercept': True,
}
print "parameters:", parameters
t0 = time()
clf = SGDClassifier(**parameters).fit(X_train, y_train)
print "done in %fs" % (time() - t0)
print "Percentage of non zeros coef: %f" % (np.mean(clf.coef_ != 0) * 100)

print "Loading 20 newsgroups test set... "
```

```
news_test = load_mlcomp('20news-18828', 'test')
t0 = time()
print "done in %fs" % (time() - t0)

print "Predicting the labels of the test set..."
print "%d documents" % len(news_test.filenames)
print "%d categories" % len(news_test.target_names)

print "Extracting features from the dataset using the same vectorizer"
t0 = time()
X_test = vectorizer.transform((open(f).read() for f in news_test.filenames))
y_test = news_test.target
print "done in %fs" % (time() - t0)
print "n_samples: %d, n_features: %d" % X_test.shape

print "Predicting the outcomes of the testing set"
t0 = time()
pred = clf.predict(X_test)
print "done in %fs" % (time() - t0)

print "Classification report on test set for classifier:"
print clf
print
print classification_report(y_test, pred, target_names=news_test.target_names)

cm = confusion_matrix(y_test, pred)
print "Confusion matrix:"
print cm

# Show confusion matrix
pl.matshow(cm)
pl.title('Confusion matrix')
pl.colorbar()
pl.show()
```

Gaussian Naive Bayes

A classification example using Gaussian Naive Bayes (GNB).

Python source code: `naive_bayes.py`

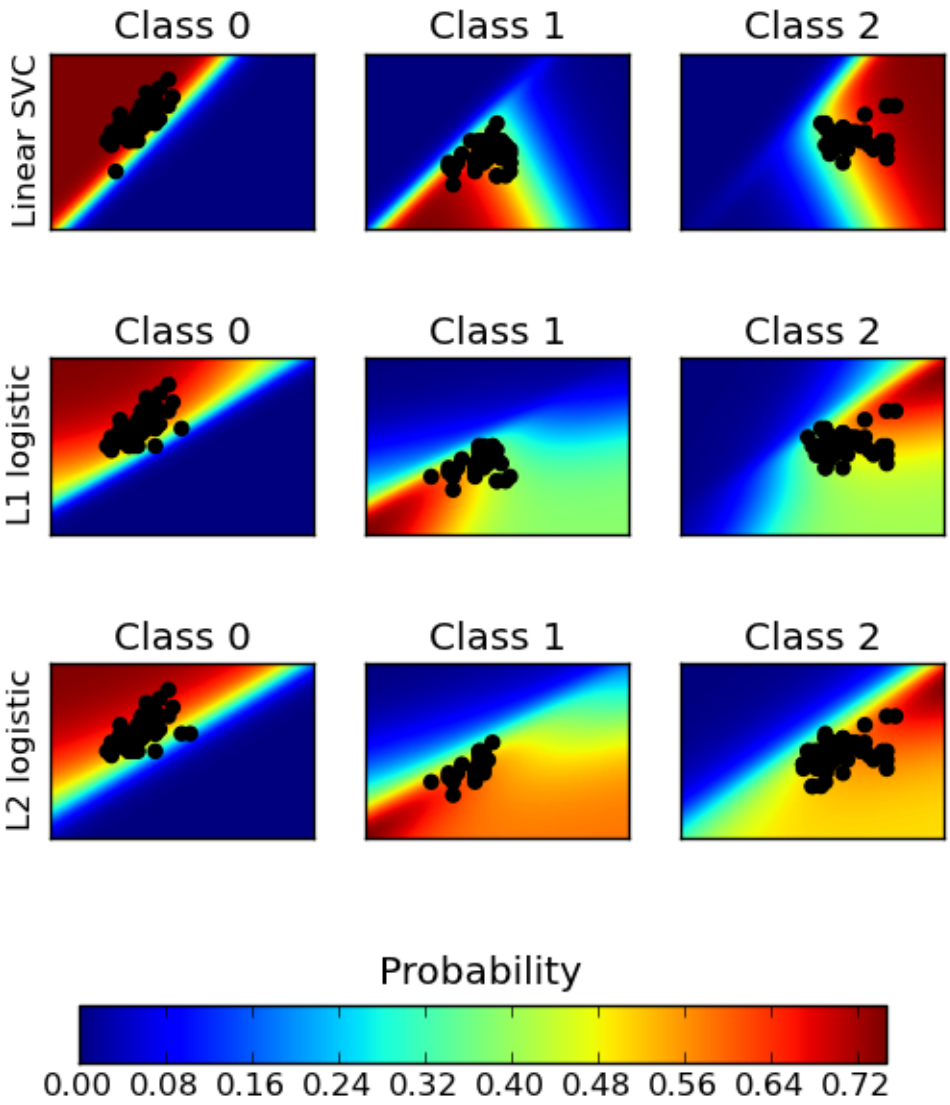
```
################################################################################
# import some data to play with

# The IRIS dataset
from scikits.learn import datasets
iris = datasets.load_iris()

X = iris.data
y = iris.target

################################################################################
# GNB
from scikits.learn.naive_bayes import GNB
gnb = GNB()

y_pred = gnb.fit(X, y).predict(X)
```

```
print "Number of mislabeled points : %d" % (y != y_pred).sum()
```

Plot classification probability

Plot the classification probability for different classifiers. We use a 3 class dataset, and we classify it with a Support Vector classifier, as well as L1 and L2 penalized logistic regression.

The logistic regression is not a multiclass classifier out of the box. As a result it can identify only the first class.



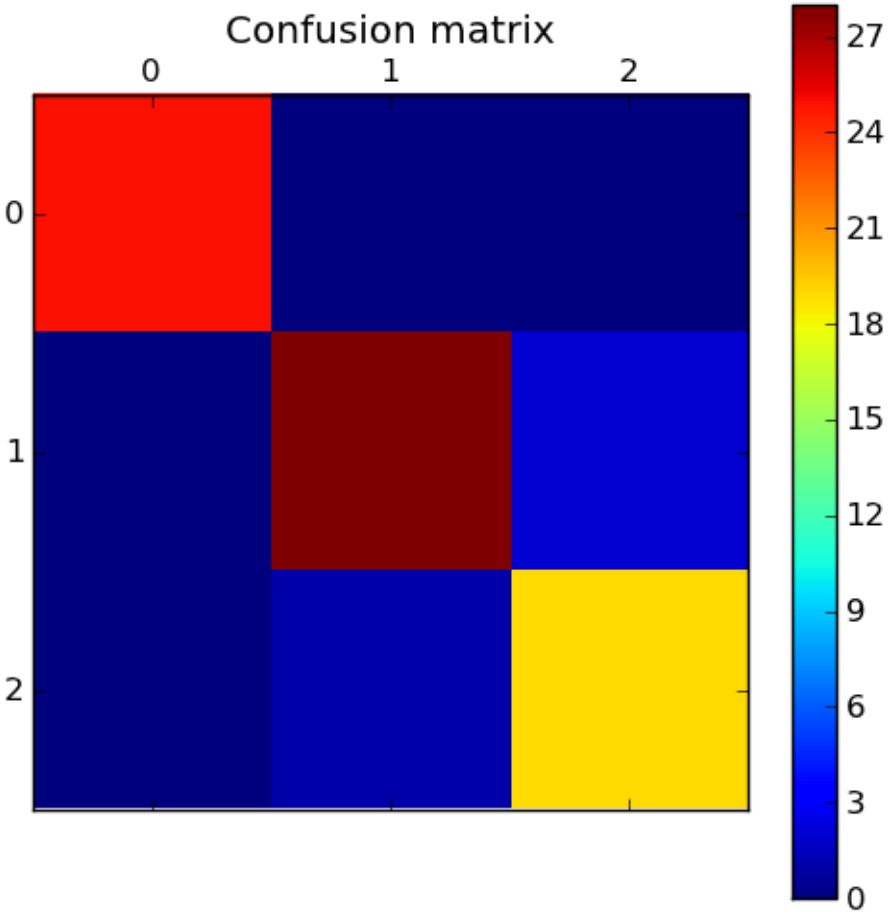
Python source code: `plot_classification_probability.py`

```
# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

import pylab as pl
import numpy as np
```

```
from scikits.learn.linear_model import LogisticRegression
from scikits.learn.svm import SVC
from scikits.learn import datasets

iris = datasets.load_iris()
X = iris.data[:, :2] # we only take the first two features for visualization
y = iris.target

n_features = X.shape[1]

C = 1.0

# Create different classifiers. The logistic regression cannot do
# multiclass out of the box.
classifiers = {
                'L1 logistic': LogisticRegression(C=C, penalty='l1'),
                'L2 logistic': LogisticRegression(C=C, penalty='l2'),
                'Linear SVC': SVC(kernel='linear', C=C, probability=True),
              }

n_classifiers = len(classifiers)

pl.figure(figsize=(3*2, n_classifiers*2))
pl.subplots_adjust(bottom=.2, top=.95)

for index, (name, classifier) in enumerate(classifiers.iteritems()):
    classifier.fit(X, y)

    y_pred = classifier.predict(X)
    classif_rate = np.mean(y_pred.ravel() == y.ravel()) * 100
    print  "classif_rate for %s : %f " % (name, classif_rate)

    # View probabilities=
    xx = np.linspace(3,9,100)
    yy = np.linspace(1,5,100).T
    xx, yy = np.meshgrid(xx, yy)
    Xfull = np.c_[xx.ravel(),yy.ravel()]
    probas = classifier.predict_proba(Xfull)
    n_classes = np.unique(y_pred).size
    for k in range(n_classes):
        pl.subplot(n_classifiers, n_classes, index*n_classes + k + 1)
        pl.title("Class %d" % k)
        if k == 0:
            pl.ylabel(name)
        imshow_handle = pl.imshow(probas[:, k].reshape((100, 100)),
                                  extent=(3, 9, 1, 5), origin='lower')
        pl.xticks(())
        pl.yticks(())
        idx = (y_pred == k)
        if idx.any():
            pl.scatter(X[idx, 0], X[idx, 1], marker='o', c='k')

ax = pl.axes([0.15, 0.04, 0.7, 0.05])
pl.title("Probability")
pl.colorbar(imshow_handle, cax=ax, orientation='horizontal')

pl.show()
```

Confusion matrix

Example of confusion matrix usage to evaluate the quality of the output of a classifier.



Python source code: `plot_confusion_matrix.py`

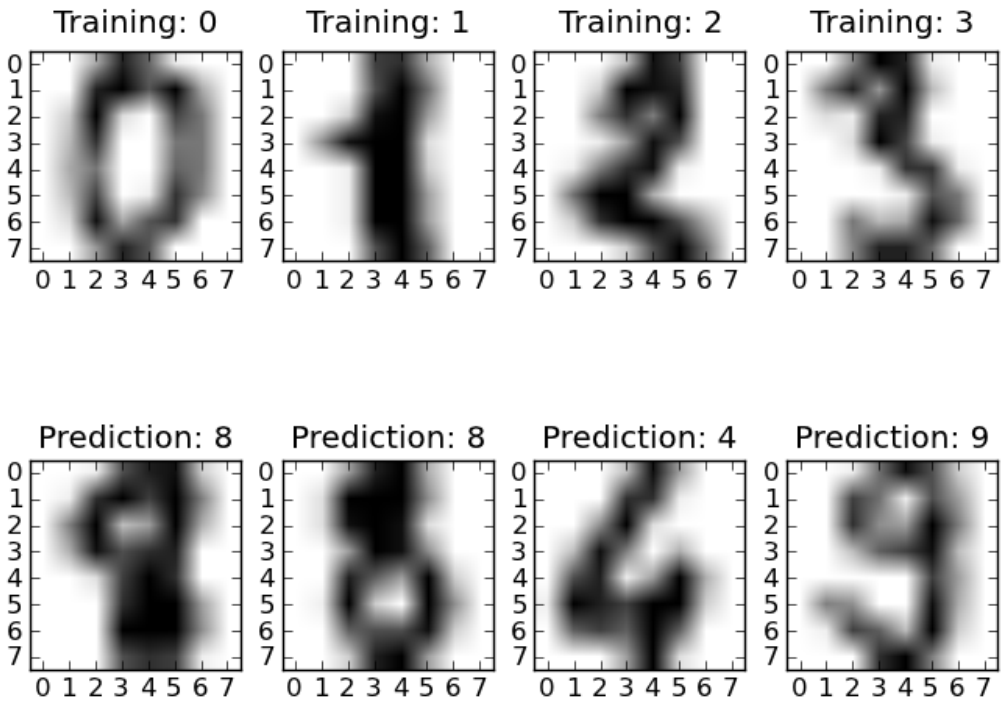
```
print __doc__

import random
import pylab as pl
from scikits.learn import svm, datasets
from scikits.learn.metrics import confusion_matrix

# import some data to play with
iris = datasets.load_iris()
X = iris.data
y = iris.target
n_samples, n_features = X.shape
p = range(n_samples)
```

```
random.seed(0)
random.shuffle(p)
X, y = X[p], y[p]
half = int(n_samples/2)

# Run classifier
classifier = svm.SVC(kernel='linear')
y_ = classifier.fit(X[:half],y[:half]).predict(X[half:])

# Compute confusion matrix
cm = confusion_matrix(y[half:], y_)

print cm

# Show confusion matrix
pl.matshow(cm)
pl.title('Confusion matrix')
pl.colorbar()
pl.show()
```

Recognizing hand-written digits

An example showing how the scikit-learn can be used to recognize images of hand-written digits.

This example is commented in the *tutorial section of the user manual*.



Python source code: `plot_digits_classification.py`

```
print __doc__

# Author: Gael Varoquaux <gael dot varoquaux at normalesup dot org>
# License: Simplified BSD

# Standard scientific Python imports
import pylab as pl

# Import datasets, classifiers and performance metrics
from scikits.learn import datasets, svm, metrics

# The digits dataset
digits = datasets.load_digits()

# The data that we are interested in is made of 8x8 images of digits,
# let's have a look at the first 3 images, stored in the `images`
# attribute of the dataset. If we were working from image files, we
# could load them using pylab.imread. For these images know which
# digit they represent: it is given in the 'target' of the dataset.
for index, (image, label) in enumerate(zip(digits.images, digits.target)[:4]):
    pl.subplot(2, 4, index+1)
    pl.imshow(image, cmap=pl.cm.gray_r)
    pl.title('Training: %i' % label)
```

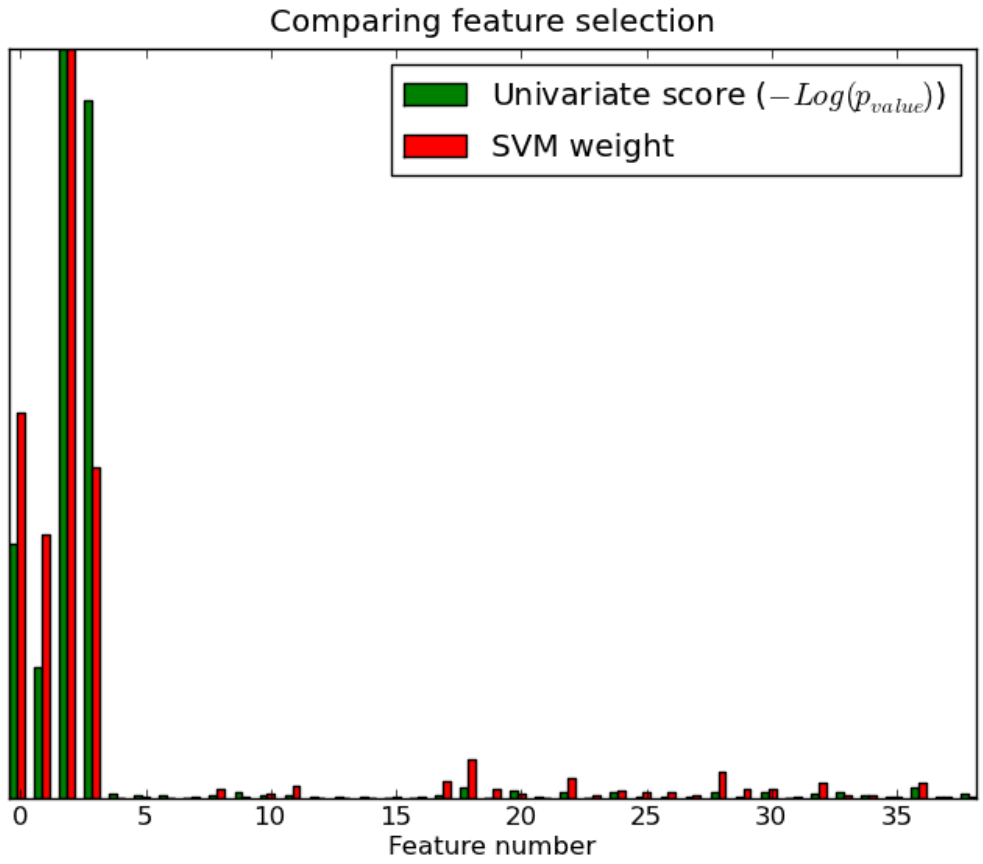
```
# To apply an classifier on this data, we need to flatten the image, to
# turn the data in a (samples, feature) matrix:
n_samples = len(digits.images)
data = digits.images.reshape((n_samples, -1))

# Create a classifier: a support vector classifier
classifier = svm.SVC()

# We learn the digits on the first half of the digits
classifier.fit(data[:n_samples/2], digits.target[:n_samples/2])

# Now predict the value of the digit on the second half:
expected = digits.target[n_samples/2:]
predicted = classifier.predict(data[n_samples/2:])

print "Classification report for classifier %s:\n%s\n" % (
    classifier, metrics.classification_report(expected, predicted))
print "Confusion matrix:\n%s" % metrics.confusion_matrix(expected, predicted)

for index, (image, prediction) in enumerate(
    zip(digits.images[n_samples/2:], predicted)[:4]):
    pl.subplot(2, 4, index+5)
    pl.imshow(image, cmap=pl.cm.gray_r)
    pl.title('Prediction: %i' % prediction)

pl.show()
```

Univariate Feature Selection

An example showing univariate feature selection.

Noisy (non informative) features are added to the iris data and univariate feature selection is applied. For each feature, we plot the p-values for the univariate feature selection and the corresponding weights of an SVM. We can see that univariate feature selection selects the informative features and that these have larger SVM weights.

In the total set of features, only the 4 first ones are significant. We can see that they have the highest score with univariate feature selection. The SVM attributes small weights to these features, but these weight are non zero. Applying univariate feature selection before the SVM increases the SVM weight attributed to the significant features, and will thus improve classification.



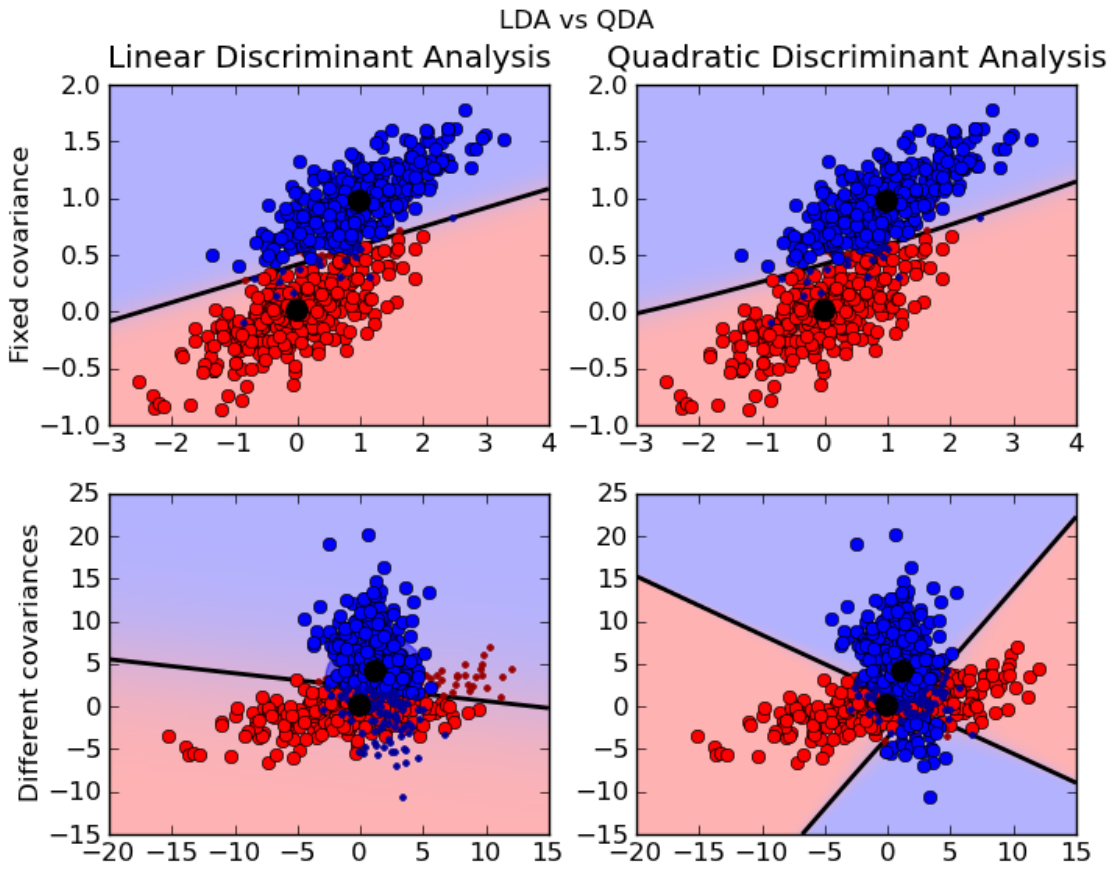
Python source code: `plot_feature_selection.py`

```
print __doc__

import numpy as np
import pylab as pl

###############################################################################
# import some data to play with

# The IRIS dataset
from scikits.learn import datasets, svm
iris = datasets.load_iris()

# Some noisy data not correlated
E = np.random.normal(size=(len(iris.data), 35))

# Add the noisy data to the informative features
x = np.hstack((iris.data, E))
y = iris.target

###############################################################################
pl.figure(1)
pl.clf()

x_indices = np.arange(x.shape[-1])
```

```
###############################################################################
# Univariate feature selection
from scikits.learn.feature_selection import SelectFpr, f_classif
# As a scoring function, we use a F test for classification
# We use the default selection function: the 10% most significant
# features

selector = SelectFpr(f_classif, alpha=0.1)
selector.fit(x, y)
scores = -np.log10(selector._pvalues)
scores /= scores.max()
pl.bar(x_indices-.45, scores, width=.3,
        label=r'Univariate score ($-Log(p_{value})$)',
        color='g')

###############################################################################
# Compare to the weights of an SVM
clf = svm.SVC(kernel='linear')
clf.fit(x, y)

svm_weights = (clf.coef_**2).sum(axis=0)
svm_weights /= svm_weights.max()
pl.bar(x_indices-.15, svm_weights, width=.3, label='SVM weight',
        color='r')


# ###############################################################################
# # Now fit an SVM with added feature selection
# selector = univ_selection.Univ(
#                 score_func=univ_selection.f_classif)

# selector.fit(x, clf.predict(x))
# svm_weights = (clf.support_**2).sum(axis=0)
# svm_weights /= svm_weights.max()
# full_svm_weights = np.zeros(selector.support_.shape)
# full_svm_weights[selector.support_] = svm_weights
# pl.bar(x_indices+.15, full_svm_weights, width=.3,
#         label='SVM weight after univariate selection',
#         color='b')

pl.title("Comparing feature selection")
pl.xlabel('Feature number')
pl.yticks(())
pl.axis('tight')
pl.legend(loc='upper right')
pl.show()
```

Linear Discriminant Analysis & Quadratic Discriminant Analysis with confidence

Plot the decision boundary



Python source code: `plot_lda_qda.py`

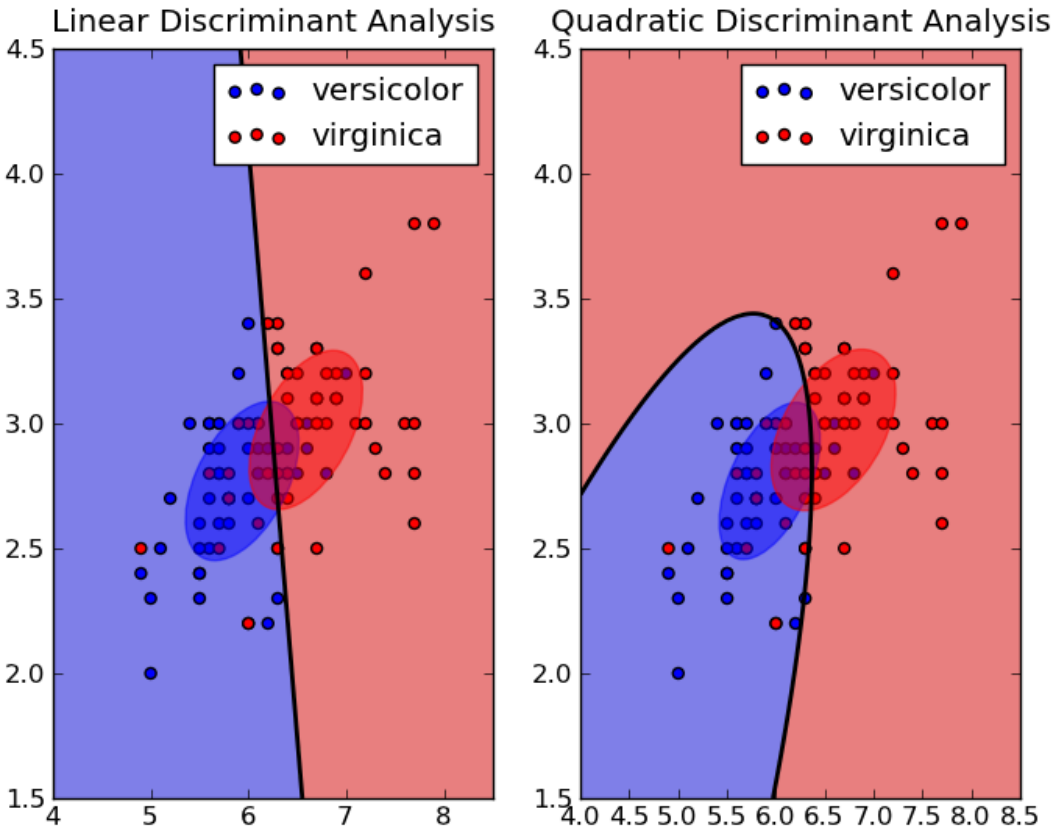
```
print __doc__

from scipy import linalg
import numpy as np
import pylab as pl
import matplotlib as mpl
from matplotlib import colors

from scikits.learn.lda import LDA
from scikits.learn.qda import QDA

###############################################################################
# colormap
cmap = colors.LinearSegmentedColormap('red_blue_classes',
    {'red' : [(0, 1, 1), (1, 0.7, 0.7)],
     'green' : [(0, 0.7, 0.7), (1, 0.7, 0.7)],
     'blue' : [(0, 0.7, 0.7), (1, 1, 1)]
    })
pl.cm.register_cmap(cmap=cmap)


###############################################################################
# generate datasets
def dataset_fixed_cov():
```

```
    '''Generate 2 Gaussians samples with the same covariance matrix'''
    n, dim = 300, 2
    np.random.seed(0)
    C = np.array([[0., -0.23], [0.83, .23]])
    X = np.r_[np.dot(np.random.randn(n, dim), C),
              np.dot(np.random.randn(n, dim), C) + np.array([1, 1])]
    y = np.hstack((np.zeros(n), np.ones(n)))
    return X, y

def dataset_cov():
    '''Generate 2 Gaussians samples with different covariance matrices'''
    n, dim = 300, 2
    np.random.seed(0)
    C = np.array([[0., -1.], [2.5, .7]]) * 2.
    X = np.r_[np.dot(np.random.randn(n, dim), C),
              np.dot(np.random.randn(n, dim), C.T) + np.array([1, 4])]
    y = np.hstack((np.zeros(n), np.ones(n)))
    return X, y

###############################################################################
# plot functions
def plot_data(lda, X, y, y_pred, fig_index):
    splot = pl.subplot(2, 2, fig_index)
    if fig_index == 1:
        pl.title('Linear Discriminant Analysis')
        pl.ylabel('Fixed covariance')
    elif fig_index == 2:
        pl.title('Quadratic Discriminant Analysis')
    elif fig_index == 3:
        pl.ylabel('Different covariances')

    tp = (y == y_pred) # True Positive
    tp0, tp1 = tp[y == 0], tp[y == 1]
    X0, X1 = X[y == 0], X[y == 1]
    X0_tp, X0_fp = X0[tp0], X0[tp0 != True]
    X1_tp, X1_fp = X1[tp1], X1[tp1 != True]
    xmin, xmax = X[:, 0].min(), X[:, 0].max()
    ymin, ymax = X[:, 1].min(), X[:, 1].max()

    # class 0: dots
    pl.plot(X0_tp[:, 0], X0_tp[:, 1], 'o', color='red')
    pl.plot(X0_fp[:, 0], X0_fp[:, 1], '.', color='#990000') # dark red

    # class 1: dots
    pl.plot(X1_tp[:, 0], X1_tp[:, 1], 'o', color='blue')
    pl.plot(X1_fp[:, 0], X1_fp[:, 1], '.', color='#000099') # dark blue

    # class 0 and 1 : areas
    nx, ny = 200, 100
    x_min, x_max = pl.xlim()
    y_min, y_max = pl.ylim()
    xx, yy = np.meshgrid(np.linspace(x_min, x_max, nx),
                         np.linspace(y_min, y_max, ny))
    Z = lda.predict_proba(np.c_[xx.ravel(), yy.ravel()])
    Z = Z[:, 1].reshape(xx.shape)
    pl.pcolormesh(xx, yy, Z, cmap='red_blue_classes',
                  norm=colors.Normalize(0., 1.))
    pl.contour(xx, yy, Z, [0.5], linewidths=2., colors='k')
```

```
    # means
    pl.plot(lda.means_[0][0], lda.means_[0][1],
            'o', color='black', markersize=10)
    pl.plot(lda.means_[1][0], lda.means_[1][1],
            'o', color='black', markersize=10)

    return splot

def plot_ellipse(splot, mean, cov, color):
    v, w = linalg.eigh(cov)
    u = w[0] / linalg.norm(w[0])
    angle = np.arctan(u[1]/u[0])
    angle = 180 * angle / np.pi # convert to degrees
    # filled gaussian at 2 standard deviation
    ell = mpl.patches.Ellipse(mean, 2 * v[0] ** 0.5, 2 * v[1] ** 0.5,
                                          180 + angle, color=color)
    ell.set_clip_box(splot.bbox)
    ell.set_alpha(0.5)
    splot.add_artist(ell)

def plot_lda_cov(lda, splot):
    plot_ellipse(splot, lda.means_[0], lda.covariance_, 'red')
    plot_ellipse(splot, lda.means_[1], lda.covariance_, 'blue')

def plot_qda_cov(qda, splot):
    plot_ellipse(splot, qda.means_[0], qda.covariances_[0], 'red')
    plot_ellipse(splot, qda.means_[1], qda.covariances_[1], 'blue')

##############################################################################
for i, (X, y) in enumerate([dataset_fixed_cov(), dataset_cov()]):
    # LDA
    lda = LDA()
    y_pred = lda.fit(X, y, store_covariance=True).predict(X)
    splot = plot_data(lda, X, y, y_pred, fig_index=2 * i + 1)
    plot_lda_cov(lda, splot)
    pl.axis('tight')

    # QDA
    qda = QDA()
    y_pred = qda.fit(X, y, store_covariances=True).predict(X)
    splot = plot_data(qda, X, y, y_pred, fig_index=2 * i + 2)
    plot_qda_cov(qda, splot)
    pl.axis('tight')
pl.suptitle('LDA vs QDA')
pl.show()
```

Linear and Quadratic Discriminant Analysis with confidence ellipsoid

Plot the confidence ellipsoids of each class and decision boundary



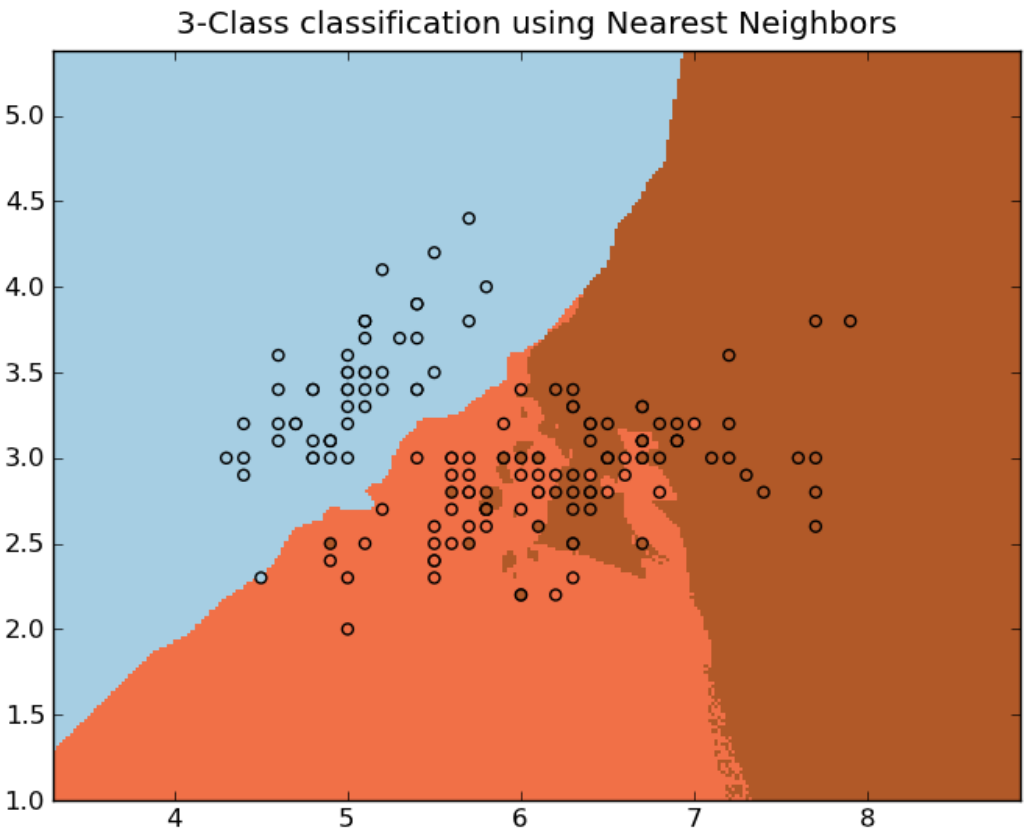
Python source code: `plot_lda_vs_qda.py`

```
print __doc__

from scipy import linalg
import numpy as np
import pylab as pl
import matplotlib as mpl

from scikits.learn.lda import LDA
from scikits.learn.qda import QDA

###############################################################################
# load sample dataset
from scikits.learn.datasets import load_iris

iris = load_iris()
X = iris.data[:,:2] # Take only 2 dimensions
y = iris.target
X = X[y > 0]
y = y[y > 0]
y -= 1
target_names = iris.target_names[1:]

###############################################################################
# LDA
```

```
lda = LDA()
y_pred = lda.fit(X, y, store_covariance=True).predict(X)

# QDA
qda = QDA()
y_pred = qda.fit(X, y, store_covariances=True).predict(X)

###############################################################################
# Plot results

def plot_ellipse(splot, mean, cov, color):
    v, w = linalg.eigh(cov)
    u = w[0] / linalg.norm(w[0])
    angle = np.arctan(u[1]/u[0])
    angle = 180 * angle / np.pi # convert to degrees
    # filled gaussian at 2 standard deviation
    ell = mpl.patches.Ellipse(mean, 2 * v[0] ** 0.5, 2 * v[1] ** 0.5,
                                          180 + angle, color=color)
    ell.set_clip_box(splot.bbox)
    ell.set_alpha(0.5)
    splot.add_artist(ell)

xx, yy = np.meshgrid(np.linspace(4, 8.5, 200), np.linspace(1.5, 4.5, 200))
X_grid = np.c_[xx.ravel(), yy.ravel()]
zz_lda = lda.predict_proba(X_grid)[:,1].reshape(xx.shape)
zz_qda = qda.predict_proba(X_grid)[:,1].reshape(xx.shape)

pl.figure()
splot = pl.subplot(1, 2, 1)
pl.contourf(xx, yy, zz_lda > 0.5, alpha=0.5)
pl.scatter(X[y==0,0], X[y==0,1], c='b', label=target_names[0])
pl.scatter(X[y==1,0], X[y==1,1], c='r', label=target_names[1])
pl.contour(xx, yy, zz_lda, [0.5], linewidths=2., colors='k')
plot_ellipse(splot, lda.means_[0], lda.covariance_, 'b')
plot_ellipse(splot, lda.means_[1], lda.covariance_, 'r')
pl.legend()
pl.axis('tight')
pl.title('Linear Discriminant Analysis')

splot = pl.subplot(1, 2, 2)
pl.contourf(xx, yy, zz_qda > 0.5, alpha=0.5)
pl.scatter(X[y==0,0], X[y==0,1], c='b', label=target_names[0])
pl.scatter(X[y==1,0], X[y==1,1], c='r', label=target_names[1])
pl.contour(xx, yy, zz_qda, [0.5], linewidths=2., colors='k')
plot_ellipse(splot, qda.means_[0], qda.covariances_[0], 'b')
plot_ellipse(splot, qda.means_[1], qda.covariances_[1], 'r')
pl.legend()
pl.axis('tight')
pl.title('Quadratic Discriminant Analysis')
pl.show()
```

Nearest Neighbors

Sample usage of Nearest Neighbors classification. It will plot the decision boundaries for each class.



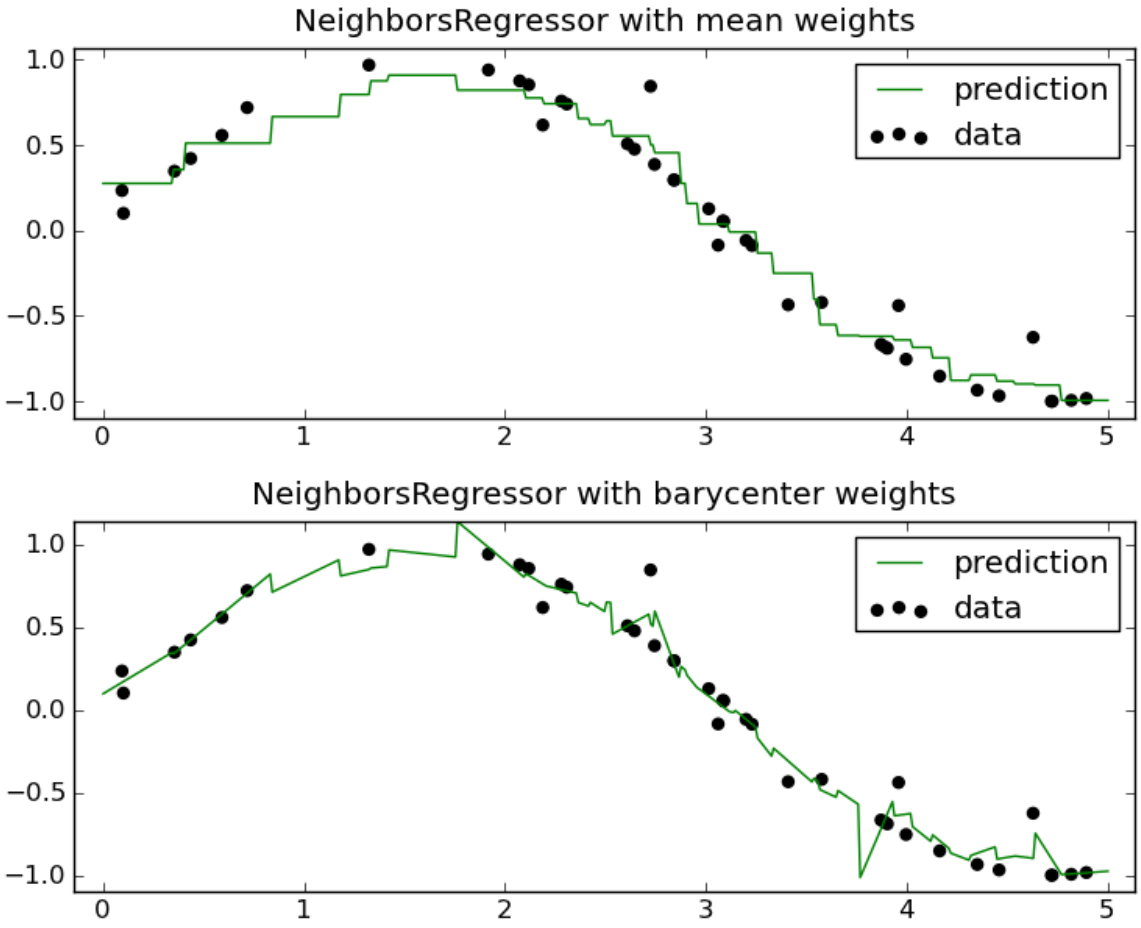
Python source code: `plot_neighbors.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import neighbors, datasets

# import some data to play with
iris = datasets.load_iris()
X = iris.data[:, :2] # we only take the first two features. We could
                     # avoid this ugly slicing by using a two-dim dataset
Y = iris.target

h = .02 # step size in the mesh

# we create an instance of Neighbours Classifier and fit the data.
clf = neighbors.NeighborsClassifier()
clf.fit(X, Y)

# Plot the decision boundary. For that, we will asign a color to each
# point in the mesh [x_min, m_max]x[y_min, y_max].
x_min, x_max = X[:,0].min()-1, X[:,0].max() + 1
y_min, y_max = X[:,1].min()-1, X[:,1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
```

```
# Put the result into a color plot
Z = Z.reshape(xx.shape)
pl.set_cmap(pl.cm.Paired)
pl.pcolormesh(xx, yy, Z)

# Plot also the training points
pl.scatter(X[:,0], X[:,1], c=Y)
pl.title('3-Class classification using Nearest Neighbors')
pl.axis('tight')
pl.show()
```

k-Nearest Neighbors regression

Demonstrate the resolution of a regression problem using a k-Nearest Neighbor and the interpolation of the target using both barycenter and constant weights.



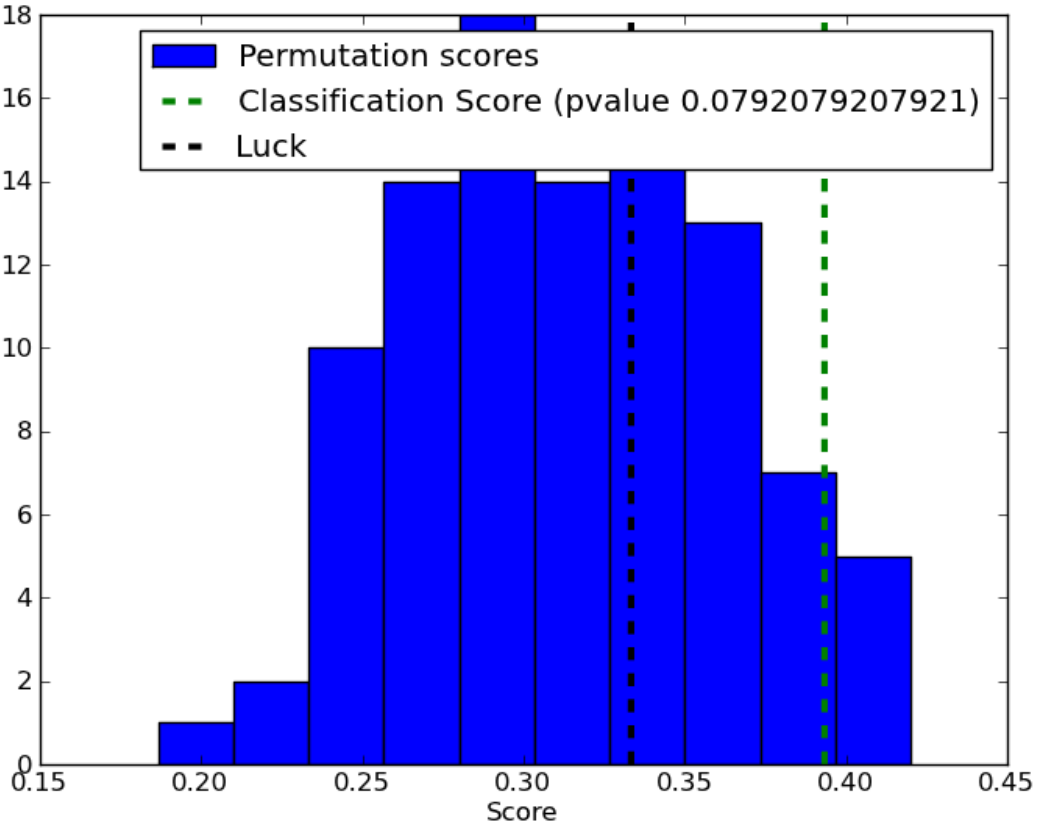
Python source code: `plot_neighbors_regression.py`

```
print __doc__

# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
#         Fabian Pedregosa <fabian.pedregosa@inria.fr>
#
# License: BSD, (C) INRIA
```

```
##############################################################################
# Generate sample data
import numpy as np
import pylab as pl
from scikits.learn import neighbors

np.random.seed(0)
X = np.sort(5*np.random.rand(40, 1), axis=0)
T = np.linspace(0, 5, 500)[:, np.newaxis]
y = np.sin(X).ravel()

# Add noise to targets
y[::5] += 1*(0.5 - np.random.rand(8))

##############################################################################
# Fit regression model

for i, mode in enumerate(('mean', 'barycenter')):
    knn = neighbors.NeighborsRegressor(n_neighbors=4, mode=mode)
    y_ = knn.fit(X, y).predict(T)

    pl.subplot(2, 1, 1 + i)
    pl.scatter(X, y, c='k', label='data')
    pl.plot(T, y_, c='g', label='prediction')
    pl.axis('tight')
    pl.legend()
    pl.title('NeighborsRegressor with %s weights' % mode)

pl.subplots_adjust(0.1, 0.04, 0.95, 0.94, 0.3, 0.28)
pl.show()
```

Test with permutations the significance of a classification score

In order to test if a classification score is significative a technique in repeating the classification procedure after randomizing, permuting, the labels. The p-value is then given by the percentage of runs for which the score obtained is greater than the classification score obtained in the first place.



Python source code: `plot_permutation_test_for_classification.py`

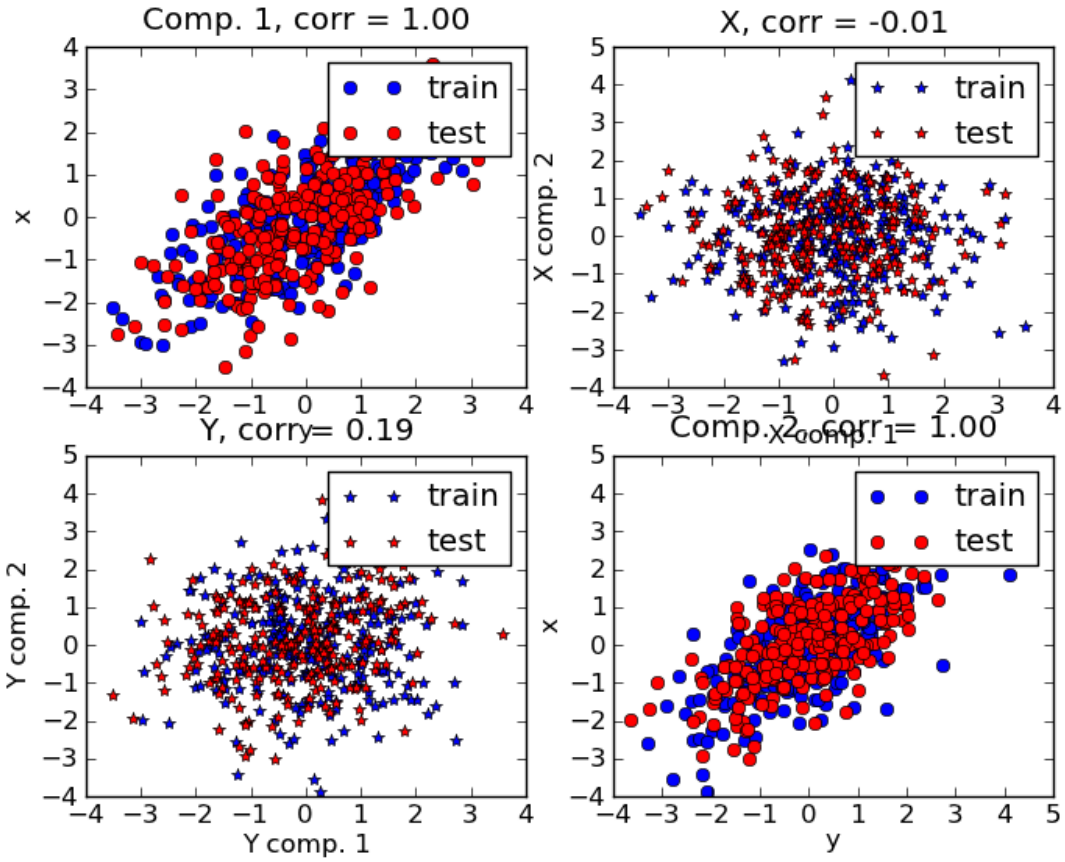
```
# Author:  Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD

print __doc__

import numpy as np
import pylab as pl

from scikits.learn.svm import SVC
from scikits.learn.cross_val import StratifiedKFold, permutation_test_score
from scikits.learn import datasets
from scikits.learn.metrics import zero_one_score


##############################################################################
# Loading a dataset
iris = datasets.load_iris()
X = iris.data
y = iris.target
n_classes = np.unique(y).size

# Some noisy data not correlated
random = np.random.RandomState(seed=0)
E = random.normal(size=(len(X), 2200))
```

```
# Add noisy data to the informative features for make the task harder
X = np.c_[X, E]

svm = SVC(kernel='linear')
cv = StratifiedKFold(y, 2)

score, permutation_scores, pvalue = permutation_test_score(svm, X, y,
                                         zero_one_score, cv=cv,
                                         n_permutations=100, n_jobs=1)

print "Classification score %s (pvalue : %s)" % (score, pvalue)

###############################################################################
# View histogram of permutation scores
pl.hist(permutation_scores, label='Permutation scores')
ylim = pl.ylim()
pl.vlines(score, ylim[0], ylim[1], linestyle='--',
          color='g', linewidth=3, label='Classification Score'
          ' (pvalue %s)' % pvalue)
pl.vlines(1.0 / n_classes, ylim[0], ylim[1], linestyle='--',
          color='k', linewidth=3, label='Luck')
pl.ylim(ylim)
pl.legend()
pl.xlabel('Score')
pl.show()
```

PLS Partial Least Squares

Simple usage of various PLS flavor: - PLSCanonical - PLSRegression, with multivariate response, a.k.a. PLS2 - PLSRegression, with univariate response, a.k.a. PLS1 - CCA

Given 2 multivariate covarying two-dimensional datasets, X, and Y, PLS extracts the 'directions of covariance', i.e. the components of each datasets that explain the most shared variance between both datasets. This is apparent on the **scatterplot matrix** display: components 1 in dataset X and dataset Y are maximaly correlated (points lie around the first diagonal). This is also true for components 2 in both dataset, however, the correlation across datasets for different components is weak: the point cloud is very spherical.



Python source code: `plot_pls.py`

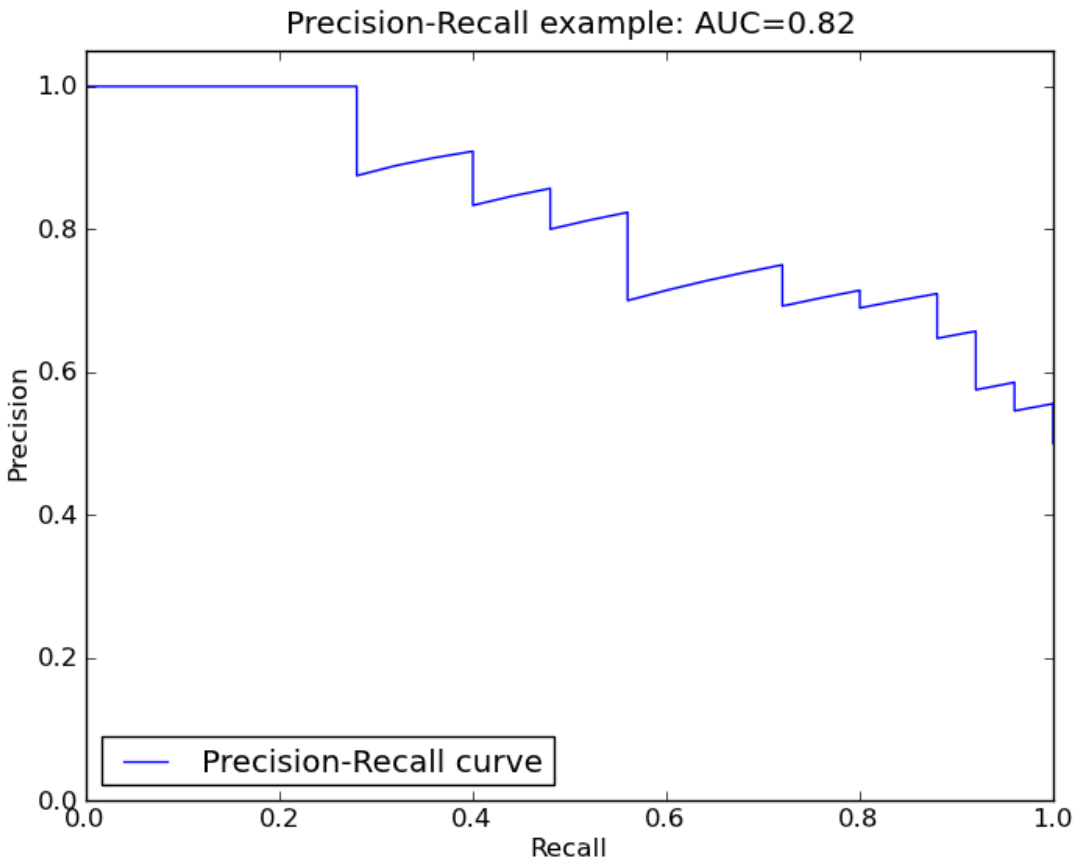
```
import numpy as np
import pylab as pl
from scikits.learn.pls import PLSCanonical, PLSRegression, CCA

#############################################################################
# Dataset based latent variables model

n = 500
# 2 latents vars:
l1 = np.random.normal(size=n)
l2 = np.random.normal(size=n)

latents = np.array([l1, l1, l2, l2]).T
X = latents + np.random.normal(size=4*n).reshape((n, 4))
Y = latents + np.random.normal(size=4*n).reshape((n, 4))

X_train = X[:n/2, :]
Y_train = Y[:n/2, :]
X_test = X[n/2:, :]
Y_test = Y[n/2:, :]

print "Corr(X)"
print np.round(np.corrcoef(X.T), 2)
print "Corr(Y)"
```

```
print np.round(np.corrcoef(Y.T), 2)

##############################################################################
# Canonical (symetric) PLS

# Transform data
# ~~~~~~~~~~~~~~
plsca = PLSCanonical()
plsca.fit(X_train, Y_train, n_components=2)
X_train_r, Y_train_r = plsca.transform(X_train, Y_train)
X_test_r, Y_test_r = plsca.transform(X_test, Y_test)

# Scatter plot of scores
# ~~~~~~~~~~~~~~~~~~~~~~
# 1) on diagonal plot X vs Y scores on each components
pl.subplot(221)
pl.plot(X_train_r[:, 0], Y_train_r[:, 0], "ob", label="train")
pl.plot(X_test_r[:, 0], Y_test_r[:, 0], "or", label="test")
pl.xlabel("y")
pl.ylabel("x")
pl.title('Comp. 1, corr = %.2f' %
         np.corrcoef(X_test_r[:, 0], X_test_r[:, 0])[0, 1])
pl.legend()

pl.subplot(224)
pl.plot(X_train_r[:, 1], Y_train_r[:, 1], "ob", label="train")
pl.plot(X_test_r[:, 1], Y_test_r[:, 1], "or", label="test")
pl.xlabel("y")
pl.ylabel("x")
pl.title('Comp. 2, corr = %.2f' %
         np.corrcoef(X_test_r[:, 1], X_test_r[:, 1])[0, 1])
pl.legend()

# 2) Off diagonal plot components 1 vs 2 for X and Y
pl.subplot(222)
pl.plot(X_train_r[:, 0], X_train_r[:, 1], "*b", label="train")
pl.plot(X_test_r[:, 0], X_test_r[:, 1], "*r", label="test")
pl.xlabel("X comp. 1")
pl.ylabel("X comp. 2")
pl.title('X, corr = %.2f' % np.corrcoef(X_test_r[:, 0], X_test_r[:, 1])[0, 1])
pl.legend()

pl.subplot(223)
pl.plot(Y_train_r[:, 0], Y_train_r[:, 1], "*b", label="train")
pl.plot(Y_test_r[:, 0], Y_test_r[:, 1], "*r", label="test")
pl.xlabel("Y comp. 1")
pl.ylabel("Y comp. 2")
pl.title('Y, corr = %.2f' % np.corrcoef(Y_test_r[:, 0], Y_test_r[:, 1])[0, 1])
pl.legend()
pl.show()

##############################################################################
# PLS regression, with multivariate response, a.k.a. PLS2

n = 1000
q = 3
p = 10
X = np.random.normal(size=n * p).reshape((n, p))
```

```
B = np.array([[1, 2] + [0] * (p - 2)] * q).T
# each Yj = 1*X1 + 2*X2 + noize
Y = np.dot(X, B) + np.random.normal(size=n * q).reshape((n, q)) + 5

pls2 = PLSRegression()
pls2.fit(X, Y, n_components=3)
print "True B (such that: Y = XB + Err)"
print B
# compare pls2.coefs with B
print "Estimated B"
print np.round(pls2.coefs, 1)
pls2.predict(X)

##########################################################################
# PLS regression, with univariate response, a.k.a. PLS1

n = 1000
p = 10
X = np.random.normal(size=n*p).reshape((n, p))
y = X[:, 0] + 2 * X[:, 1] + np.random.normal(size=n * 1) + 5
pls1 = PLSRegression()
pls1.fit(X, y, n_components=3)
# note that the number of compements exceeds 1 (the dimension of y)
print "Estimated betas"
print np.round(pls1.coefs, 1)

##########################################################################
# CCA (PLS mode B with symetric deflation)

cca = CCA()
cca.fit(X_train, Y_train, n_components=2)
X_train_r, Y_train_r = plsca.transform(X_train, Y_train)
X_test_r, Y_test_r = plsca.transform(X_test, Y_test)
```

Precision-Recall

Example of Precision-Recall metric to evaluate the quality of the output of a classifier.



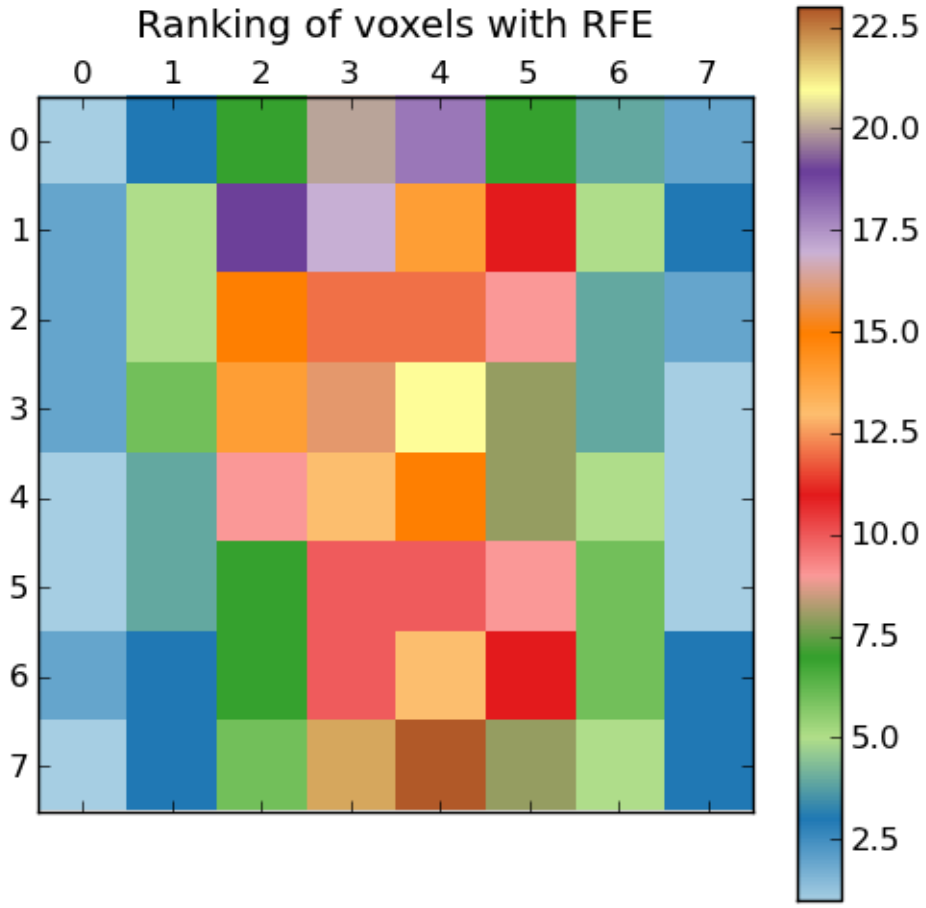
Python source code: `plot_precision_recall.py`

```
print __doc__

import random
import pylab as pl
import numpy as np
from scikits.learn import svm, datasets
from scikits.learn.metrics import precision_recall_curve
from scikits.learn.metrics import auc

# import some data to play with
iris = datasets.load_iris()
X = iris.data
y = iris.target
X, y = X[y!=2], y[y!=2] # Keep also 2 classes (0 and 1)
n_samples, n_features = X.shape
p = range(n_samples) # Shuffle samples
random.seed(0)
random.shuffle(p)
X, y = X[p], y[p]
half = int(n_samples/2)

# Add noisy features
np.random.seed(0)
X = np.c_[X,np.random.randn(n_samples, 200 * n_features)]
```

```
# Run classifier
classifier = svm.SVC(kernel='linear', probability=True)
probas_ = classifier.fit(X[:half], y[:half]).predict_proba(X[half:])

# Compute Precision-Recall and plot curve
precision, recall, thresholds = precision_recall_curve(y[half:], probas_[:,1])
area = auc(recall, precision)
print "Area Under Curve: %0.2f" % area

pl.figure(-1)
pl.clf()
pl.plot(recall, precision, label='Precision-Recall curve')
pl.xlabel('Recall')
pl.ylabel('Precision')
pl.ylim([0.0,1.05])
pl.xlim([0.0,1.0])
pl.title('Precision-Recall example: AUC=%0.2f' % area)
pl.legend(loc="lower left")
pl.show()
```

Recursive feature elimination

A recursive feature elimination is performed prior to SVM classification.



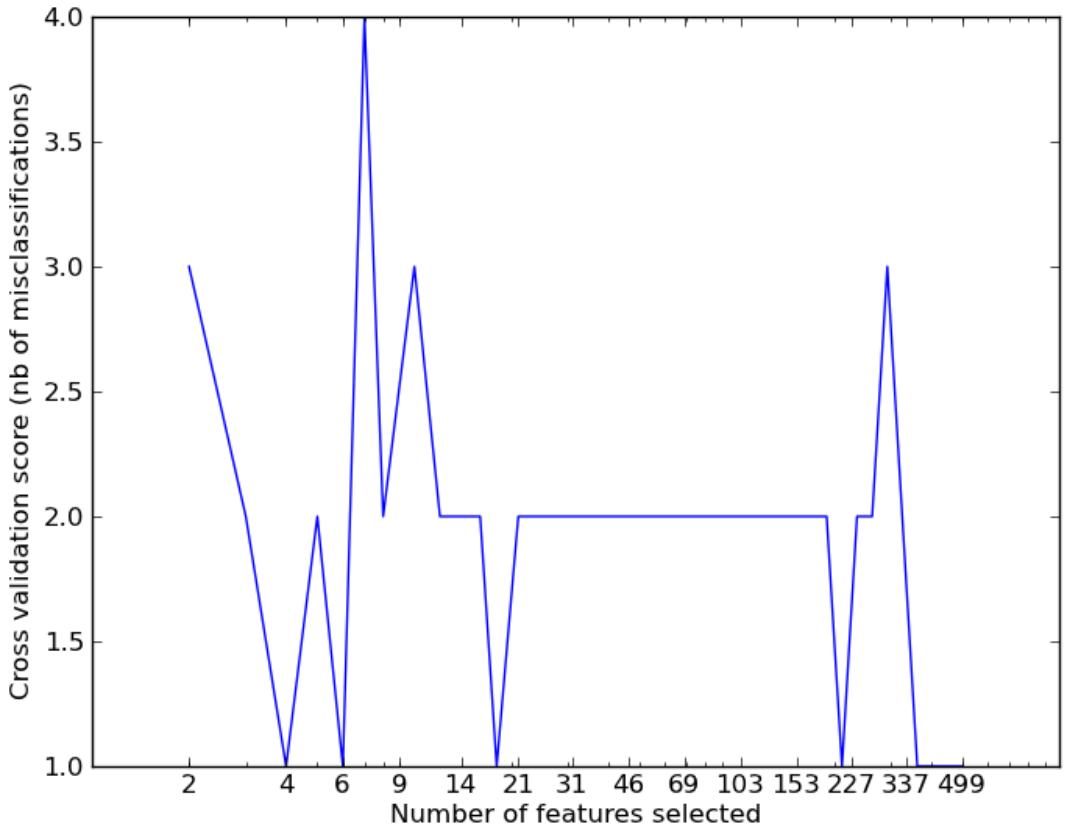
Python source code: `plot_rfe_digits.py`

```
print __doc__

from scikits.learn.svm import SVC
from scikits.learn import datasets
from scikits.learn.feature_selection import RFE

###############################################################################
# Loading the Digits dataset
digits = datasets.load_digits()

# To apply an classifier on this data, we need to flatten the image, to
# turn the data in a (samples, feature) matrix:
n_samples = len(digits.images)
X = digits.images.reshape((n_samples, -1))
y = digits.target
```

```
###############################################################################
# Create the RFE object and compute a cross-validated score

svc = SVC(kernel="linear", C=1)
rfe = RFE(estimator=svc, n_features=1, percentage=0.1)
rfe.fit(X, y)

image_ranking_ = rfe.ranking_.reshape(digits.images[0].shape)

import pylab as pl
pl.matshow(image_ranking_)
pl.colorbar()
pl.title('Ranking of voxels with RFE')
pl.show()
```

Recursive feature elimination with cross-validation

Recursive feature elimination with automatic tuning of the number of features selected with cross-validation



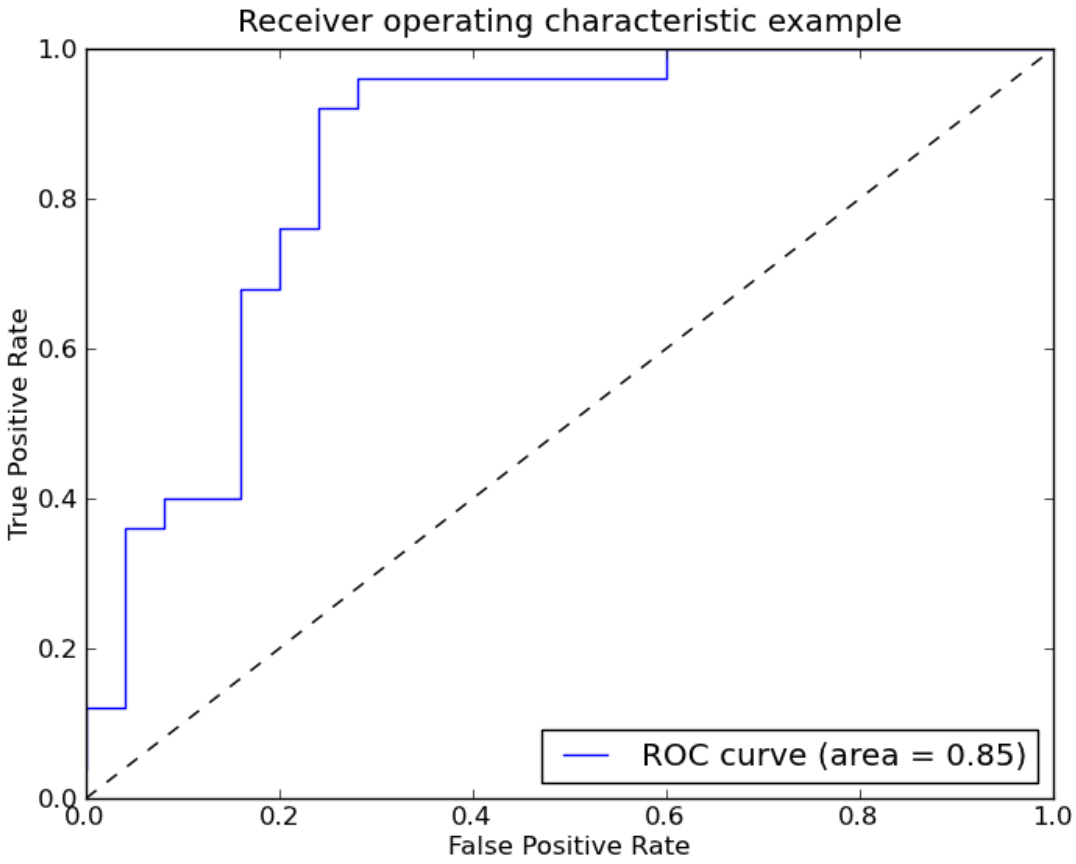
Python source code: `plot_rfe_with_cross_validation.py`

```
print __doc__
import numpy as np
```

```
from scikits.learn.svm import SVC
from scikits.learn.cross_val import StratifiedKFold
from scikits.learn.feature_selection import RFECV
from scikits.learn.datasets import samples_generator
from scikits.learn.metrics import zero_one

################################################################################
# Loading a dataset

X, y = samples_generator.test_dataset_classif(n_features=500, k=5, seed=0)

################################################################################
# Create the RFE object and compute a cross-validated score

svc = SVC(kernel='linear')
rfecv = RFECV(estimator=svc, n_features=2, percentage=0.1, loss_func=zero_one)
rfecv.fit(X, y, cv=StratifiedKFold(y, 2))

print 'Optimal number of features : %d' % rfecv.support_.sum()

import pylab as pl
pl.figure()
pl.semilogx(rfecv.n_features_, rfecv.cv_scores_)
pl.xlabel('Number of features selected')
pl.ylabel('Cross validation score (nb of misclassifications)')
# 15 ticks regularly-space in log
x_ticks = np.unique(np.logspace(np.log10(2),
                                np.log10(rfecv.n_features_.max()),
                                15,
                    ).astype(np.int))
pl.xticks(x_ticks, x_ticks)
pl.show()
```

Receiver operating characteristic (ROC)

Example of Receiver operating characteristic (ROC) metric to evaluate the quality of the output of a classifier.



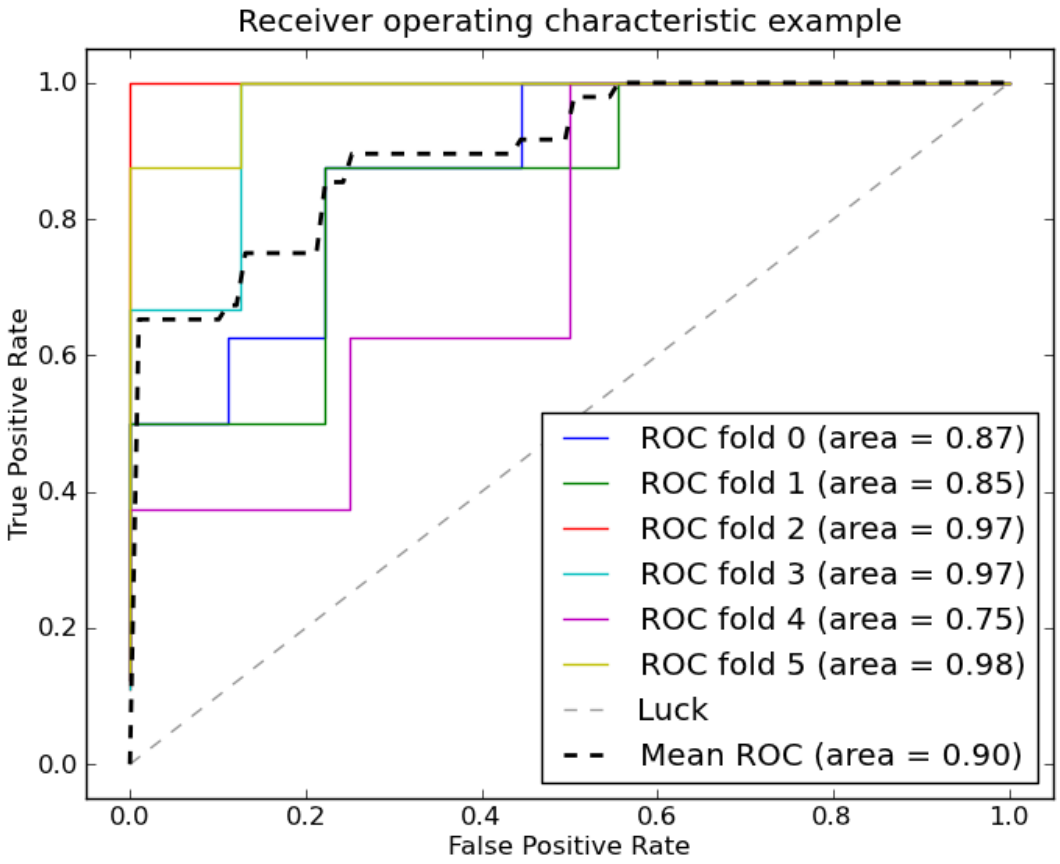
Python source code: `plot_roc.py`

```
print __doc__

import random
import numpy as np
import pylab as pl
from scikits.learn import svm, datasets
from scikits.learn.metrics import roc_curve, auc

# import some data to play with
iris = datasets.load_iris()
X = iris.data
y = iris.target
X, y = X[y!=2], y[y!=2]
n_samples, n_features = X.shape
p = range(n_samples)
random.seed(0)
random.shuffle(p)
X, y = X[p], y[p]
half = int(n_samples/2)

# Add noisy features
X = np.c_[X,np.random.randn(n_samples, 200*n_features)]

# Run classifier
```

```
classifier = svm.SVC(kernel='linear', probability=True)
probas_ = classifier.fit(X[:half],y[:half]).predict_proba(X[half:])

# Compute ROC curve and area the curve
fpr, tpr, thresholds = roc_curve(y[half:], probas_[:,1])
roc_auc = auc(fpr, tpr)
print "Area under the ROC curve : %f" % roc_auc

# Plot ROC curve
pl.figure(-1)
pl.clf()
pl.plot(fpr, tpr, label='ROC curve (area = %0.2f)' % roc_auc)
pl.plot([0, 1], [0, 1], 'k--')
pl.xlim([0.0,1.0])
pl.ylim([0.0,1.0])
pl.xlabel('False Positive Rate')
pl.ylabel('True Positive Rate')
pl.title('Receiver operating characteristic example')
pl.legend(loc="lower right")
pl.show()
```

Receiver operating characteristic (ROC) with cross validation

Example of Receiver operating characteristic (ROC) metric to evaluate the quality of the output of a classifier using cross-validation.



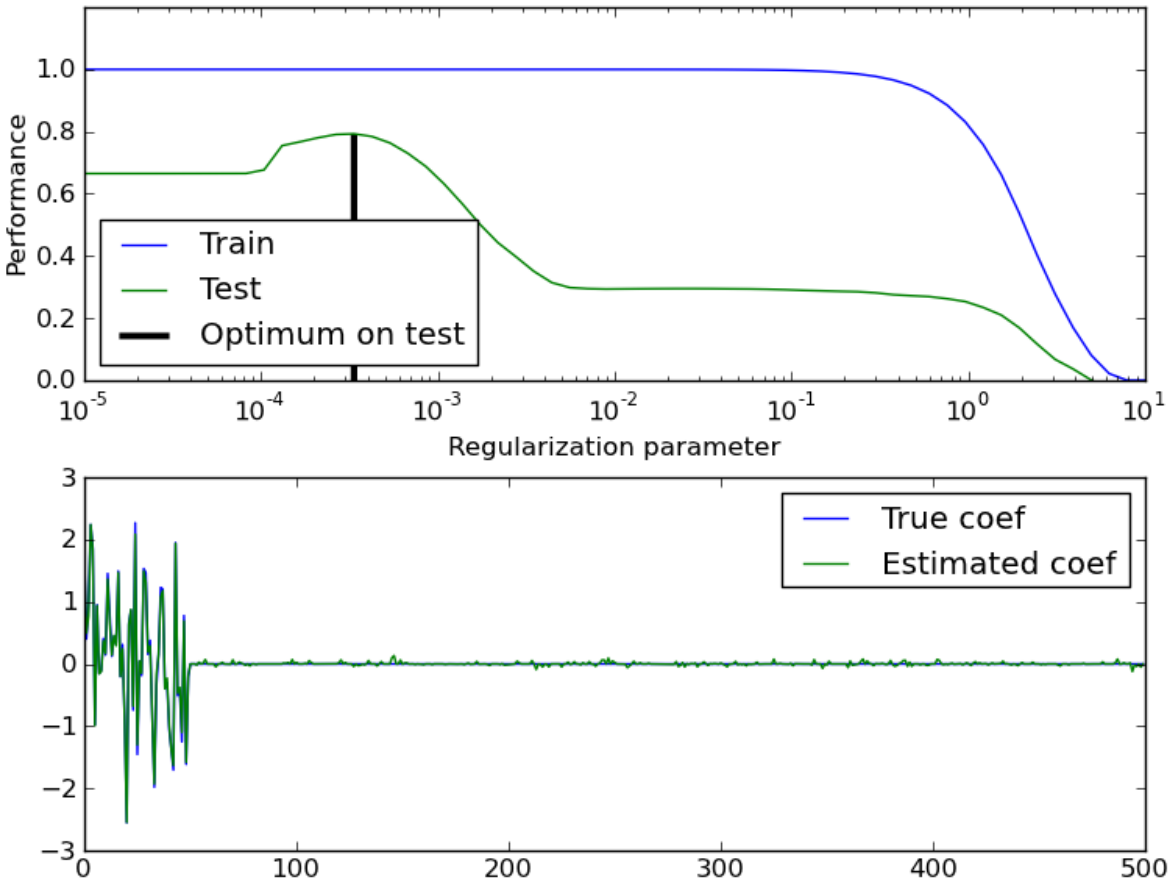
Python source code: `plot_roc_crossval.py`

```
print __doc__

import numpy as np
from scipy import interp
import pylab as pl

from scikits.learn import svm, datasets
from scikits.learn.metrics import roc_curve, auc
from scikits.learn.cross_val import StratifiedKFold

###############################################################################
# Data IO and generation

# import some data to play with
iris = datasets.load_iris()
X = iris.data
y = iris.target
X, y = X[y!=2], y[y!=2]
n_samples, n_features = X.shape

# Add noisy features
X = np.c_[X,np.random.randn(n_samples, 200*n_features)]

###############################################################################
```

```
# Classification and ROC analysis

# Run classifier with crossvalidation and plot ROC curves
cv = StratifiedKFold(y, k=6)
classifier = svm.SVC(kernel='linear', probability=True)

mean_tpr = 0.0
mean_fpr = np.linspace(0, 1, 100)
all_tpr = []

for i, (train, test) in enumerate(cv):
    probas_ = classifier.fit(X[train], y[train]).predict_proba(X[test])
    # Compute ROC curve and area the curve
    fpr, tpr, thresholds = roc_curve(y[test], probas_[:,1])
    mean_tpr += interp(mean_fpr, fpr, tpr)
    mean_tpr[0] = 0.0
    roc_auc = auc(fpr, tpr)
    pl.plot(fpr, tpr, lw=1, label='ROC fold %d (area = %0.2f)' % (i, roc_auc))

pl.plot([0, 1], [0, 1], '--', color=(0.6,0.6,0.6), label='Luck')

mean_tpr /= len(cv)
mean_tpr[-1] = 1.0
mean_auc = auc(mean_fpr, mean_tpr)
pl.plot(mean_fpr, mean_tpr, 'k--',
        label='Mean ROC (area = %0.2f)' % mean_auc, lw=2)

pl.xlim([-0.05,1.05])
pl.ylim([-0.05,1.05])
pl.xlabel('False Positive Rate')
pl.ylabel('True Positive Rate')
pl.title('Receiver operating characteristic example')
pl.legend(loc="lower right")
pl.show()
```

Train error vs Test error

Illustration of how the performance of an estimator on unseen data (test data) is not the same as the performance on training data. As the regularization increases the performance on train decreases while the performance on test is optimal within a range of values of the regularization parameter. The example with an Elastic-Net regression model and the performance is measured using the explained variance a.k.a. R^2.



Python source code: `plot_train_error_vs_test_error.py`

```
print __doc__

# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

import numpy as np
from scikits.learn import linear_model

##############################################################################
# Generate sample data
n_samples_train, n_samples_test, n_features = 75, 150, 500
np.random.seed(0)
coef = np.random.randn(n_features)
coef[50:] = 0.0 # only the top 10 features are impacting the model
X = np.random.randn(n_samples_train + n_samples_test, n_features)
y = np.dot(X, coef)

# Split train and test data
X_train, X_test = X[:n_samples_train], X[n_samples_train:]
y_train, y_test = y[:n_samples_train], y[n_samples_train:]

##############################################################################
# Compute train and test errors
alphas = np.logspace(-5, 1, 60)
```

```
enet = linear_model.ElasticNet(rho=0.7)
train_errors = list()
test_errors = list()
for alpha in alphas:
    enet.fit(X_train, y_train, alpha=alpha)
    train_errors.append(enet.score(X_train, y_train))
    test_errors.append(enet.score(X_test, y_test))

i_alpha_optim = np.argmax(test_errors)
alpha_optim = alphas[i_alpha_optim]
print "Optimal regularization parameter : %s" % alpha_optim

# Estimate the coef_ on full data with optimal regularization parameter
coef_ = enet.fit(X, y, alpha=alpha_optim).coef_

##############################################################################
# Plot results functions

import pylab as pl
pl.subplot(2, 1, 1)
pl.semilogx(alphas, train_errors, label='Train')
pl.semilogx(alphas, test_errors, label='Test')
pl.vlines(alpha_optim, pl.ylim()[0], np.max(test_errors),
                        color='k', linewidth=3, label='Optimum on test')
pl.legend(loc='lower left')
pl.ylim([0, 1.2])
pl.xlabel('Regularization parameter')
pl.ylabel('Performance')

# Show estimated coef_ vs true coef
pl.subplot(2, 1, 2)
pl.plot(coef, label='True coef')
pl.plot(coef_, label='Estimated coef')
pl.legend()
pl.subplots_adjust(0.09, 0.04, 0.94, 0.94, 0.26, 0.26)
pl.show()
```

2.1.2 Examples based on real world datasets

Applications to real world problems with some medium sized datasets or interactive user interface.

Faces recognition example using eigenfaces and SVMs

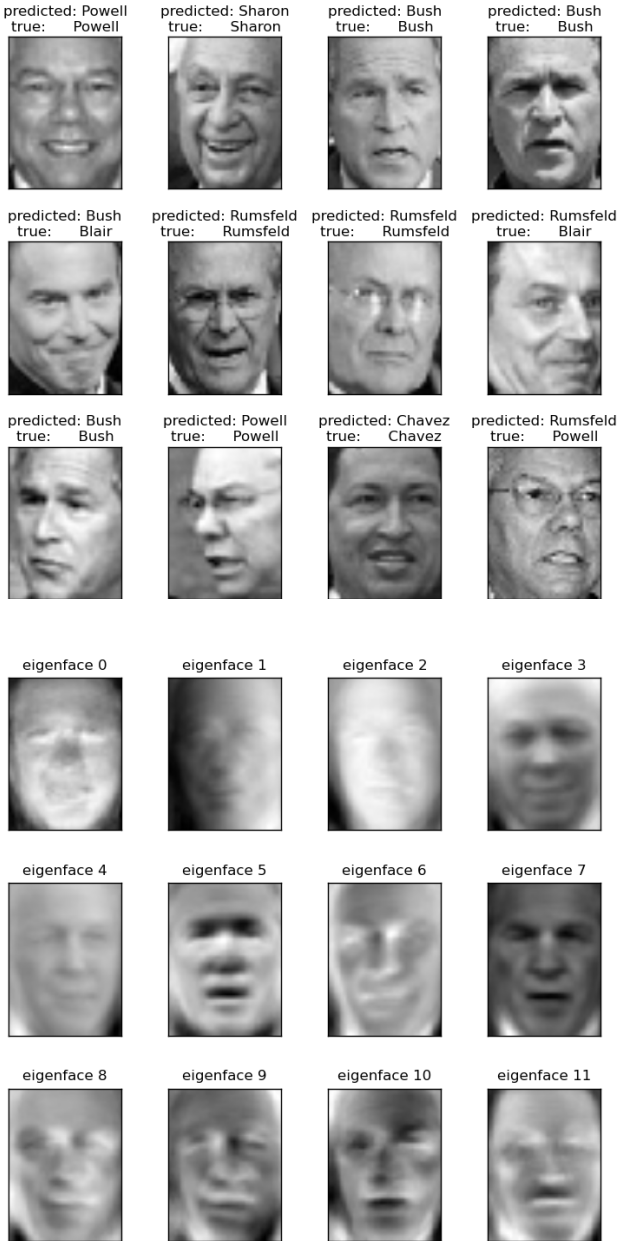
The dataset used in this example is a preprocessed excerpt of the "Labeled Faces in the Wild", aka LFW:

http://vis-www.cs.umass.edu/lfw/lfw-funneled.tgz (233MB)

Expected results for the top 5 most represented people in the dataset:

```
                   precision    recall  f1-score   support

Gerhard_Schroeder       0.91      0.75      0.82        28
  Donald_Rumsfeld       0.84      0.82      0.83        33
       Tony_Blair       0.65      0.82      0.73        34
     Colin_Powell       0.78      0.88      0.83        58
    George_W_Bush       0.93      0.86      0.90       129
```

```
avg / total       0.86      0.84      0.85       282
```



Python source code: `face_recognition.py`

```
print __doc__

from time import time
import logging
import pylab as pl

from scikits.learn.cross_val import StratifiedKFold
from scikits.learn.datasets import fetch_lfw_people
from scikits.learn.grid_search import GridSearchCV
from scikits.learn.metrics import classification_report
```

```
from scikits.learn.metrics import confusion_matrix
from scikits.learn.decomposition import RandomizedPCA
from scikits.learn.svm import SVC

# Display progress logs on stdout
logging.basicConfig(level=logging.INFO, format='%(asctime)s %(message)s')


###############################################################################
# Download the data, if not already on disk and load it as numpy arrays

lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)

# reshape the data using the traditional (n_samples, n_features) shape
faces = lfw_people.data
n_samples, h, w = faces.shape

X = faces.reshape((n_samples, h * w))
n_features = X.shape[1]

# the label to predict is the id of the person
y = lfw_people.target
target_names = lfw_people.target_names
n_classes = target_names.shape[0]

print "Total dataset size:"
print "n_samples: %d" % n_samples
print "n_features: %d" % n_features
print "n_classes: %d" % n_classes


###############################################################################
# Split into a training set and a test set using a stratified k fold

# split into a training and testing set
train, test = iter(StratifiedKFold(y, k=4)).next()
X_train, X_test = X[train], X[test]
y_train, y_test = y[train], y[test]


###############################################################################
# Compute a PCA (eigenfaces) on the face dataset (treated as unlabeled
# dataset): unsupervised feature extraction / dimensionality reduction
n_components = 150

print "Extracting the top %d eigenfaces from %d faces" % (
    n_components, X_train.shape[0])
t0 = time()
pca = RandomizedPCA(n_components=n_components, whiten=True).fit(X_train)
print "done in %0.3fs" % (time() - t0)

eigenfaces = pca.components_.reshape((n_components, h, w))

print "Projecting the input data on the eigenfaces orthonormal basis"
t0 = time()
X_train_pca = pca.transform(X_train)
X_test_pca = pca.transform(X_test)
print "done in %0.3fs" % (time() - t0)
```

```
###############################################################################
# Train a SVM classification model

print "Fitting the classifier to the training set"
t0 = time()
param_grid = {
 'C': [1, 5, 10, 50, 100],
 'gamma': [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.1],
}
clf = GridSearchCV(SVC(kernel='rbf'), param_grid,
                   fit_params={'class_weight': 'auto'})
clf = clf.fit(X_train_pca, y_train)
print "done in %0.3fs" % (time() - t0)
print "Best estimator found by grid search:"
print clf.best_estimator


###############################################################################
# Quantitative evaluation of the model quality on the test set

print "Predicting the people names on the testing set"
t0 = time()
y_pred = clf.predict(X_test_pca)
print "done in %0.3fs" % (time() - t0)

print classification_report(y_test, y_pred, target_names=target_names)
print confusion_matrix(y_test, y_pred, labels=range(n_classes))


###############################################################################
# Qualitative evaluation of the predictions using matplotlib

def plot_gallery(images, titles, h, w, n_row=3, n_col=4):
    """Helper function to plot a gallery of portraits"""
    pl.figure(figsize=(1.8 * n_col, 2.4 * n_row))
    pl.subplots_adjust(bottom=0, left=.01, right=.99, top=.90, hspace=.35)
    for i in range(n_row * n_col):
        pl.subplot(n_row, n_col, i + 1)
        pl.imshow(images[i].reshape((h, w)), cmap=pl.cm.gray)
        pl.title(titles[i], size=12)
        pl.xticks(())
        pl.yticks(())

# plot the result of the prediction on a portion of the test set

def title(y_pred, y_test, target_names, i):
    pred_name = target_names[y_pred[i]].rsplit(' ', 1)[-1]
    true_name = target_names[y_test[i]].rsplit(' ', 1)[-1]
    return 'predicted: %s\ntrue:      %s' % (pred_name, true_name)

prediction_titles = [title(y_pred, y_test, target_names, i)
                     for i in range(y_pred.shape[0])]

plot_gallery(X_test, prediction_titles, h, w)

# plot the gallery of the most significative eigenfaces
```

```
eigenface_titles = ["eigenface %d" % i for i in range(eigenfaces.shape[0])]
plot_gallery(eigenfaces, eigenface_titles, h, w)

pl.show()
```

Species distribution modeling

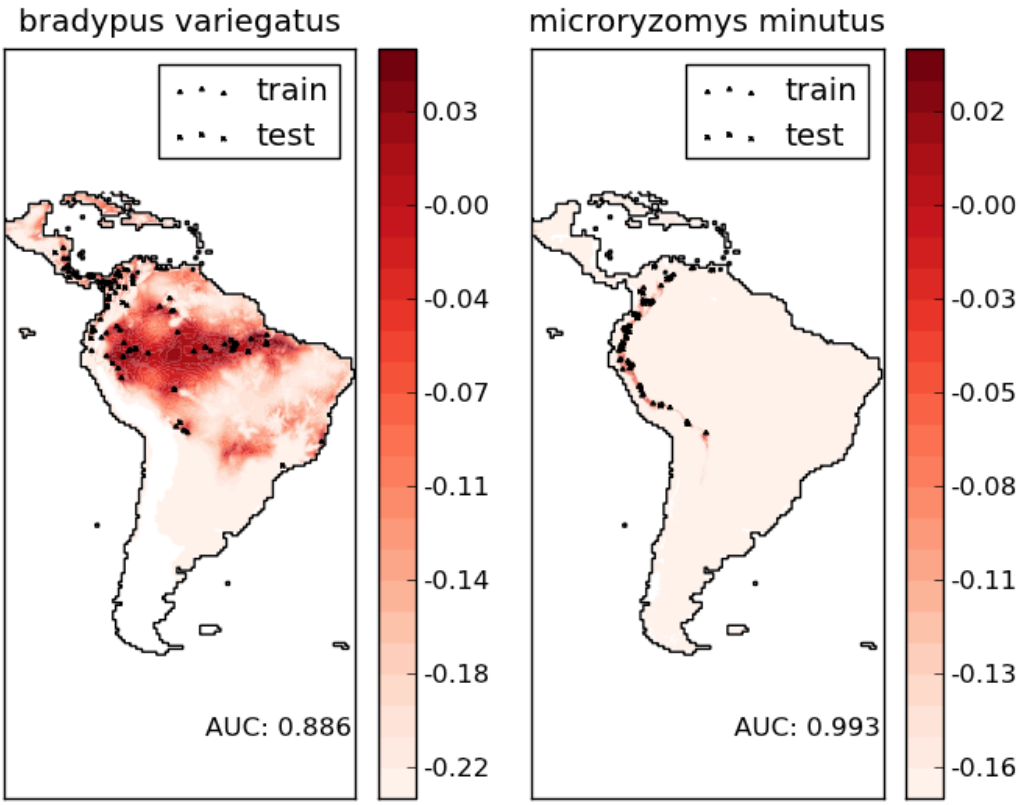
Modeling species' geographic distributions is an important problem in conservation biology. In this example we model the geographic distribution of two south american mammals given past observations and 14 environmental variables. Since we have only positive examples (there are no unsuccessful observations), we cast this problem as a density estimation problem and use the *OneClassSVM* provided by the package *scikits.learn.svm* as our modeling tool. The dataset is provided by Phillips et. al. (2006). If available, the example uses basemap to plot the coast lines and national boundaries of South America.

The two species are:

- Bradypus variegatus , the Brown-throated Sloth.
- Microryzomys minutus , also known as the Forest Small Rice Rat, a rodent that lives in Peru, Colombia, Ecuador, Peru, and Venezuela.

References:

- "Maximum entropy modeling of species geographic distributions" S. J. Phillips, R. P. Anderson, R. E. Schapire - Ecological Modelling, 190:231-259, 2006.



Python source code: plot_species_distribution_modeling.py

```
from __future__ import division

# Author: Peter Prettenhofer <peter.prettenhofer@gmail.com>
#
# License: Simplified BSD

print __doc__

import os
from os.path import normpath, split, exists
from glob import glob
from time import time

import pylab as pl
import numpy as np

try:
    from mpl_toolkits.basemap import Basemap
    basemap = True
except ImportError:
    basemap = False

from scikits.learn import svm
from scikits.learn.metrics import roc_curve, auc
from scikits.learn.datasets.base import Bunch

###############################################################################
# Download the data, if not already on disk
samples_url = "http://www.cs.princeton.edu/~schapire/maxent/datasets/" \
              "samples.zip"
coverage_url = "http://www.cs.princeton.edu/~schapire/maxent/datasets/" \
               "coverages.zip"
samples_archive_name = "samples.zip"
coverage_archive_name = "coverages.zip"


def download(url, archive_name):
    if not exists(archive_name[:-4]):
        if not exists(archive_name):
            import urllib
            print "Downloading data, please wait ..."
            print url
            opener = urllib.urlopen(url)
            open(archive_name, 'wb').write(opener.read())
            print

        import zipfile
        print "Decompressiong the archive: " + archive_name
        zipfile.ZipFile(archive_name).extractall()
        # Remove the archive: we don't need it as we have expanded it
        # to directory
        os.unlink(archive_name)
        print


download(samples_url, samples_archive_name)
download(coverage_url, coverage_archive_name)
```

```
t0 = time()


###############################################################################
# Preprocess data

species = ["bradypus_variegatus_0", "microryzomys_minutus_0"]
species_map = dict([(s, i) for i, s in enumerate(species)])

# x,y coordinates of study area
x_left_lower_corner = -94.8
y_left_lower_corner = -56.05
n_cols = 1212
n_rows = 1592
grid_size = 0.05  # ~5.5 km

# x,y coordinates for each cell
xmin = x_left_lower_corner + grid_size
xmax = xmin + (n_cols * grid_size)
ymin = y_left_lower_corner + grid_size
ymax = ymin + (n_rows * grid_size)

# x coordinates of the grid cells
xx = np.arange(xmin, xmax, grid_size)
# y coordinates of the grid cells
yy = np.arange(ymin, ymax, grid_size)

print "Data grid"
print "---------"
print "xmin, xmax:", xmin, xmax
print "ymin, ymax:", ymin, ymax
print "grid size:", grid_size
print

###############################################################################
# Load data

print "loading data from disk..."
def read_file(fname):
    """Read coverage grid data; returns array of
    shape [n_rows, n_cols]. """
    f = open(fname)
    # Skip header
    for i in range(6):
        f.readline()
    X = np.fromfile(f, dtype=np.float32, sep=" ", count=-1)
    f.close()
    return X.reshape((n_rows, n_cols))

def load_dir(directory):
    """Loads each of the coverage grids and returns a
    tensor of shape [14, n_rows, n_cols].
    """
    data = []
    for fpath in glob("%s/*.asc" % normpath(directory)):
        fname = split(fpath)[-1]
        fname = fname[:fname.index(".")]
```

```
        X = read_file(fpath)  #np.loadtxt(fpath, skiprows=6, dtype=np.float32)
        data.append(X)
    return np.array(data, dtype=np.float32)

def get_coverages(points, coverages, xx, yy):
    """
    Returns
    -------
    array : shape = [n_points, 14]
    """
    rows = []
    cols = []
    for n in range(points.shape[0]):
        i = np.searchsorted(xx, points[n, 0])
        j = np.searchsorted(yy, points[n, 1])
        rows.append(-j)
        cols.append(i)
    return coverages[:, rows, cols].T

species2id = lambda s: species_map.get(s, -1)
train = np.loadtxt('samples/alltrain.csv', converters={0: species2id},
                   skiprows=1, delimiter=",")
test = np.loadtxt('samples/alltest.csv', converters={0: species2id},
                  skiprows=1, delimiter=",")
# Load env variable grids
coverage = load_dir("coverages")

# Per species data
bv = Bunch(name=" ".join(species[0].split("_")[:2]),
           train=train[train[:,0] == 0, 1:],
           test=test[test[:,0] == 0, 1:])
mm = Bunch(name=" ".join(species[1].split("_")[:2]),
           train=train[train[:,0] == 1, 1:],
           test=test[test[:,0] == 1, 1:])

# Get features (=coverages)
bv.train_cover = get_coverages(bv.train, coverage, xx, yy)
bv.test_cover = get_coverages(bv.test, coverage, xx, yy)
mm.train_cover = get_coverages(mm.train, coverage, xx, yy)
mm.test_cover = get_coverages(mm.test, coverage, xx, yy)


def predict(clf, mean, std):
    """Predict the density of the land grid cells
    under the model `clf`.

    Returns
    -------
    array : shape [n_rows, n_cols]
    """
    Z = np.ones((n_rows, n_cols), dtype=np.float64)
    # the land points
    idx = np.where(coverage[2] > -9999)
    X = coverage[:, idx[0], idx[1]].T
    pred = clf.decision_function((X-mean)/std)[:,0]
    Z *= pred.min()
    Z[idx[0], idx[1]] = pred
    return Z
```

```
# background points (grid coordinates) for evaluation
np.random.seed(13)
background_points = np.c_[np.random.randint(low=0, high=n_rows, size=10000),
                          np.random.randint(low=0, high=n_cols, size=10000)].T

# The grid in x,y coordinates
X, Y = np.meshgrid(xx, yy[::-1])
#basemap = False
for i, species in enumerate([bv, mm]):
    print "_" * 80
    print "Modeling distribution of species '%s'" % species.name
    print
    # Standardize features
    mean = species.train_cover.mean(axis=0)
    std = species.train_cover.std(axis=0)
    train_cover_std = (species.train_cover - mean) / std

    # Fit OneClassSVM
    print "fit OneClassSVM ... ",
    clf = svm.OneClassSVM(nu=0.1, kernel="rbf", gamma=0.5)
    clf.fit(train_cover_std)
    print "done. "

    # Plot map of South America
    pl.subplot(1, 2, i + 1)
    if basemap:
        print "plot coastlines using basemap"
        m = Basemap(projection='cyl', llcrnrlat=ymin,
                urcrnrlat=ymax, llcrnrlon=xmin,
                urcrnrlon=xmax, resolution='c')
        m.drawcoastlines()
        m.drawcountries()
        #m.drawrivers()
    else:
        print "plot coastlines from coverage"
        CS = pl.contour(X, Y, coverage[2,:,:], levels=[-9999], colors="k",
                        linestyles="solid")
        pl.xticks([])
        pl.yticks([])

    print "predict species distribution"
    Z = predict(clf, mean, std)
    levels = np.linspace(Z.min(), Z.max(), 25)
    Z[coverage[2,:,:] == -9999] = -9999
    CS = pl.contourf(X, Y, Z, levels=levels, cmap=pl.cm.Reds)
    pl.colorbar(format='%.2f')
    pl.scatter(species.train[:, 0], species.train[:, 1], s=2**2, c='black',
               marker='^', label='train')
    pl.scatter(species.test[:, 0], species.test[:, 1], s=2**2, c='black',
               marker='x', label='test')
    pl.legend()
    pl.title(species.name)
    pl.axis('equal')

    # Compute AUC w.r.t. background points
    pred_background = Z[background_points[0], background_points[1]]
    pred_test = clf.decision_function((species.test_cover-mean)/std)[:,0]
    scores = np.r_[pred_test, pred_background]
```

```
    y = np.r_[np.ones(pred_test.shape), np.zeros(pred_background.shape)]
    fpr, tpr, thresholds = roc_curve(y, scores)
    roc_auc = auc(fpr, tpr)
    pl.text(-35, -70, "AUC: %.3f" % roc_auc, ha="right")
    print "Area under the ROC curve : %f" % roc_auc

print "time elapsed: %.3fs" % (time() - t0)

pl.show()
```

Finding structure in the stock market

An example of playing with stock market data to try and find some structure in it.

Python source code: `stock_market.py`

```
print __doc__

# Author: Gael Varoquaux gael.varoquaux@normalesup.org
# License: BSD

import datetime
from matplotlib import finance
import numpy as np

from scikits.learn import cluster

# Choose a time period reasonnably calm (not too long ago so that we get
# high-tech firms, and before the 2008 crash)
d1 = datetime.datetime(2003, 01, 01)
d2 = datetime.datetime(2008, 01, 01)

symbol_dict = {
        'TOT'  : 'Total',
        'XOM'  : 'Exxon',
        'CVX'  : 'Chevron',
        'COP'  : 'ConocoPhillips',
        'VLO'  : 'Valero Energy',
        'MSFT' : 'Microsoft',
        'IBM'  : 'IBM',
        'TWX'  : 'Time Warner',
        'CMCSA': 'Comcast',
        'CVC'  : 'Cablevision',
        'YHOO' : 'Yahoo',
        'DELL' : 'Dell',
        'HPQ'  : 'Hewlett-Packard',
        'AMZN' : 'Amazon',
        'TM'   : 'Toyota',
        'CAJ'  : 'Canon',
        'MTU'  : 'Mitsubishi',
        'SNE'  : 'Sony',
        'F'    : 'Ford',
        'HMC'  : 'Honda',
        'NAV'  : 'Navistar',
        'NOC'  : 'Northrop Grumman',
        'BA'   : 'Boeing',
        'KO'   : 'Coca Cola',
```

```
        'MMM'  : '3M',
        'MCD'  : 'Mc Donalds',
        'PEP'  : 'Pepsi',
        'KFT'  : 'Kraft Foods',
        'K'    : 'Kellogg',
        'UN'   : 'Unilever',
        'MAR'  : 'Marriott',
        'PG'   : 'Procter Gamble',
        'CL'   : 'Colgate-Palmolive',
        'NWS'  : 'News Corporation',
        'GE'   : 'General Electrics',
        'WFC'  : 'Wells Fargo',
        'JPM'  : 'JPMorgan Chase',
        'AIG'  : 'AIG',
        'AXP'  : 'American express',
        'BAC'  : 'Bank of America',
        'GS'   : 'Goldman Sachs',
        'AAPL' : 'Apple',
        'SAP'  : 'SAP',
        'CSCO' : 'Cisco',
        'TXN'  : 'Texas instruments',
        'XRX'  : 'Xerox',
        'LMT'  : 'Lookheed Martin',
        'WMT'  : 'Wal-Mart',
        'WAG'  : 'Walgreen',
        'HD'   : 'Home Depot',
        'GSK'  : 'GlaxoSmithKline',
        'PFE'  : 'Pfizer',
        'SNY'  : 'Sanofi-Aventis',
        'NVS'  : 'Novartis',
        'KMB'  : 'Kimberly-Clark',
        'R'    : 'Ryder',
        'GD'   : 'General Dynamics',
        'RTN'  : 'Raytheon',
        'CVS'  : 'CVS',
        'CAT'  : 'Caterpillar',
        'DD'   : 'DuPont de Nemours',
    }

symbols, names = np.array(symbol_dict.items()).T

quotes = [finance.quotes_historical_yahoo(symbol, d1, d2, asobject=True)
                for symbol in symbols]

#volumes = np.array([q.volume for q in quotes]).astype(np.float)
open    = np.array([q.open   for q in quotes]).astype(np.float)
close   = np.array([q.close  for q in quotes]).astype(np.float)
variation = close - open
correlations = np.corrcoef(variation)

_, labels = cluster.affinity_propagation(correlations)

for i in range(labels.max()+1):
    print 'Cluster %i: %s' % ((i+1),
                              ', '.join(names[labels==i]))
```

Libsvm GUI

A simple graphical frontend for Libsvm mainly intended for didactic purposes. You can create data points by point and click and visualize the decision region induced by different kernels and parameter settings.

To create positive examples click the left mouse button; to create negative examples click the right button.

If all examples are from the same class, it uses a one-class SVM.

TODO add labels to the panel.

Requirements

- Tkinter
- scikits.learn
- matplotlib with TkAgg

Python source code: `svm_gui.py`

```
from __future__ import division

print __doc__

# Author: Peter Prettenhoer <peter.prettenhofer@gmail.com>
#
# License: BSD Style.

import matplotlib
matplotlib.use('TkAgg')

from matplotlib.backends.backend_tkagg import FigureCanvasTkAgg
#from matplotlib.backends.backend_tkagg import NavigationToolbar2TkAgg
from matplotlib.figure import Figure
from matplotlib.contour import ContourSet

import Tkinter as Tk
import sys
import numpy as np

from scikits.learn import svm

y_min, y_max = -50, 50
x_min, x_max = -50, 50


class Model(object):
    """The Model which hold the data. It implements the
    observable in the observer pattern and notifies the
    registered observers on change event.
    """

    def __init__(self):
        self.observers = []
        self.surface = None
        self.data = []
        self.cls = None
        self.surface_type = 0
```

```
    def changed(self, event):
        """Notify the observers. """
        for observer in self.observers:
            observer.update(event, self)

    def add_observer(self, observer):
        """Register an observer. """
        self.observers.append(observer)

    def set_surface(self, surface):
        self.surface = surface


class Controller(object):
    def __init__(self, model):
        self.model = model
        self.kernel = Tk.IntVar()
        self.surface_type = Tk.IntVar()
        # Whether or not a model has been fitted
        self.fitted = False

    def fit(self):
        print "fit the model"
        train = np.array(self.model.data)
        X = train[:, :2]
        y = train[:, 2]

        C = float(self.complexity.get())
        gamma = float(self.gamma.get())
        coef0 = float(self.coef0.get())
        degree = int(self.degree.get())
        kernel_map = {0: "linear", 1: "rbf", 2: "poly"}
        if len(np.unique(y)) == 1:
            clf = svm.OneClassSVM(kernel=kernel_map[self.kernel.get()],
                      gamma=gamma, coef0=coef0, degree=degree)
            clf.fit(X)
        else:
            clf = svm.SVC(kernel=kernel_map[self.kernel.get()], C=C,
                          gamma=gamma, coef0=coef0, degree=degree)
            clf.fit(X, y)
        if hasattr(clf, 'score'):
            print "Accuracy:", clf.score(X, y) * 100
        X1, X2, Z = self.decision_surface(clf)
        self.model.clf = clf
        self.model.set_surface((X1, X2, Z))
        self.model.surface_type = self.surface_type.get()
        self.fitted = True
        self.model.changed("surface")

    def decision_surface(self, cls):
        delta = 1
        x = np.arange(x_min, x_max + delta, delta)
        y = np.arange(y_min, y_max + delta, delta)
        X1, X2 = np.meshgrid(x, y)
        Z = cls.decision_function(np.c_[X1.ravel(), X2.ravel()])
        Z = Z.reshape(X1.shape)
        return X1, X2, Z
```

```
    def clear_data(self):
        self.model.data = []
        self.fitted = False
        self.model.changed("clear")

    def add_example(self, x, y, label):
        self.model.data.append((x, y, label))
        self.model.changed("example_added")

        # update decision surface if already fitted.
        self.refit()

    def refit(self):
        """Refit the model if already fitted. """
        if self.fitted:
            self.fit()


class View(object):
    """Test docstring. """
    def __init__(self, root, controller):
        f = Figure()
        ax = f.add_subplot(111)
        ax.set_xticks([])
        ax.set_yticks([])
        ax.set_xlim((x_min, x_max))
        ax.set_ylim((y_min, y_max))
        canvas = FigureCanvasTkAgg(f, master=root)
        canvas.show()
        canvas.get_tk_widget().pack(side=Tk.TOP, fill=Tk.BOTH, expand=1)
        canvas._tkcanvas.pack(side=Tk.TOP, fill=Tk.BOTH, expand=1)
        canvas.mpl_connect('button_press_event', self.onclick)
#         toolbar = NavigationToolbar2TkAgg(canvas, root)
#         toolbar.update()
        self.controllbar = ControllBar(root, controller)
        self.f = f
        self.ax = ax
        self.canvas = canvas
        self.controller = controller
        self.contours = []
        self.c_labels = None
        self.plot_kernels()

    def plot_kernels(self):
        self.ax.text(-50, -60, "Linear: $u^T v$")
        self.ax.text(-20, -60, "RBF: $\exp (-\gamma \| u-v \|^2)$")
        self.ax.text(10, -60, "Poly: $(\gamma \, u^T v + r)^d$")

    def onclick(self, event):
        if event.xdata and event.ydata:
            if event.button == 1:
                self.controller.add_example(event.xdata, event.ydata, 1)
            elif event.button == 3:
                self.controller.add_example(event.xdata, event.ydata, -1)

    def update(self, event, model):
        if event == "example_added":
            x, y, l = model.data[-1]
```

```
            if l == 1:
                color = 'w'
            elif l == -1:
                color = 'k'
            self.ax.plot([x], [y], "%so" % color, scalex=0.0, scaley=0.0)

        if event == "clear":
            self.ax.clear()
            self.ax.set_xticks([])
            self.ax.set_yticks([])
            self.contours = []
            self.c_labels = None
            self.plot_kernels()

        if event == "surface":
            self.remove_surface()
            self.plot_support_vectors(model.clf.support_vectors_)
            self.plot_decision_surface(model.surface, model.surface_type)

        self.canvas.draw()

    def remove_surface(self):
        """Remove old decision surface."""
        if len(self.contours) > 0:
            for contour in self.contours:
                if isinstance(contour, ContourSet):
                    for lineset in contour.collections:
                        lineset.remove()
                else:
                    contour.remove()
            self.contours = []

    def plot_support_vectors(self, support_vectors):
        """Plot the support vectors by placing circles over the
        corresponding data points and adds the circle collection
        to the contours list."""
        cs = self.ax.scatter(support_vectors[:, 0], support_vectors[:, 1],
                             s=80, edgecolors="k", facecolors="none")
        self.contours.append(cs)

    def plot_decision_surface(self, surface, type):
        X1, X2, Z = surface
        if type == 0:
            levels = [-1.0, 0.0, 1.0]
            linestyles = ['dashed', 'solid', 'dashed']
            colors = 'k'
            self.contours.append(self.ax.contour(X1, X2, Z, levels,
                                                 colors=colors,
                                                 linestyles=linestyles))
        elif type == 1:
            self.contours.append(self.ax.contourf(X1, X2, Z, 10,
                                                  cmap=matplotlib.cm.bone,
                                                  origin='lower',
                                                  alpha=0.85))
            self.contours.append(self.ax.contour(X1, X2, Z, [0.0],
                                                 colors='k',
                                                 linestyles=['solid']))
        else:
```

```
            raise ValueError("surface type unknown")


class ControllBar(object):
    def __init__(self, root, controller):
        fm = Tk.Frame(root)
        kernel_group = Tk.Frame(fm)
        Tk.Radiobutton(kernel_group, text="Linear", variable=controller.kernel,
                       value=0, command=controller.refit).pack(anchor=Tk.W)
        Tk.Radiobutton(kernel_group, text="RBF", variable=controller.kernel,
                       value=1, command=controller.refit).pack(anchor=Tk.W)
        Tk.Radiobutton(kernel_group, text="Poly", variable=controller.kernel,
                       value=2, command=controller.refit).pack(anchor=Tk.W)
        kernel_group.pack(side=Tk.LEFT)

        valbox = Tk.Frame(fm)
        controller.complexity = Tk.StringVar()
        controller.complexity.set("1.0")
        c = Tk.Frame(valbox)
        Tk.Label(c, text="C:", anchor="e", width=7).pack(side=Tk.LEFT)
        Tk.Entry(c, width=6, textvariable=controller.complexity).pack(
            side=Tk.LEFT)
        c.pack()

        controller.gamma = Tk.StringVar()
        controller.gamma.set("0.01")
        g = Tk.Frame(valbox)
        Tk.Label(g, text="gamma:", anchor="e", width=7).pack(side=Tk.LEFT)
        Tk.Entry(g, width=6, textvariable=controller.gamma).pack(side=Tk.LEFT)
        g.pack()

        controller.degree = Tk.StringVar()
        controller.degree.set("3")
        d = Tk.Frame(valbox)
        Tk.Label(d, text="degree:", anchor="e", width=7).pack(side=Tk.LEFT)
        Tk.Entry(d, width=6, textvariable=controller.degree).pack(side=Tk.LEFT)
        d.pack()

        controller.coef0 = Tk.StringVar()
        controller.coef0.set("0")
        r = Tk.Frame(valbox)
        Tk.Label(r, text="coef0:", anchor="e", width=7).pack(side=Tk.LEFT)
        Tk.Entry(r, width=6, textvariable=controller.coef0).pack(side=Tk.LEFT)
        r.pack()
        valbox.pack(side=Tk.LEFT)

        cmap_group = Tk.Frame(fm)
        Tk.Radiobutton(cmap_group, text="Hyperplanes",
                       variable=controller.surface_type, value=0,
                       command=controller.refit).pack(anchor=Tk.W)
        Tk.Radiobutton(cmap_group, text="Surface",
                       variable=controller.surface_type, value=1,
                       command=controller.refit).pack(anchor=Tk.W)

        cmap_group.pack(side=Tk.LEFT)

        train_button = Tk.Button(fm, text='Fit', width=5,
                                 command=controller.fit)
```

```
        train_button.pack()
        fm.pack(side=Tk.LEFT)
        Tk.Button(fm, text='Clear', width=5,
                  command=controller.clear_data).pack(side=Tk.LEFT)


def main(argv):
    root = Tk.Tk()
    model = Model()
    controller = Controller(model)
    root.wm_title("Scikit-learn Libsvm GUI")
    view = View(root, controller)
    model.add_observer(view)
    Tk.mainloop()

if __name__ == "__main__":
    main(sys.argv)
```

Wikipedia princial eigenvector

A classical way to assert the relative importance of vertices in a graph is to compute the principal eigenvector of the adjacency matrix so as to assign to each vertex the values of the components of the first eigenvector as a centrality score:

http://en.wikipedia.org/wiki/Eigenvector_centrality

On the graph of webpages and links those values are called the PageRank scores by Google.

The goal of this example is to analyze the graph of links inside wikipedia articles to rank articles by relative importance according to this eigenvector centrality.

The traditional way to compute the principal eigenvector is to use the power iteration method:

http://en.wikipedia.org/wiki/Power_iteration

Here the computation is achieved thanks to Martinsson's Randomized SVD algoritm implemented in the scikit.

The graph data is fetched from the DBpedia dumps. DBpedia is an extraction of the latent structured data of the Wikipedia content.

Python source code: `wikipedia_principal_eigenvector.py`

```
print __doc__

# Author: Olivier Grisel <olivier.grisel@ensta.org>
# License: Simplified BSD

from bz2 import BZ2File
import os
from datetime import datetime
from pprint import pprint
from time import time

import numpy as np

from scipy import sparse

from scikits.learn.utils.extmath import fast_svd
from scikits.learn.externals.joblib import Memory
```

```
################################################################################
# Where to download the data, if not already on disk
redirects_url = "http://downloads.dbpedia.org/3.5.1/en/redirects_en.nt.bz2"
redirects_filename = redirects_url.rsplit("/", 1)[1]

page_links_url = "http://downloads.dbpedia.org/3.5.1/en/page_links_en.nt.bz2"
page_links_filename = page_links_url.rsplit("/", 1)[1]

resources = [
    (redirects_url, redirects_filename),
    (page_links_url, page_links_filename),
]

for url, filename in resources:
    if not os.path.exists(filename):
        import urllib
        print "Downloading data from '%s', please wait..." % url
        opener = urllib.urlopen(url)
        open(filename, 'wb').write(opener.read())
        print


################################################################################
# Loading the redirect files

memory = Memory(cachedir=".")


def index(redirects, index_map, k):
    """Find the index of an article name after redirect resolution"""
    k = redirects.get(k, k)
    return index_map.setdefault(k, len(index_map))


DBPEDIA_RESOURCE_PREFIX_LEN = len("http://dbpedia.org/resource/")
SHORTNAME_SLICE = slice(DBPEDIA_RESOURCE_PREFIX_LEN + 1, -1)


def short_name(nt_uri):
    """Remove the < and > URI markers and the common URI prefix"""
    return nt_uri[SHORTNAME_SLICE]


def get_redirects(redirects_filename):
    """Parse the redirections and build a transitively closed map out of it"""
    redirects = {}
    print "Parsing the NT redirect file"
    for l, line in enumerate(BZ2File(redirects_filename)):
        split = line.split()
        if len(split) != 4:
            print "ignoring malformed line: " + line
            continue
        redirects[short_name(split[0])] = short_name(split[2])
        if l % 1000000 == 0:
            print "[%s] line: %08d" % (datetime.now().isoformat(), l)

    # compute the transitive closure
```

```
    print "Computing the transitive closure of the redirect relation"
    for l, source in enumerate(redirects.keys()):
        transitive_target = None
        target = redirects[source]
        seen = set([source])
        while True:
            transitive_target = target
            target = redirects.get(target)
            if target is None or target in seen:
                break
            seen.add(target)
        redirects[source] = transitive_target
        if l % 1000000 == 0:
            print "[%s] line: %08d" % (datetime.now().isoformat(), l)

    return redirects


# disabling joblib as the pickling of large dicts seems much too slow
#@memory.cache
def get_adjacency_matrix(redirects_filename, page_links_filename, limit=None):
    """Extract the adjacency graph as a scipy sparse matrix

    Redirects are resolved first.

    Returns X, the scipy sparse adjacency matrix, redirects as python
    dict from article names to article names and index_map a python dict
    from article names to python int (article indexes).
    """

    print "Computing the redirect map"
    redirects = get_redirects(redirects_filename)

    print "Computing the integer index map"
    index_map = dict()
    links = list()
    for l, line in enumerate(BZ2File(page_links_filename)):
        split = line.split()
        if len(split) != 4:
            print "ignoring malformed line: " + line
            continue
        i = index(redirects, index_map, short_name(split[0]))
        j = index(redirects, index_map, short_name(split[2]))
        links.append((i, j))
        if l % 1000000 == 0:
            print "[%s] line: %08d" % (datetime.now().isoformat(), l)

        if limit is not None and l >= limit - 1:
            break

    print "Computing the adjacency matrix"
    X = sparse.lil_matrix((len(index_map), len(index_map)), dtype=np.float32)
    for i, j in links:
        X[i, j] = 1.0
    del links
    print "Converting to CSR representation"
    X = X.tocsr()
    print "CSR conversion done"
```

```
    return X, redirects, index_map


# stop after 5M links to make it possible to work in RAM
X, redirects, index_map = get_adjacency_matrix(
    redirects_filename, page_links_filename, limit=5000000)
names = dict((i, name) for name, i in index_map.iteritems())

print "Computing the principal singular vectors using fast_svd"
t0 = time()
U, s, V = fast_svd(X, 5, q=3)
print "done in %0.3fs" % (time() - t0)

# print the names of the wikipedia related strongest compenents of the the
# principal singular vector which should be similar to the highest eigenvector
print "Top wikipedia pages according to principal singular vectors"
pprint([names[i] for i in np.abs(U.T[0]).argsort()[-10:]])
pprint([names[i] for i in np.abs(V[0]).argsort()[-10:]])


def centrality_scores(X, alpha=0.85, max_iter=100, tol=1e-10):
    """Power iteration computation of the principal eigenvector

    This method is also known as Google PageRank and the implementation
    is based on the one from the NetworkX project (BSD licensed too)
    with copyrights by:

      Aric Hagberg <hagberg@lanl.gov>
      Dan Schult <dschult@colgate.edu>
      Pieter Swart <swart@lanl.gov>
    """
    n = X.shape[0]
    X = X.copy()
    incoming_counts = np.asarray(X.sum(axis=1)).ravel()

    print "Normalizing the graph"
    for i in incoming_counts.nonzero()[0]:
        X.data[X.indptr[i]:X.indptr[i + 1]] *= 1.0 / incoming_counts[i]
    dangle = np.asarray(np.where(X.sum(axis=1) == 0, 1.0 / n, 0)).ravel()

    scores = np.ones(n, dtype=np.float32) / n  # initial guess
    for i in range(max_iter):
        print "power iteration #%d" % i
        prev_scores = scores
        scores = (alpha * (scores * X + np.dot(dangle, prev_scores))
                  + (1 - alpha) * prev_scores.sum() / n)
        # check convergence: normalized l_inf norm
        scores_max = np.abs(scores).max()
        if scores_max == 0.0:
            scores_max = 1.0
        err = np.abs(scores - prev_scores).max() / scores_max
        print "error: %0.6f" % err
        if err < n * tol:
            return scores

    return scores

print "Computing principal eigenvector score using a power iteration method"
```

```
t0 = time()
scores = centrality_scores(X, max_iter=100, tol=1e-10)
print "done in %0.3fs" % (time() - t0)
pprint([names[i] for i in np.abs(scores).argsort()[-10:]])
```

2.1.3 Clustering

Examples concerning the *scikits.learn.cluster* package.

A demo of K-Means clustering on the handwritten digits data

Comparing various initialization strategies in terms of runtime and quality of the results.

TODO: explode the ouput of the cluster labeling and digits.target groundtruth as categorical boolean arrays of shape (n_sample, n_unique_labels) and measure the Pearson correlation as an additional measure of the clustering quality.

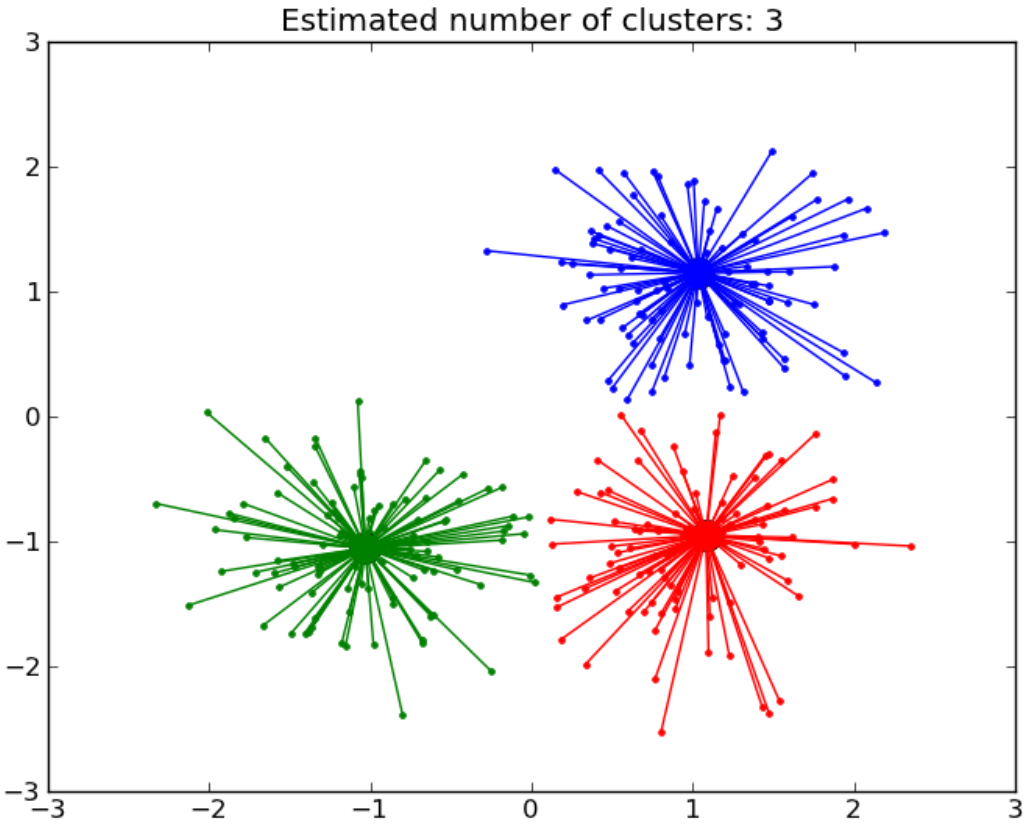
Python source code: `kmeans_digits.py`

```
print __doc__

from time import time
import numpy as np

from scikits.learn.cluster import KMeans
from scikits.learn.datasets import load_digits
from scikits.learn.decomposition import PCA
from scikits.learn.preprocessing import scale

np.random.seed(42)

digits = load_digits()
data = scale(digits.data)

n_samples, n_features = data.shape
n_digits = len(np.unique(digits.target))

print "n_digits: %d" % n_digits
print "n_features: %d" % n_features
print "n_samples: %d" % n_samples
print

print "Raw k-means with k-means++ init..."
t0 = time()
km = KMeans(init='k-means++', k=n_digits, n_init=10).fit(data)
print "done in %0.3fs" % (time() - t0)
print "inertia: %f" % km.inertia_
print

print "Raw k-means with random centroid init..."
t0 = time()
km = KMeans(init='random', k=n_digits, n_init=10).fit(data)
print "done in %0.3fs" % (time() - t0)
print "inertia: %f" % km.inertia_
print

print "Raw k-means with PCA-based centroid init..."
```

```
# in this case the seeding of the centers is deterministic, hence we run the
# kmeans algorithm only once with n_init=1
t0 = time()
pca = PCA(n_components=n_digits).fit(data)
km = KMeans(init=pca.components_, k=n_digits, n_init=1).fit(data)
print "done in %0.3fs" % (time() - t0)
print "inertia: %f" % km.inertia_
print
```

Demo of affinity propagation clustering algorithm

Reference: Brendan J. Frey and Delbert Dueck, "Clustering by Passing Messages Between Data Points", Science Feb. 2007



Python source code: `plot_affinity_propagation.py`

```
print __doc__

import numpy as np
from scikits.learn.cluster import AffinityPropagation

##############################################################################
# Generate sample data
##############################################################################
np.random.seed(0)
```

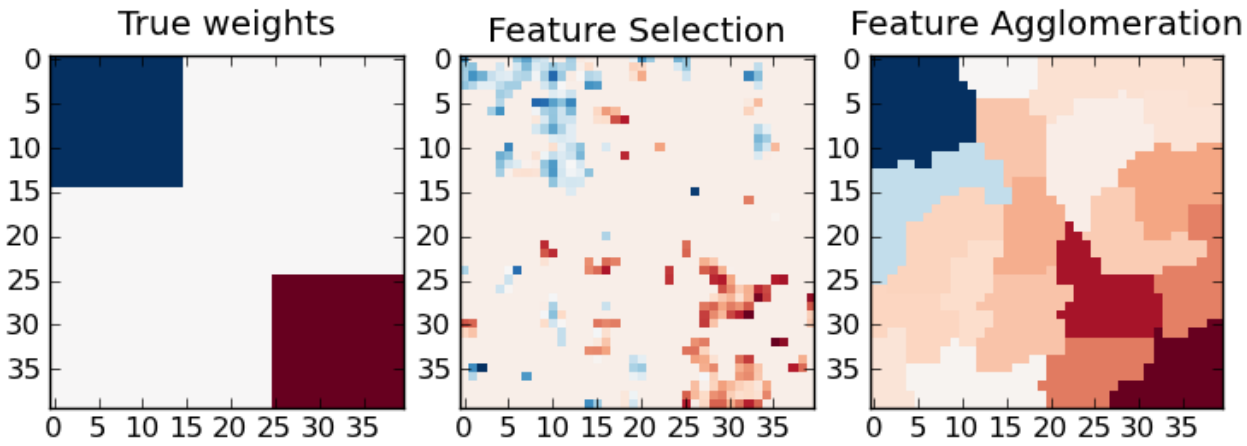
```
n_points_per_cluster = 100
n_clusters = 3
n_points = n_points_per_cluster*n_clusters
means = np.array([[1,1],[-1,-1],[1,-1]])
std = .5

X = np.empty((0, 2))
for i in range(n_clusters):
    X = np.r_[X, means[i] + std * np.random.randn(n_points_per_cluster, 2)]

##############################################################################
# Compute similarities
##############################################################################
X_norms = np.sum(X*X, axis=1)
S = - X_norms[:,np.newaxis] - X_norms[np.newaxis,:] + 2 * np.dot(X, X.T)
p = 10*np.median(S)

##############################################################################
# Compute Affinity Propagation
##############################################################################

af = AffinityPropagation()
af.fit(S, p)
cluster_centers_indices = af.cluster_centers_indices_
labels = af.labels_

n_clusters_ = len(cluster_centers_indices)

print 'Estimated number of clusters: %d' % n_clusters_

##############################################################################
# Plot result
##############################################################################

import pylab as pl
from itertools import cycle

pl.close('all')
pl.figure(1)
pl.clf()

colors = cycle('bgrcmykbgrcmykbgrcmykbgrcmyk')
for k, col in zip(range(n_clusters_), colors):
    class_members = labels == k
    cluster_center = X[cluster_centers_indices[k]]
    pl.plot(X[class_members,0], X[class_members,1], col+'.')
    pl.plot(cluster_center[0], cluster_center[1], 'o', markerfacecolor=col,
                                    markeredgecolor='k', markersize=14)
    for x in X[class_members]:
        pl.plot([cluster_center[0], x[0]], [cluster_center[1], x[1]], col)

pl.title('Estimated number of clusters: %d' % n_clusters_)
pl.show()
```

Feature agglomeration vs. univariate selection

This example compares 2 dimensionality reduction strategies:

- univariate feature selection with Anova
- feature agglomeration with Ward hierarchical clustering

Both methods are compared in a regression problem using a BayesianRidge as supervised estimator.



Python source code: `plot_feature_agglomeration_vs_univariate_selection.py`

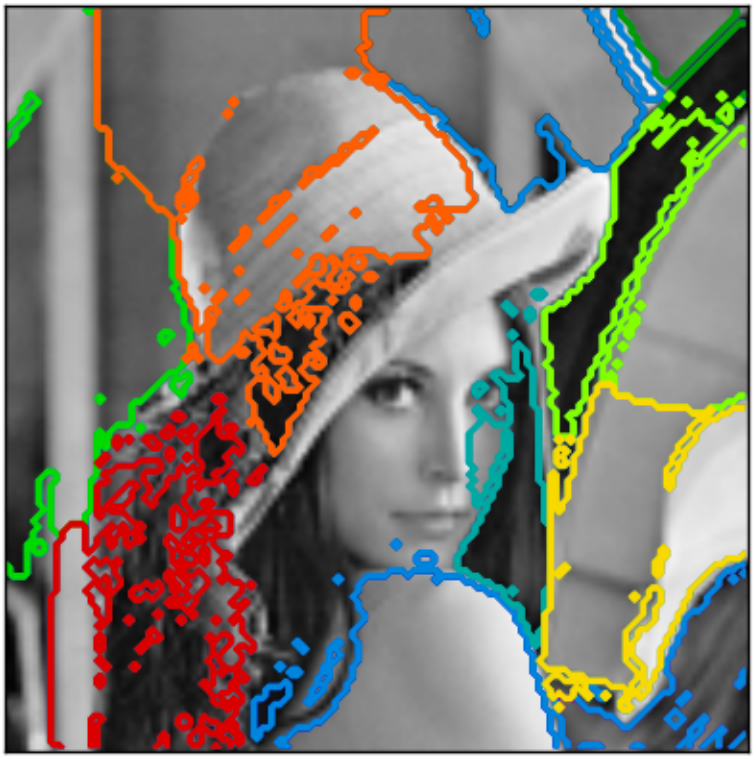
```
# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

print __doc__

import numpy as np
import pylab as pl
from scipy import linalg, ndimage

from scikits.learn.feature_extraction.image import grid_to_graph
from scikits.learn import feature_selection
from scikits.learn.cluster import WardAgglomeration
from scikits.learn.linear_model import BayesianRidge
from scikits.learn.pipeline import Pipeline
from scikits.learn.grid_search import GridSearchCV
from scikits.learn.externals.joblib import Memory
from scikits.learn.cross_val import KFold

###############################################################################
# Generate data
n_samples = 200
size = 40 # image size
roi_size = 15
snr = 5.
np.random.seed(0)
mask = np.ones([size, size], dtype=np.bool)

coef = np.zeros((size, size))
coef[0:roi_size, 0:roi_size] = -1.
coef[-roi_size:, -roi_size:] = 1.
```

```
X = np.random.randn(n_samples, size**2)
for x in X: # smooth data
    x[:] = ndimage.gaussian_filter(x.reshape(size, size), sigma=1.0).ravel()
X -= X.mean(axis=0)
X /= X.std(axis=0)

y = np.dot(X, coef.ravel())
noise = np.random.randn(y.shape[0])
noise_coef = (linalg.norm(y, 2) / np.exp(snr / 20.)) / linalg.norm(noise, 2)
y += noise_coef * noise # add noise

###############################################################################
# Compute the coefs of a Bayesian Ridge with GridSearch
cv = KFold(len(y), 2) # cross-validation generator for model selection
ridge = BayesianRidge()
mem = Memory(cachedir='.', verbose=1)

# Ward agglomeration followed by BayesianRidge
A = grid_to_graph(n_x=size, n_y=size)
ward = WardAgglomeration(n_clusters=10, connectivity=A, memory=mem,
                         n_components=1)
clf = Pipeline([('ward', ward), ('ridge', ridge)])
parameters = {'ward__n_clusters': [10, 20, 30]}
# Select the optimal number of parcels with grid search
clf = GridSearchCV(clf, parameters, n_jobs=1)
clf.fit(X, y, cv=cv) # set the best parameters
coef_ = clf.best_estimator.steps[-1][1].coef_
coef_ = clf.best_estimator.steps[0][1].inverse_transform(coef_)
coef_agglomeration_ = coef_.reshape(size, size)

# Anova univariate feature selection followed by BayesianRidge
f_regression = mem.cache(feature_selection.f_regression) # caching function
anova = feature_selection.SelectPercentile(f_regression)
clf = Pipeline([('anova', anova), ('ridge', ridge)])
parameters = {'anova__percentile': [5, 10, 20]}
# Select the optimal percentage of features with grid search
clf = GridSearchCV(clf, parameters)
clf.fit(X, y, cv=cv) # set the best parameters
coef_ = clf.best_estimator.steps[-1][1].coef_
coef_ = clf.best_estimator.steps[0][1].inverse_transform(coef_)
coef_selection_ = coef_.reshape(size, size)

###############################################################################
# Inverse the transformation to plot the results on an image
pl.close('all')
pl.figure(figsize=(7.3, 2.7))
pl.subplot(1, 3, 1)
pl.imshow(coef, interpolation="nearest", cmap=pl.cm.RdBu_r)
pl.title("True weights")
pl.subplot(1, 3, 2)
pl.imshow(coef_selection_, interpolation="nearest", cmap=pl.cm.RdBu_r)
pl.title("Feature Selection")
pl.subplot(1, 3, 3)
pl.imshow(coef_agglomeration_, interpolation="nearest", cmap=pl.cm.RdBu_r)
pl.title("Feature Agglomeration")
pl.subplots_adjust(0.04, 0.0, 0.98, 0.94, 0.16, 0.26)
pl.show()
```

Segmenting the picture of Lena in regions

This example uses spectral clustering on a graph created from voxel-to-voxel difference on an image to break this image into multiple partly-homogenous regions.

This procedure (spectral clustering on an image) is an efficient approximate solution for finding normalized graph cuts.



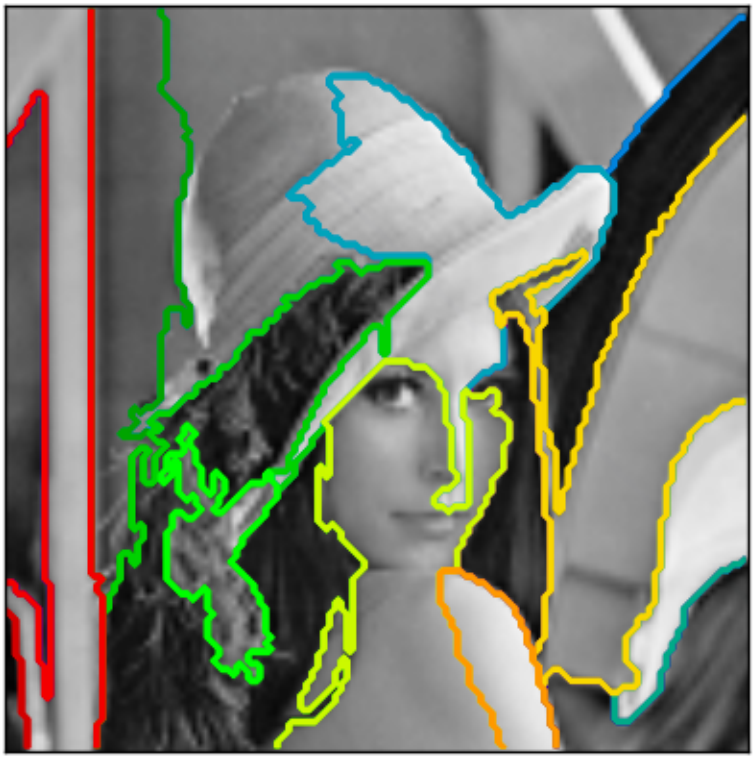
Python source code: `plot_lena_segmentation.py`

```
print __doc__

# Author: Gael Varoquaux <gael.varoquaux@normalesup.org>
# License: BSD

import numpy as np
import scipy as sp
import pylab as pl

from scikits.learn.feature_extraction import image
from scikits.learn.cluster import spectral_clustering

lena = sp.lena()
# Downsample the image by a factor of 4
lena = lena[::2, ::2] + lena[1::2, ::2] + lena[::2, 1::2] + lena[1::2, 1::2]
lena = lena[::2, ::2] + lena[1::2, ::2] + lena[::2, 1::2] + lena[1::2, 1::2]
```

```
# Convert the image into a graph with the value of the gradient on the
# edges.
graph = image.img_to_graph(lena)

# Take a decreasing function of the gradient: an exponential
# The smaller beta is, the more independant the segmentation is of the
# actual image. For beta=1, the segmentation is close to a voronoi
beta = 5
eps  = 1e-6
graph.data = np.exp(-beta*graph.data/lena.std()) + eps

# Apply spectral clustering (this step goes much faster if you have pyamg
# installed)
N_REGIONS = 11
labels = spectral_clustering(graph, k=N_REGIONS)
labels = labels.reshape(lena.shape)

###############################################################################
# Visualize the resulting regions
pl.figure(figsize=(5, 5))
pl.imshow(lena,   cmap=pl.cm.gray)
for l in range(N_REGIONS):
    pl.contour(labels == l, contours=1,
            colors=[pl.cm.spectral(l/float(N_REGIONS)), ])
pl.xticks(())
pl.yticks(())
pl.show()
```

A demo of structured Ward hierarchical clustering on Lena image

Compute the segmentation of a 2D image with Ward hierarchical clustering. The clustering is spatially constrained in order for each segmented region to be in one piece.



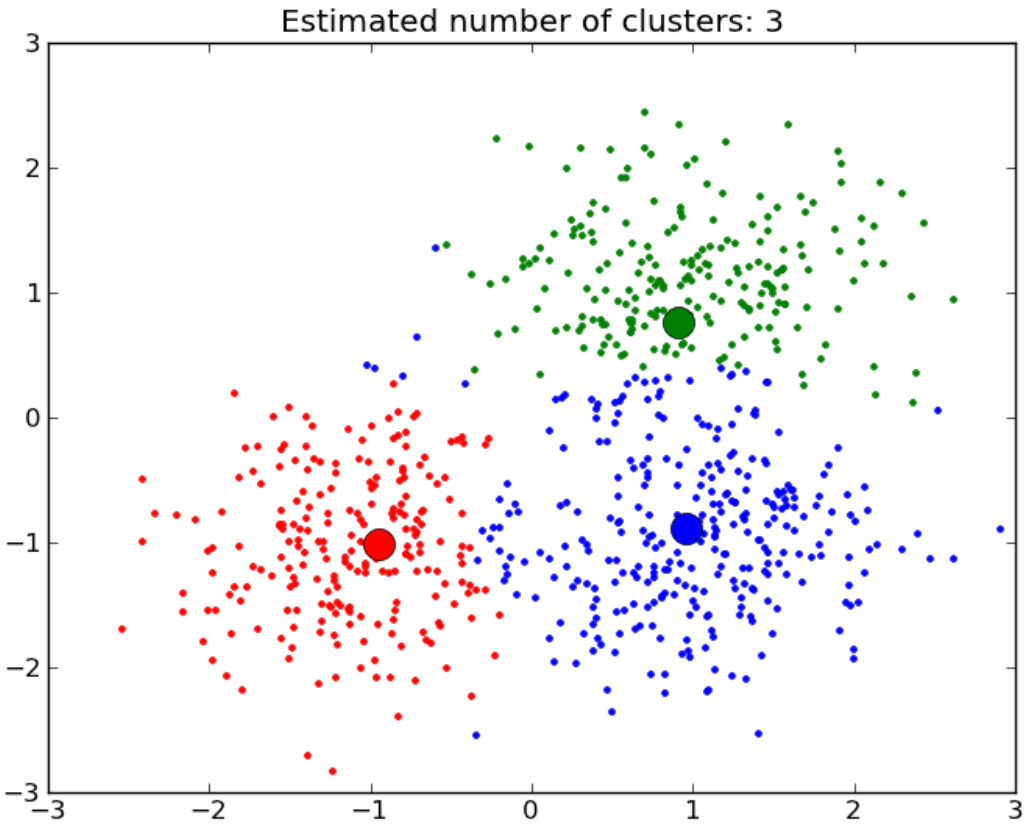
Python source code: `plot_lena_ward_segmentation.py`

```
# Author : Vincent Michel, 2010
#          Alexandre Gramfort, 2011
# License: BSD Style.

print __doc__

import time as time
import numpy as np
import scipy as sp
import pylab as pl
from scikits.learn.feature_extraction.image import grid_to_graph
from scikits.learn.cluster import Ward

###############################################################################
# Generate data
lena = sp.lena()
# Downsample the image by a factor of 4
lena = lena[::2, ::2] + lena[1::2, ::2] + lena[::2, 1::2] + lena[1::2, 1::2]
lena = lena[::2, ::2] + lena[1::2, ::2] + lena[::2, 1::2] + lena[1::2, 1::2]
mask = np.ones_like(lena).astype(bool)
X = np.atleast_2d(lena[mask]).T

###############################################################################
```

```
# Define the structure A of the data. Pixels connected to their neighbors.
connectivity = grid_to_graph(*lena.shape)

###############################################################################
# Compute clustering
print "Compute structured hierarchical clustering..."
st = time.time()
n_clusters = 15 # number of regions
ward = Ward(n_clusters=n_clusters).fit(X, connectivity=connectivity)
label = np.reshape(ward.labels_, mask.shape)
print "Elaspsed time: ", time.time() - st
print "Number of pixels: ", label.size
print "Number of clusters: ", np.unique(label).size

###############################################################################
# Plot the results on an image
pl.figure(figsize=(5, 5))
pl.imshow(lena, cmap=pl.cm.gray)
for l in range(n_clusters):
    pl.contour(label == l, contours=1,
            colors=[pl.cm.spectral(l/float(n_clusters)), ])
pl.xticks(())
pl.yticks(())
pl.show()
```

A demo of the mean-shift clustering algorithm

Reference: K. Funkunaga and L.D. Hosteler, "The Estimation of the Gradient of a Density Function, with Applications in Pattern Recognition"



Python source code: `plot_mean_shift.py`

```
print __doc__

import numpy as np
from scikits.learn.cluster import MeanShift, estimate_bandwidth

###############################################################################
# Generate sample data
np.random.seed(0)

n_points_per_cluster = 250
n_clusters = 3
n_points = n_points_per_cluster*n_clusters
means = np.array([[1,1],[-1,-1],[1,-1]])
std = .6
clustMed = []

X = np.empty((0, 2))
for i in range(n_clusters):
    X = np.r_[X, means[i] + std * np.random.randn(n_points_per_cluster, 2)]

###############################################################################
# Compute clustering with MeanShift
bandwidth = estimate_bandwidth(X, quantile=0.3)
ms = MeanShift(bandwidth=bandwidth)
```

```
ms.fit(X)
labels = ms.labels_
cluster_centers = ms.cluster_centers_

labels_unique = np.unique(labels)
n_clusters_ = len(labels_unique)

print "number of estimated clusters : %d" % n_clusters_

##############################################################################
# Plot result
import pylab as pl
from itertools import cycle

pl.figure(1)
pl.clf()

colors = cycle('bgrcmykbgrcmykbgrcmykbgrcmyk')
for k, col in zip(range(n_clusters_), colors):
    my_members = labels == k
    cluster_center = cluster_centers[k]
    pl.plot(X[my_members,0], X[my_members,1], col+'.')
    pl.plot(cluster_center[0], cluster_center[1], 'o', markerfacecolor=col,
                                    markeredgecolor='k', markersize=14)
pl.title('Estimated number of clusters: %d' % n_clusters_)
pl.show()
```

Spectral clustering for image segmentation

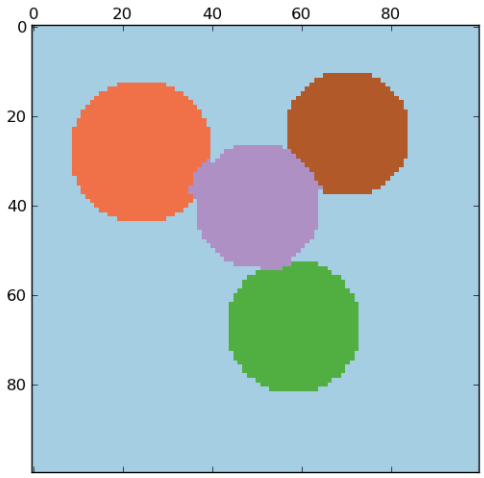
In this example, an image with connected circles is generated and spectral clustering is used to separate the circles.

In these settings, the spectral clustering approach solves the problem know as 'normalized graph cuts': the image is seen as a graph of connected voxels, and the spectral clustering algorithm amounts to choosing graph cuts defining regions while minimizing the ratio of the gradient along the cut, and the volume of the region.

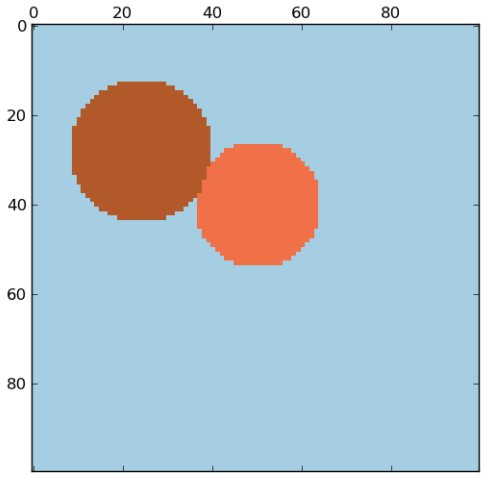
As the algorithm tries to balance the volume (ie balance the region sizes), if we take circles with different sizes, the segmentation fails.

In addition, as there is no useful information in the intensity of the image, or its gradient, we choose to perform the spectral clustering on a graph that is only weakly informed by the gradient. This is close to performing a Voronoi partition of the graph.

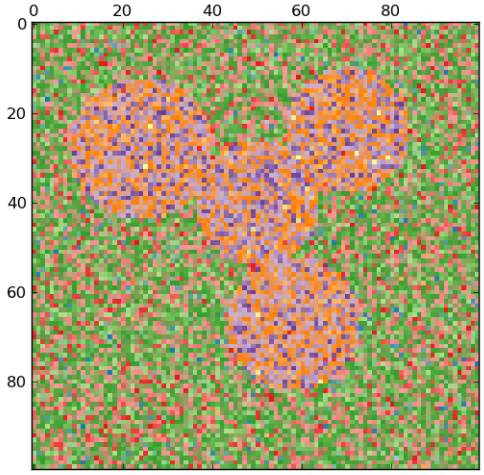
In addition, we use the mask of the objects to restrict the graph to the outline of the objects. In this example, we are interested in separating the objects one from the other, and not from the background.

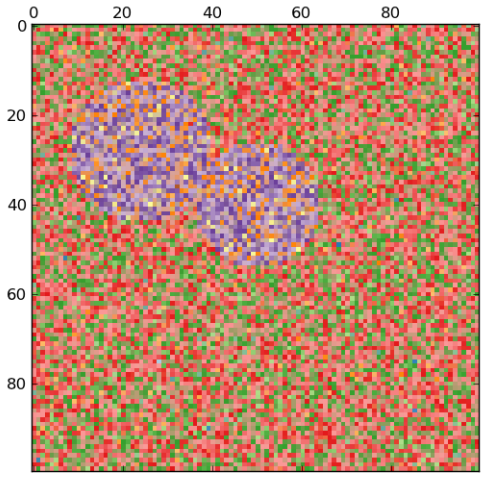

0
20
40
60
80
0
20
40
60
80

-


0
20
40
60
80
0
20
40
60
80

-



- 

Python source code: `plot_segmentation_toy.py`

```
print __doc__

# Authors:  Emmanuelle Gouillart <emmanuelle.gouillart@normalesup.org>
#           Gael Varoquaux <gael.varoquaux@normalesup.org>
# License: BSD

import numpy as np
import pylab as pl

from scikits.learn.feature_extraction import image
from scikits.learn.cluster import spectral_clustering

################################################################################
l = 100
x, y = np.indices((l, l))
```

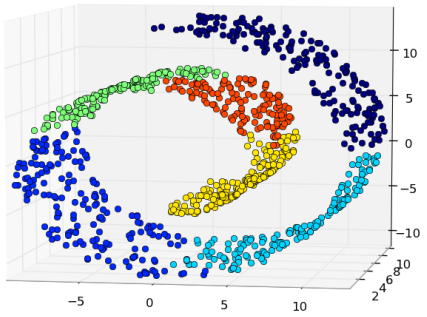
```
center1 = (28, 24)
center2 = (40, 50)
center3 = (67, 58)
center4 = (24, 70)

radius1, radius2, radius3, radius4 = 16, 14, 15, 14

circle1 = (x - center1[0])**2 + (y - center1[1])**2 < radius1**2
circle2 = (x - center2[0])**2 + (y - center2[1])**2 < radius2**2
circle3 = (x - center3[0])**2 + (y - center3[1])**2 < radius3**2
circle4 = (x - center4[0])**2 + (y - center4[1])**2 < radius4**2

##############################################################################
# 4 circles
img = circle1 + circle2 + circle3 + circle4
mask = img.astype(bool)
img = img.astype(float)

img += 1 + 0.2*np.random.randn(*img.shape)

# Convert the image into a graph with the value of the gradient on the
# edges.
graph = image.img_to_graph(img, mask=mask)

# Take a decreasing function of the gradient: we take it weakly
# dependant from the gradient the segmentation is close to a voronoi
graph.data = np.exp(-graph.data/graph.data.std())

labels = spectral_clustering(graph, k=4)
label_im = -np.ones(mask.shape)
label_im[mask] = labels

pl.matshow(img)
pl.matshow(label_im)

##############################################################################
# 2 circles
img = circle1 + circle2
mask = img.astype(bool)
img = img.astype(float)

img += 1 + 0.2*np.random.randn(*img.shape)

graph = image.img_to_graph(img, mask=mask)
graph.data = np.exp(-graph.data/graph.data.std())

labels = spectral_clustering(graph, k=2)
label_im = -np.ones(mask.shape)
label_im[mask] = labels

pl.matshow(img)
pl.matshow(label_im)

pl.show()
```

Hierarchical clustering: structured vs unstructured ward

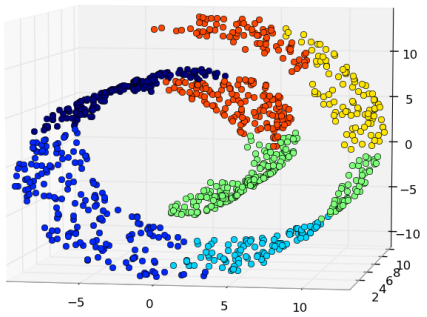
Example builds a swiss roll dataset and runs *Hierarchical clustering* on their position.

In a first step, the hierarchical clustering without connectivity constraints on structure, solely based on distance, whereas in a second step clustering restricted to the k-Nearest Neighbors graph: it's a hierarchical clustering with structure prior.

Some of the clusters learned without connectivity constraints do not respect the structure of the swiss roll and extend across different folds of the manifolds. On the opposite, when opposing connectivity constraints, the clusters form a nice parcellation of the swiss roll.



-



-

Python source code: `plot_ward_structured_vs_unstructured.py`

```
# Authors : Vincent Michel, 2010
#           Alexandre Gramfort, 2010
#           Gael Varoquaux, 2010
# License: BSD

print __doc__

import time as time
import numpy as np
import pylab as pl
import mpl_toolkits.mplot3d.axes3d as p3
from scikits.learn.cluster import Ward
from scikits.learn.datasets.samples_generator import swiss_roll
```

```
###############################################################################
# Generate data (swiss roll dataset)
n_samples = 1000
noise = 0.05
X, _ = swiss_roll(n_samples, noise)
# Make it thinner
X[:, 1] *= .5

###############################################################################
# Compute clustering
print "Compute unstructured hierarchical clustering..."
st = time.time()
ward = Ward(n_clusters=6).fit(X)
label = ward.labels_
print "Elapsed time: ", time.time() - st
print "Number of points: ", label.size

###############################################################################
# Plot result
fig = pl.figure()
ax = p3.Axes3D(fig)
ax.view_init(7, -80)
for l in np.unique(label):
    ax.plot3D(X[label == l, 0], X[label == l, 1], X[label == l, 2],
              'o', color=pl.cm.jet(np.float(l) / np.max(label + 1)))
pl.title('Without connectivity constraints')


###############################################################################
# Define the structure A of the data. Here a 10 nearest neighbors
from scikits.learn.neighbors import kneighbors_graph
connectivity = kneighbors_graph(X, n_neighbors=10)

###############################################################################
# Compute clustering
print "Compute structured hierarchical clustering..."
st = time.time()
ward = Ward(n_clusters=6).fit(X, connectivity=connectivity)
label = ward.labels_
print "Elapsed time: ", time.time() - st
print "Number of points: ", label.size

###############################################################################
# Plot result
fig = pl.figure()
ax = p3.Axes3D(fig)
ax.view_init(7, -80)
for l in np.unique(label):
    ax.plot3D(X[label == l, 0], X[label == l, 1], X[label == l, 2],
              'o', color=pl.cm.jet(float(l) / np.max(label + 1)))
pl.title('With connectivity constraints')

pl.show()
```

2.1.4 Covariance estimation

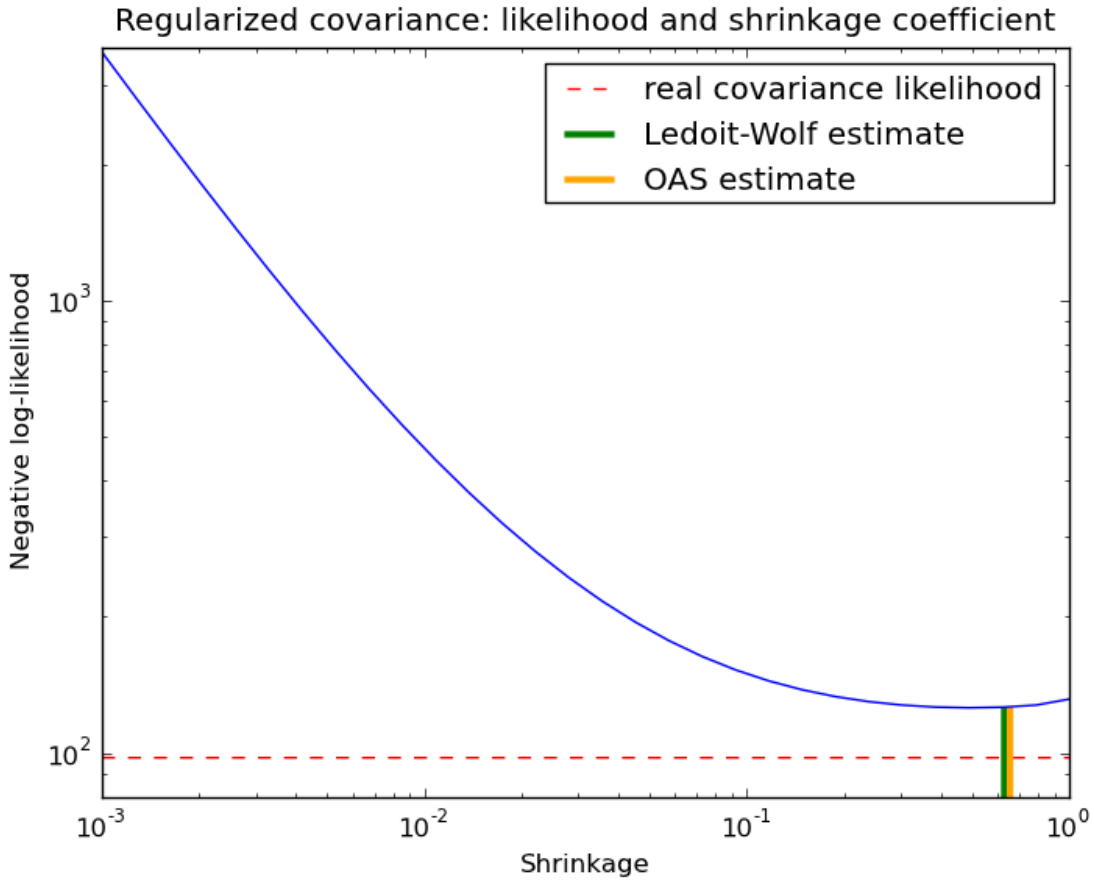
Examples concerning the *scikits.learn.covariance* package.

Ledoit-Wolf vs Covariance simple estimation

The usual covariance maximum likelihood estimate can be regularized using shrinkage. Ledoit and Wolf proposed a close formula to compute the asymptotical optimal shrinkage parameter (minimizing a MSE criterion), yielding the Ledoit-Wolf covariance estimate.

Chen et al. proposed an improvement of the Ledoit-Wolf shrinkage parameter, the OAS coefficient, whose convergence is significantly better under the assumption that the data are gaussian.

In this example, we compute the likelihood of unseen data for different values of the shrinkage parameter, highlighting the LW and OAS estimates. The Ledoit-Wolf estimate stays close to the likelihood criterion optimal value, which is an artifact of the method since it is asymptotic and we are working with a small number of observations. The OAS estimate deviates from the likelihood criterion optimal value but better approximate the MSE optimal value, especially for a small number a observations.



Python source code: `plot_covariance_estimation.py`

```
print __doc__

import numpy as np
import pylab as pl
from scipy import linalg

###############################################################################
# Generate sample data
n_features, n_samples = 30, 20
```

```
base_X_train = np.random.normal(size=(n_samples, n_features))
base_X_test = np.random.normal(size=(n_samples, n_features))

# Color samples
coloring_matrix = np.random.normal(size=(n_features, n_features))
X_train = np.dot(base_X_train, coloring_matrix)
X_test = np.dot(base_X_test, coloring_matrix)

##############################################################################
# Compute Ledoit-Wolf and Covariances on a grid of shrinkages

from scikits.learn.covariance import LedoitWolf, OAS, ShrunkCovariance, \
    log_likelihood, empirical_covariance

# Ledoit-Wolf optimal shrinkage coefficient estimate
lw = LedoitWolf()
loglik_lw = lw.fit(X_train, assume_centered=True).score(
    X_test, assume_centered=True)

# OAS coefficient estimate
oa = OAS()
loglik_oa = oa.fit(X_train, assume_centered=True).score(
    X_test, assume_centered=True)

# spanning a range of possible shrinkage coefficient values
shrinkages = np.logspace(-3, 0, 30)
negative_logliks = [-ShrunkCovariance(shrinkage=s).fit(
        X_train, assume_centered=True).score(X_test, assume_centered=True) \
                        for s in shrinkages]

# getting the likelihood under the real model
real_cov = np.dot(coloring_matrix.T, coloring_matrix)
emp_cov = empirical_covariance(X_train)
loglik_real = -log_likelihood(emp_cov, linalg.inv(real_cov))

##############################################################################
# Plot results
pl.figure(-1)
pl.title("Regularized covariance: likelihood and shrinkage coefficient")
pl.xlabel('Shrinkage')
pl.ylabel('Negative log-likelihood')
# range shrinkage curve
pl.loglog(shrinkages, negative_logliks)
# real likelihood reference
pl.hlines(loglik_real, pl.xlim()[0], pl.xlim()[1], color='red',
          label="real covariance likelihood", linestyle='--')
# adjust view
lik_max = np.amax(negative_logliks)
lik_min = np.amin(negative_logliks)
ylim0 = lik_min - 5.*np.log((pl.ylim()[1]-pl.ylim()[0]))
ylim1 = lik_max + 10.*np.log(lik_max-lik_min)
# LW likelihood
pl.vlines(lw.shrinkage_, ylim0, -loglik_lw, color='g',
          linewidth=3, label='Ledoit-Wolf estimate')
# OAS likelihood
pl.vlines(oa.shrinkage_, ylim0, -loglik_oa, color='orange',
          linewidth=3, label='OAS estimate')
```

```
pl.ylim(ylim0, ylim1)
pl.xlim(shrinkages[0], shrinkages[-1])
pl.legend()
pl.show()
```

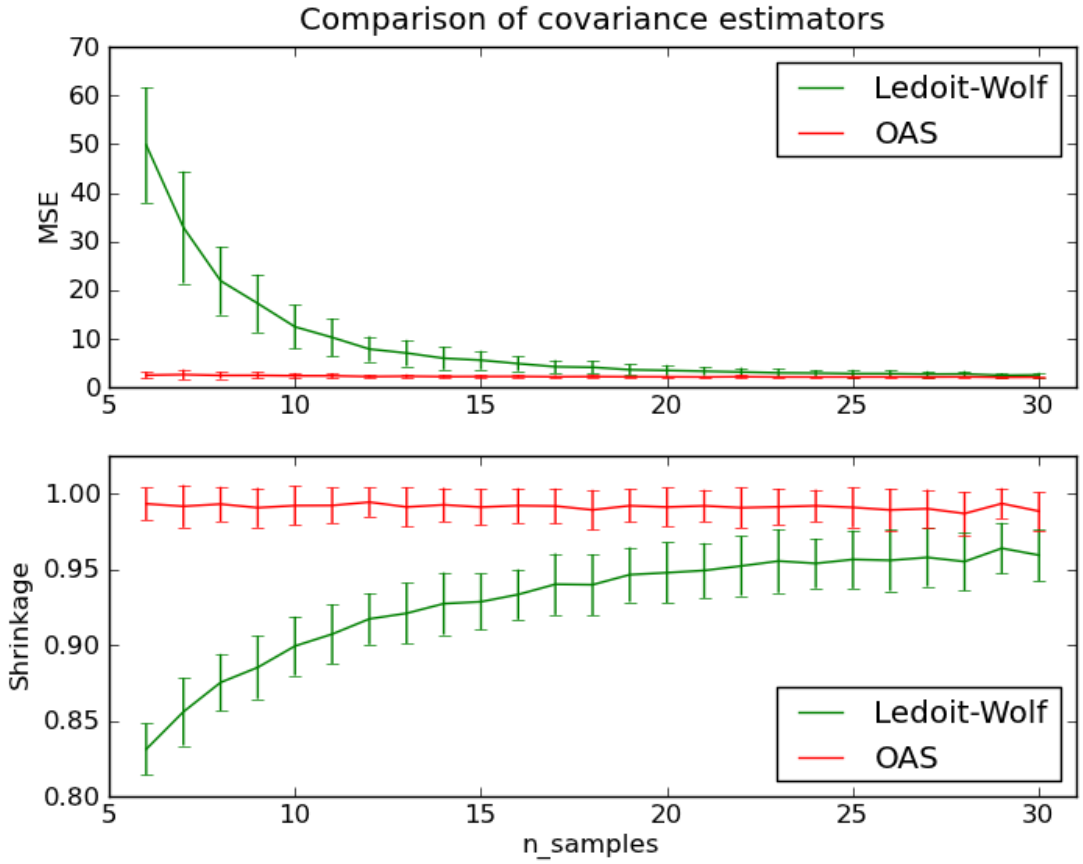
Ledoit-Wolf vs OAS estimation

The usual covariance maximum likelihood estimate can be regularized using shrinkage. Ledoit and Wolf proposed a close formula to compute the asymptotical optimal shrinkage parameter (minimizing a MSE criterion), yielding the Ledoit-Wolf covariance estimate.

Chen et al. proposed an improvement of the Ledoit-Wolf shrinkage parameter, the OAS coefficient, whose convergence is significantly better under the assumption that the data are gaussian.

This example, inspired from Chen's publication [1], shows a comparison of the estimated MSE of the LW and OAS methods, using gaussian distributed data.

[1] "Shrinkage Algorithms for MMSE Covariance Estimation" Chen et al., IEEE Trans. on Sign. Proc., Volume 58, Issue 10, October 2010.



Python source code: `plot_lw_vs_oas.py`

```
print __doc__

import numpy as np
```

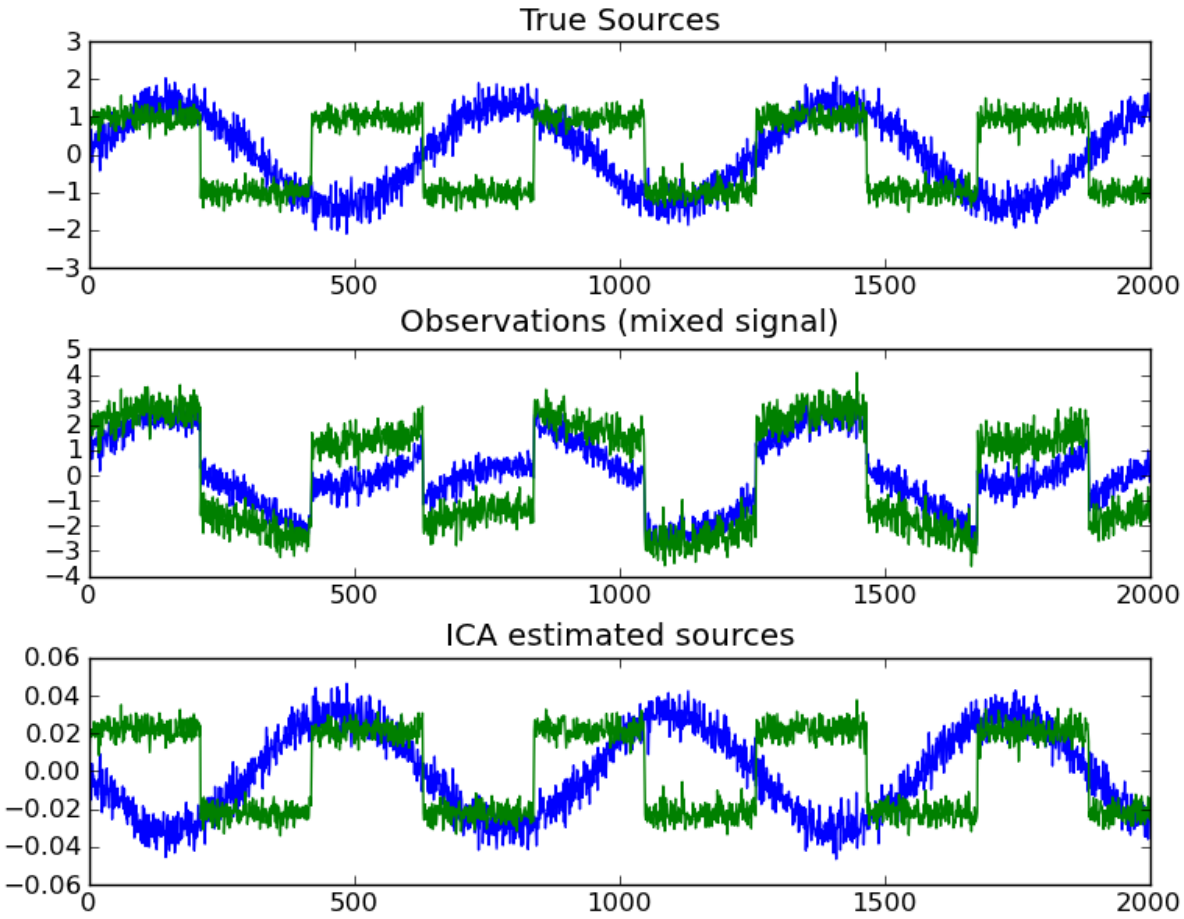
```
import pylab as pl
from scipy.linalg import toeplitz, cholesky

from scikits.learn.covariance import LedoitWolf, OAS

###############################################################################
n_features = 100
# simulation covariance matrix (AR(1) process)
r = 0.1
real_cov = toeplitz(r**np.arange(n_features))
coloring_matrix = cholesky(real_cov)

n_samples_range = np.arange(6, 31, 1)
repeat = 100
lw_mse = np.zeros((n_samples_range.size, repeat))
oa_mse = np.zeros((n_samples_range.size, repeat))
lw_shrinkage = np.zeros((n_samples_range.size, repeat))
oa_shrinkage = np.zeros((n_samples_range.size, repeat))
for i, n_samples in enumerate(n_samples_range):
    for j in range(repeat):
        X = np.dot(
            np.random.normal(size=(n_samples, n_features)), coloring_matrix.T)

        lw = LedoitWolf(store_precision=False)
        lw.fit(X, assume_centered=True)
        lw_mse[i,j] = lw.mse(real_cov)
        lw_shrinkage[i,j] = lw.shrinkage_

        oa = OAS(store_precision=False)
        oa.fit(X, assume_centered=True)
        oa_mse[i,j] = oa.mse(real_cov)
        oa_shrinkage[i,j] = oa.shrinkage_

# plot MSE
pl.subplot(2,1,1)
pl.errorbar(n_samples_range, lw_mse.mean(1), yerr=lw_mse.std(1),
            label='Ledoit-Wolf', color='g')
pl.errorbar(n_samples_range, oa_mse.mean(1), yerr=oa_mse.std(1),
            label='OAS', color='r')
pl.ylabel("MSE")
pl.legend(loc="upper right")
pl.title("Comparison of covariance estimators")
pl.xlim(5, 31)

# plot shrinkage coefficient
pl.subplot(2,1,2)
pl.errorbar(n_samples_range, lw_shrinkage.mean(1), yerr=lw_shrinkage.std(1),
            label='Ledoit-Wolf', color='g')
pl.errorbar(n_samples_range, oa_shrinkage.mean(1), yerr=oa_shrinkage.std(1),
            label='OAS', color='r')
pl.xlabel("n_samples")
pl.ylabel("Shrinkage")
pl.legend(loc="lower right")
pl.ylim(pl.ylim()[0], 1. + (pl.ylim()[1] - pl.ylim()[0])/10.)
pl.xlim(5, 31)

pl.show()
```

2.1.5 Decomposition

Examples concerning the *scikits.learn.decomposition* package.

Blind source separation using FastICA

Independent component analysis (ICA) is used to estimate sources given noisy measurements. Imagine 2 instruments playing simultaneously and 2 microphones recording the mixed signals. ICA is used to recover the sources ie. what is played by each instrument.



Python source code: `plot_ica_blind_source_separation.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn.decomposition import FastICA

###############################################################################
# Generate sample data
np.random.seed(0)
n_samples = 2000
time = np.linspace(0, 10, n_samples)
s1 = np.sin(2*time) # Signal 1 : sinusoidal signal
s2 = np.sign(np.sin(3*time)) # Signal 2 : square signal
```

```
S = np.c_[s1,s2].T
S += 0.2*np.random.normal(size=S.shape) # Add noise

S /= S.std(axis=1)[:,np.newaxis] # Standardize data
# Mix data
A = [[1, 1], [0.5, 2]] # Mixing matrix
X = np.dot(A, S) # Generate observations
# Compute ICA
ica = FastICA()
S_ = ica.fit(X).transform(X) # Get the estimated sources
A_ = ica.get_mixing_matrix() # Get estimated mixing matrix

assert np.allclose(X, np.dot(A_, S_))

###############################################################################
# Plot results
pl.figure()
pl.subplot(3, 1, 1)
pl.plot(S.T)
pl.title('True Sources')
pl.subplot(3, 1, 2)
pl.plot(X.T)
pl.title('Observations (mixed signal)')
pl.subplot(3, 1, 3)
pl.plot(S_.T)
pl.title('ICA estimated sources')
pl.subplots_adjust(0.09, 0.04, 0.94, 0.94, 0.26, 0.36)
pl.show()
```

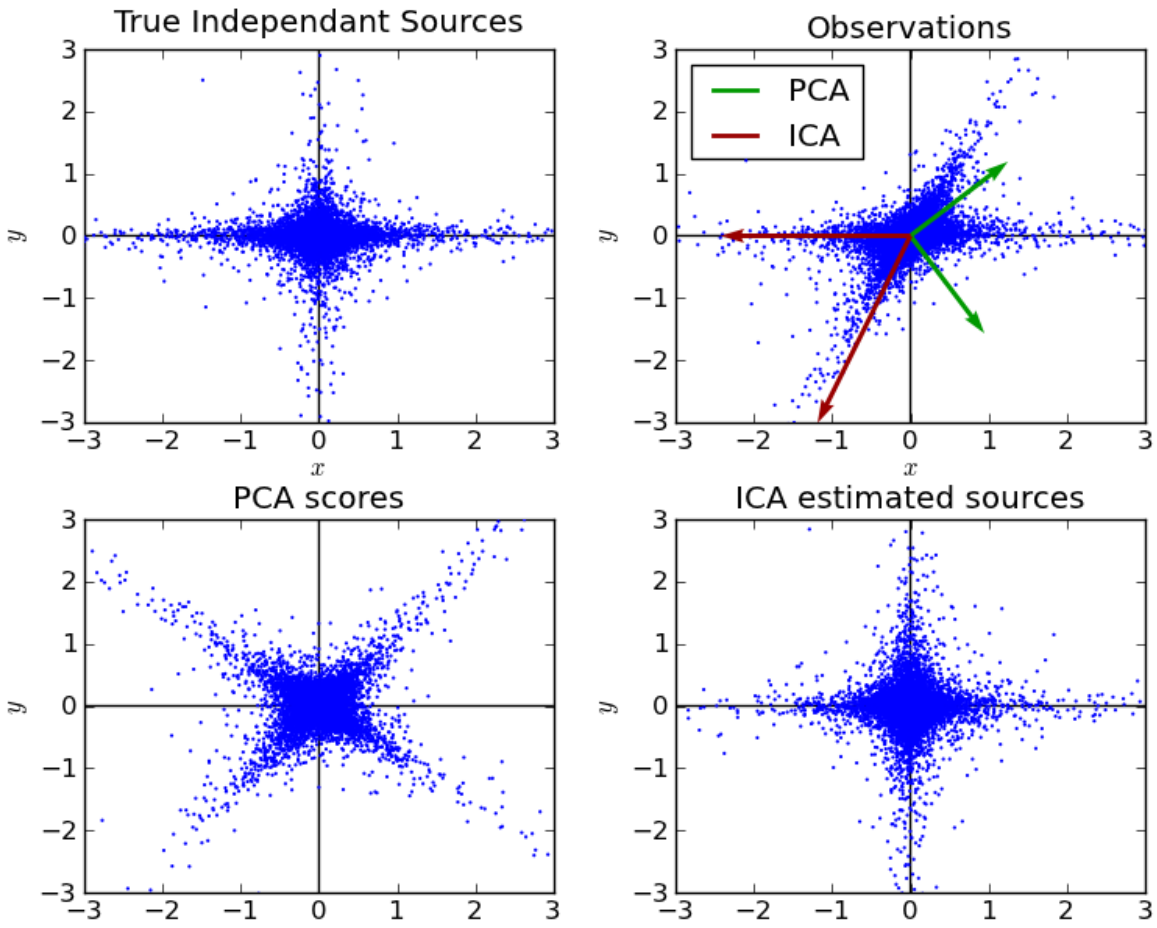
FastICA on 2D point clouds

Illustrate visually the results of *Independent component analysis (ICA)* vs *Principal component analysis (PCA)* in the feature space.

Representing ICA in the feature space gives the view of 'geometric ICA': ICA is an algorithm that finds directions in the feature space corresponding to projections with high non-Gaussianity. These directions need not be orthogonal in the original feature space, but they are orthogonal in the whitened feature space, in which all directions correspond to the same variance.

PCA, on the other hand, finds orthogonal directions in the raw feature space that correspond to directions accounting for maximum variance.

Here we simulate independent sources using a highly non-Gaussian process, 2 student T with a low number of degrees of freedom (top left figure). We mix them to create observations (top right figure). In this raw observation space, directions identified by PCA are represented by green vectors. We represent the signal in the PCA space, after whitening by the variance corresponding to the PCA vectors (lower left). Running ICA corresponds to finding a rotation in this space to identify the directions of largest non-Gaussianity (lower right).



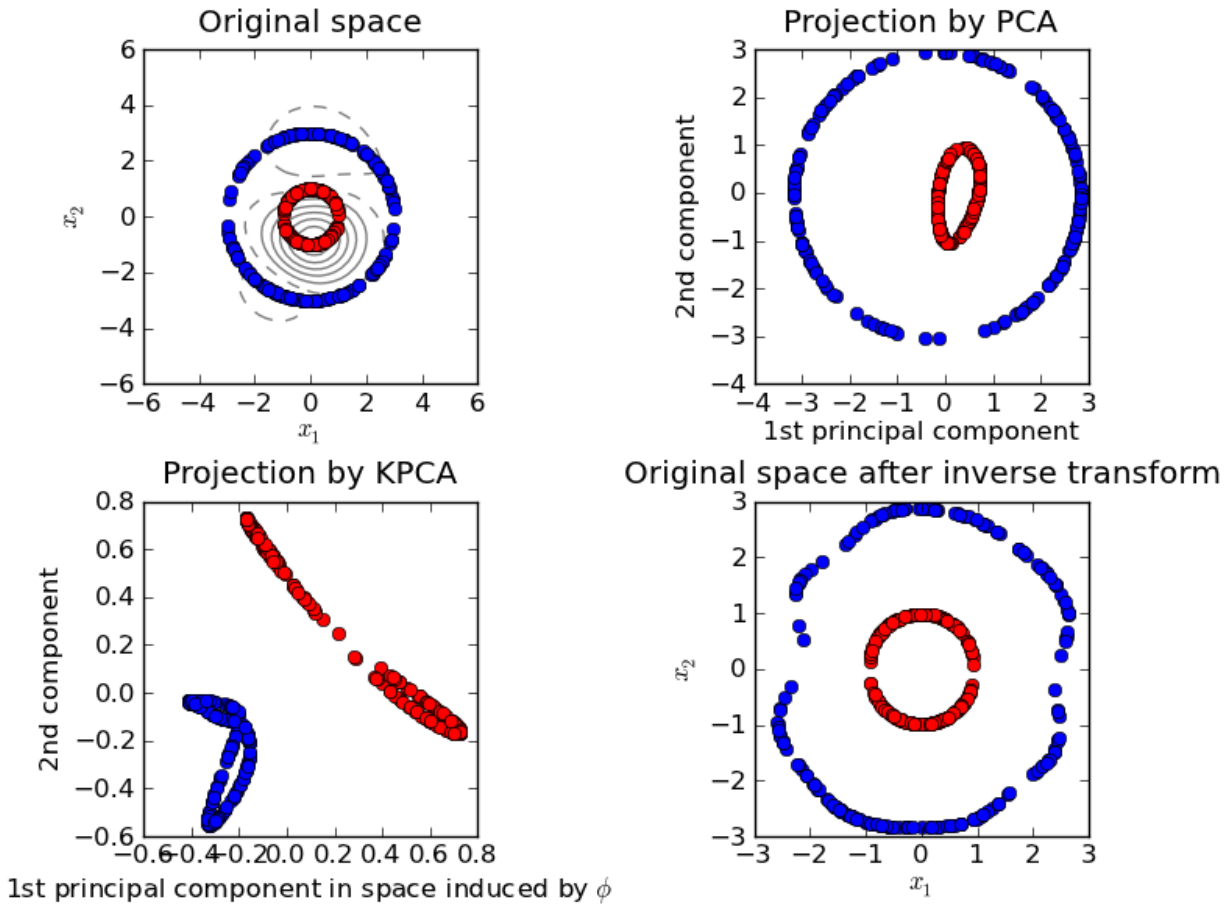
Python source code: `plot_ica_vs_pca.py`

```
print __doc__

# Authors: Alexandre Gramfort, Gael Varoquaux
# License: BSD

import numpy as np
import pylab as pl

from scikits.learn.decomposition import PCA, FastICA

###############################################################################
# Generate sample data
S = np.random.standard_t(1.5, size=(2, 10000))
S[0] *= 2.

# Mix data
A = [[1, 1], [0, 2]]  # Mixing matrix

X = np.dot(A, S)  # Generate observations

pca = PCA()
S_pca_ = pca.fit(X.T).transform(X.T).T

ica = FastICA()
```

```
S_ica_ = ica.fit(X).transform(X)  # Estimate the sources

S_ica_ /= S_ica_.std(axis=1)[:, np.newaxis]


###############################################################################
# Plot results

def plot_samples(S, axis_list=None):
    pl.scatter(S[0], S[1], s=2, marker='o', linewidths=0, zorder=10)
    if axis_list is not None:
        colors = [(0, 0.6, 0), (0.6, 0, 0)]
        for color, axis in zip(colors, axis_list):
            axis /= axis.std()
            x_axis, y_axis = axis
            # Trick to get legend to work
            pl.plot(0.1 * x_axis, 0.1 * y_axis, linewidth=2, color=color)
            # pl.quiver(x_axis, y_axis, x_axis, y_axis, zorder=11, width=0.01,
            pl.quiver(0, 0, x_axis, y_axis, zorder=11, width=0.01,
                      scale=6, color=color)

    pl.hlines(0, -3, 3)
    pl.vlines(0, -3, 3)
    pl.xlim(-3, 3)
    pl.ylim(-3, 3)
    pl.xlabel('$x$')
    pl.ylabel('$y$')

pl.subplot(2, 2, 1)
plot_samples(S / S.std())
pl.title('True Independant Sources')

axis_list = [pca.components_.T, ica.get_mixing_matrix()]
pl.subplot(2, 2, 2)
plot_samples(X / np.std(X), axis_list=axis_list)
pl.legend(['PCA', 'ICA'], loc='upper left')
pl.title('Observations')

pl.subplot(2, 2, 3)
plot_samples(S_pca_ / np.std(S_pca_, axis=-1)[:, np.newaxis])
pl.title('PCA scores')

pl.subplot(2, 2, 4)
plot_samples(S_ica_ / np.std(S_ica_))
pl.title('ICA estimated sources')

pl.subplots_adjust(0.09, 0.04, 0.94, 0.94, 0.26, 0.26)

pl.show()
```

Kernel PCA

This example shows that Kernel PCA is able to find a projection of the data that makes data linearly separable.



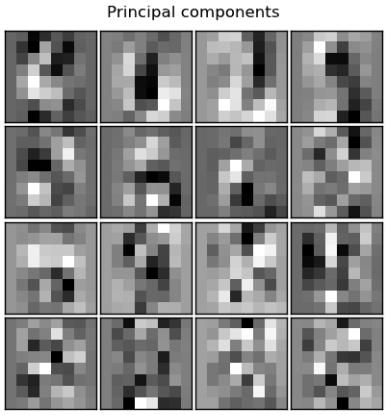
Python source code: `plot_kernel_pca.py`

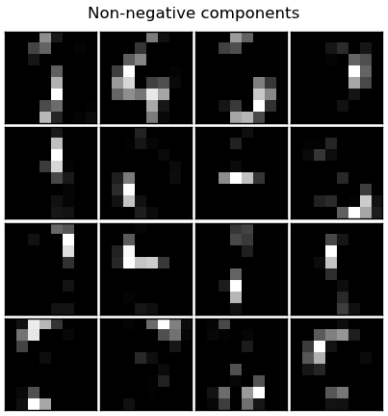
```
print __doc__

# Authors: Mathieu Blondel
# License: BSD

import numpy as np
import pylab as pl

from scikits.learn.decomposition import PCA, KernelPCA

np.random.seed(0)


def genenerate_rings(n_samples=200):
    x_red = np.random.random((n_samples,)) * 2 - 1
    signs_red = np.sign(np.random.random(x_red.shape) - 0.5)
    y_red = np.sqrt(np.abs(x_red ** 2 - 1)) * signs_red

    x_blue = np.random.random((n_samples,)) * 6 - 3
    signs_blue = np.sign(np.random.random(x_blue.shape) - 0.5)
    y_blue = np.sqrt(np.abs(x_blue ** 2 - 9)) * signs_blue

    return np.hstack(([x_red, y_red], [x_blue, y_blue])).T
```

```
def generate_clusters(n_samples=200):
    mean1 = np.array([0, 2])
    mean2 = np.array([2, 0])
    cov = np.array([[2.0, 1.0], [1.0, 2.0]])
    X_red = np.random.multivariate_normal(mean1, cov, n_samples)
    X_blue = np.random.multivariate_normal(mean2, cov, n_samples)
    return np.vstack((X_red, X_blue))

X = genenerate_rings()
#X = generate_clusters()

kpca = KernelPCA(kernel="rbf", fit_inverse_transform=True)
X_kpca = kpca.fit_transform(X)
X_back = kpca.inverse_transform(X_kpca)
pca = PCA()
X_pca = pca.fit_transform(X)

# Plot results

pl.figure()
pl.subplot(2, 2, 1, aspect='equal')
pl.title("Original space")
pl.plot(X[:200, 0], X[:200, 1], "ro")
pl.plot(X[200:, 0], X[200:, 1], "bo")
pl.xlabel("$x_1$")
pl.ylabel("$x_2$")

X1, X2 = np.meshgrid(np.linspace(-6, 6, 50), np.linspace(-6, 6, 50))
X_grid = np.array([np.ravel(X1), np.ravel(X2)]).T
# projection on the first principal component (in the phi space)
Z_grid = kpca.transform(X_grid)[:, 0].reshape(X1.shape)
pl.contour(X1, X2, Z_grid, colors='grey', linewidths=1, origin='lower')

pl.subplot(2, 2, 2, aspect='equal')
pl.plot(X_kpca[:200, 0], X_pca[:200, 1], "ro")
pl.plot(X_pca[200:, 0], X_pca[200:, 1], "bo")
pl.title("Projection by PCA")
pl.xlabel("1st principal component")
pl.ylabel("2nd component")

pl.subplot(2, 2, 3, aspect='equal')
pl.plot(X_kpca[:200, 0], X_kpca[:200, 1], "ro")
pl.plot(X_kpca[200:, 0], X_kpca[200:, 1], "bo")
pl.title("Projection by KPCA")
pl.xlabel("1st principal component in space induced by $\phi$")
pl.ylabel("2nd component")

pl.subplot(2, 2, 4, aspect='equal')
pl.plot(X_back[:200, 0], X_back[:200, 1], "ro")
pl.plot(X_back[200:, 0], X_back[200:, 1], "bo")
pl.title("Original space after inverse transform")
pl.xlabel("$x_1$")
pl.ylabel("$x_2$")

pl.subplots_adjust(0.02, 0.10, 0.98, 0.94, 0.04, 0.35)

pl.show()
```

NMF for digits feature extraction

Non-negative matrix factorization (NMF) with sparseness enforced in the components, in comparison with PCA for feature extraction.

- 

- 

Python source code: `plot_nmf.py`

```
print __doc__

from time import time
import logging
import pylab as pl

from scikits.learn.decomposition import RandomizedPCA, NMF
from scikits.learn import datasets


# Display progress logs on stdout
logging.basicConfig(level=logging.INFO,
                    format='%(asctime)s %(levelname)s %(message)s')

digits = datasets.load_digits()

# reshape the data using the traditional (n_samples, n_features) shape
n_samples = len(digits.images)
X = digits.images.reshape((n_samples, -1))
n_features = X.shape[1]
```

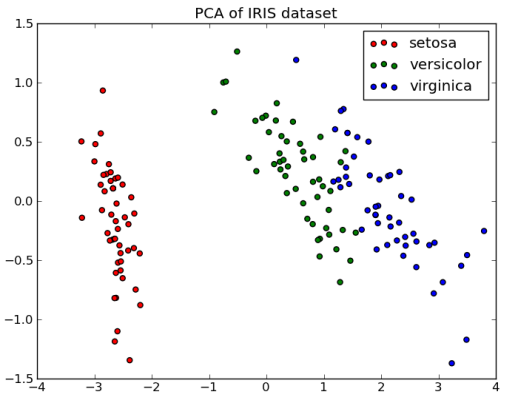
```
n_components = 16

###############################################################################
# Compute a PCA (eigendigits) on the digit dataset

print "Extracting the top %d eigendigits from %d images" % (
    n_components, X.shape[0])
t0 = time()
pca = RandomizedPCA(n_components=n_components, whiten=True).fit(X)
print "done in %0.3fs" % (time() - t0)

eigendigits = pca.components_

###############################################################################
# Compute a NMF on the digit dataset

print "Extracting %d non-negative features from %d images" % (
    n_components, X.shape[0])
t0 = time()
nmf = NMF(n_components=n_components, init='nndsvd', beta=5, tol=1e-2,
          sparseness="components").fit(X)
print "done in %0.3fs" % (time() - t0)

nmfdigits = nmf.components_

###############################################################################
# Plot the results

n_row, n_col = 4, 4

f1 = pl.figure(figsize=(1. * n_col, 1.13 * n_row))
f1.text(.5, .95, 'Principal components', horizontalalignment='center')
for i in range(n_row * n_col):
    pl.subplot(n_row, n_col, i + 1)
    pl.imshow(eigendigits[i].reshape((8, 8)), cmap=pl.cm.gray,
              interpolation='nearest')
    pl.xticks(())
    pl.yticks(())
pl.subplots_adjust(0.01, 0.05, 0.99, 0.93, 0.04, 0.)

f2 = pl.figure(figsize=(1. * n_col, 1.13 * n_row))
f2.text(.5, .95, 'Non-negative components', horizontalalignment='center')
for i in range(n_row * n_col):
    pl.subplot(n_row, n_col, i + 1)
    pl.imshow(nmfdigits[i].reshape((8, 8)), cmap=pl.cm.gray,
              interpolation='nearest')
    pl.xticks(())
    pl.yticks(())
pl.subplots_adjust(0.01, 0.05, 0.99, 0.93, 0.04, 0.)
pl.show()
```

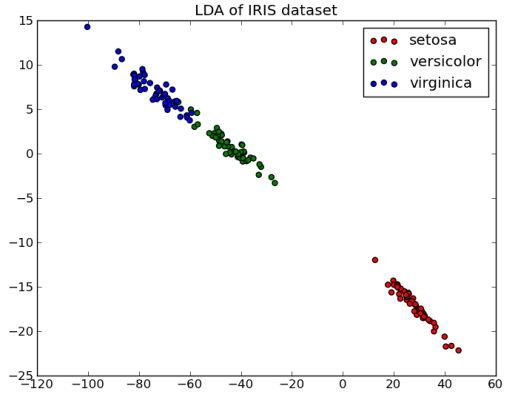
PCA 2D projection of Iris dataset

The Iris dataset represents 3 kind of Iris flowers (Setosa, Versicolour and Virginica) with 4 attributes: sepal length, sepal width, petal length and petal width.

Principal Component Analysis (PCA) applied to this data identifies the combination of attributes (principal compo-

nents, or directions in the feature space) that account for the most variance in the data. Here we plot the different samples on the 2 first principal components.



- 

Python source code: `plot_pca_vs_lda.py`

```
print __doc__

import pylab as pl

from scikits.learn import datasets
from scikits.learn.decomposition import PCA
from scikits.learn.lda import LDA

iris = datasets.load_iris()

X = iris.data
y = iris.target
target_names = iris.target_names

pca = PCA(n_components=2)
X_r = pca.fit(X).transform(X)

lda = LDA(n_components=2)
X_r2 = lda.fit(X, y).transform(X)

# Percentage of variance explained for each components
print 'explained variance ratio (first two components):', \
```

```
    pca.explained_variance_ratio_

pl.figure()
for c, i, target_name in zip("rgb", [0, 1, 2], target_names):
    pl.scatter(X_r[y == i, 0], X_r[y == i, 1], c=c, label=target_name)
pl.legend()
pl.title('PCA of IRIS dataset')

pl.figure()
for c, i, target_name in zip("rgb", [0, 1, 2], target_names):
    pl.scatter(X_r2[y == i, 0], X_r2[y == i, 1], c=c, label=target_name)
pl.legend()
pl.title('LDA of IRIS dataset')

pl.show()
```

2.1.6 Gaussian Process for Machine Learning

Examples concerning the *scikits.learn.gaussian_process* package.

Gaussian Processes regression: goodness-of-fit on the 'diabetes' dataset

This example consists in fitting a Gaussian Process model onto the diabetes dataset.

The correlation parameters are determined by means of maximum likelihood estimation (MLE). An anisotropic squared exponential correlation model with a constant regression model are assumed. We also used a nugget = 1e-2 in order to account for the (strong) noise in the targets.

We compute then compute a cross-validation estimate of the coefficient of determination (R2) without reperforming MLE, using the set of correlation parameters found on the whole dataset.

Python source code: `gp_diabetes_dataset.py`

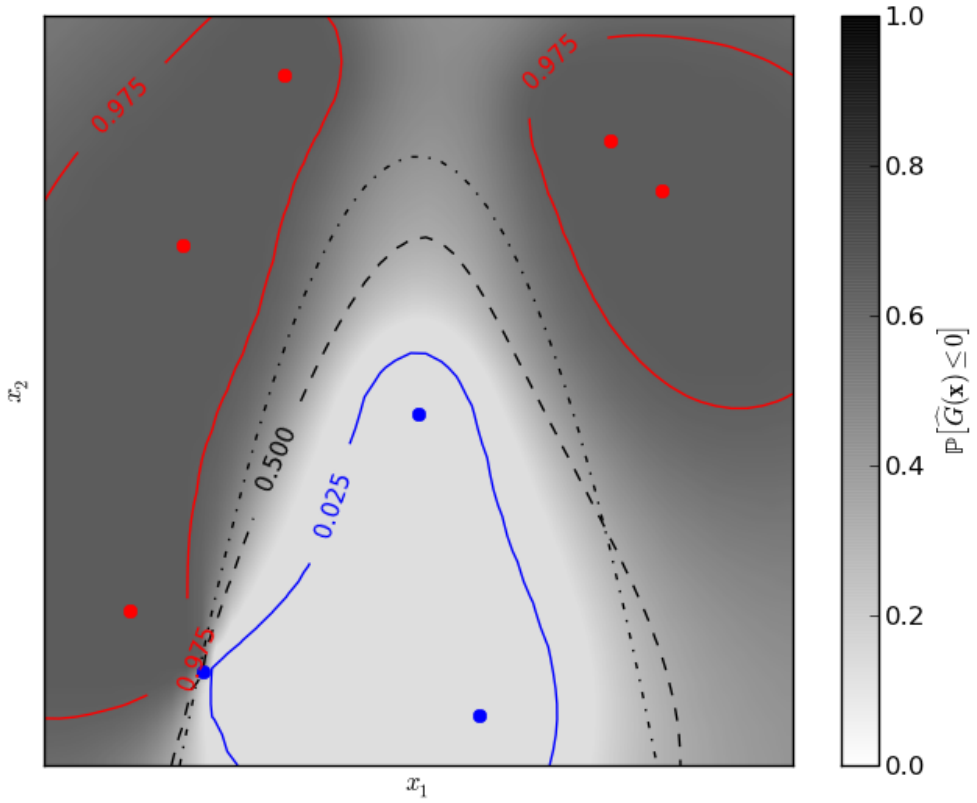
```
print __doc__

# Author: Vincent Dubourg <vincent.dubourg@gmail.com>
# License: BSD style

from scikits.learn import datasets
from scikits.learn.gaussian_process import GaussianProcess
from scikits.learn.cross_val import cross_val_score, KFold

# Load the dataset from scikits' data sets
diabetes = datasets.load_diabetes()
X, y = diabetes.data, diabetes.target

# Instanciate a GP model
gp = GaussianProcess(regr='constant', corr='absolute_exponential',
                     theta0=[1e-4] * 10, thetaL=[1e-12] * 10,
                     thetaU=[1e-2] * 10, nugget=1e-2, optimizer='Welch')

# Fit the GP model to the data performing maximum likelihood estimation
gp.fit(X, y)

# Deactivate maximum likelihood estimation for the cross-validation loop
gp.theta0 = gp.theta # Given correlation parameter = MLE
```

```
gp.thetaL, gp.thetaU = None, None # None bounds deactivate MLE

# Perform a cross-validation estimate of the coefficient of determination using
# the cross_val module using all CPUs available on the machine
K = 20 # folds
R2 = cross_val_score(gp, X, y=y, cv=KFold(y.size, K), n_jobs=-1).mean()
print("The %d-Folds estimate of the coefficient of determination is R2 = %s"
    % (K, R2))
```

Gaussian Processes classification example: exploiting the probabilistic output

A two-dimensional regression exercise with a post-processing allowing for probabilistic classification thanks to the Gaussian property of the prediction.

The figure illustrates the probability that the prediction is negative with respect to the remaining uncertainty in the prediction. The red and blue lines corresponds to the 95% confidence interval on the prediction of the zero level set.



Python source code: `plot_gp_probabilistic_classification_after_regression.py`

```
print __doc__

# Author: Vincent Dubourg <vincent.dubourg@gmail.com>
# License: BSD style

import numpy as np
```

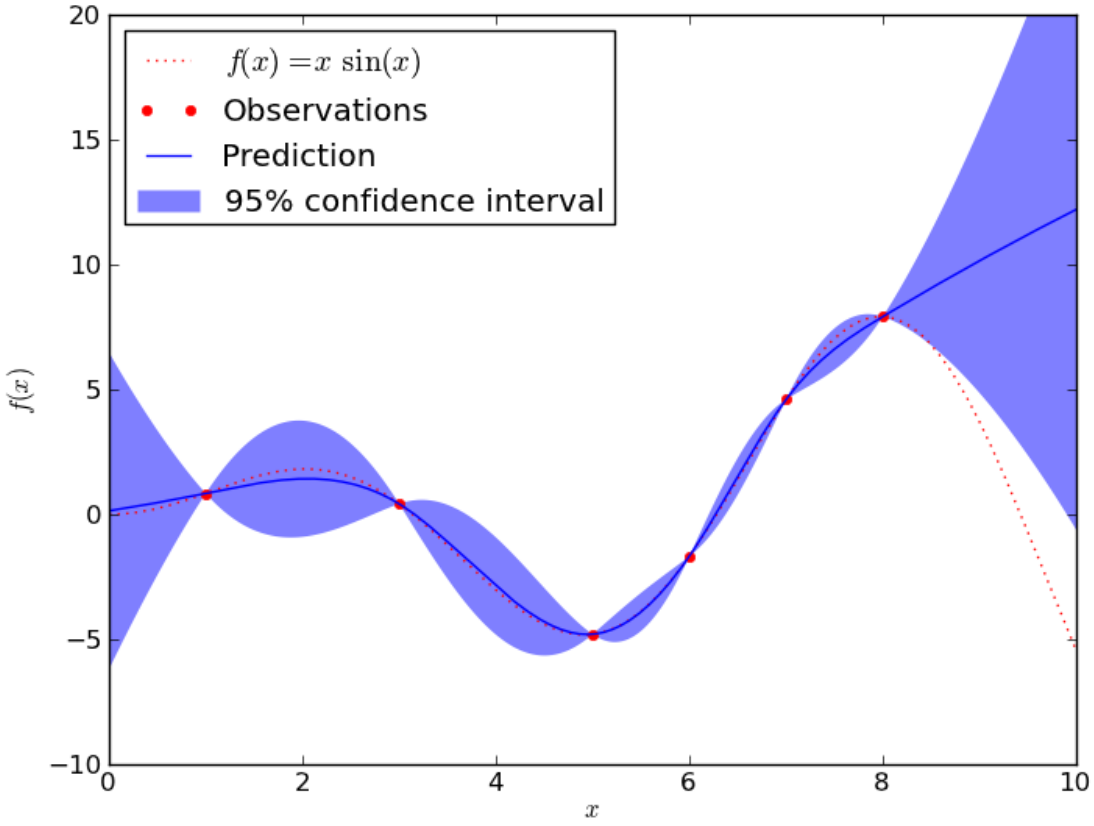
```
from scipy import stats
from scikits.learn.gaussian_process import GaussianProcess
from matplotlib import pyplot as pl
from matplotlib import cm

# Standard normal distribution functions
phi = stats.distributions.norm().pdf
PHI = stats.distributions.norm().cdf
PHIinv = stats.distributions.norm().ppf

# A few constants
lim = 8


def g(x):
    """The function to predict (classification will then consist in predicting
    whether g(x) <= 0 or not)"""
    return 5. - x[:, 1] - .5 * x[:, 0] ** 2.

# Design of experiments
X = np.array([[-4.61611719, -6.00099547],
              [4.10469096, 5.32782448],
              [0.00000000, -0.50000000],
              [-6.17289014, -4.6984743],
              [1.3109306, -6.93271427],
              [-5.03823144, 3.10584743],
              [-2.87600388, 6.74310541],
              [5.21301203, 4.26386883]])

# Observations
y = g(X)

# Instanciate and fit Gaussian Process Model
gp = GaussianProcess(theta0=5e-1)

# Don't perform MLE or you'll get a perfect prediction for this simple example!
gp.fit(X, y)

# Evaluate real function, the prediction and its MSE on a grid
res = 50
x1, x2 = np.meshgrid(np.linspace(- lim, lim, res), \
                     np.linspace(- lim, lim, res))
xx = np.vstack([x1.reshape(x1.size), x2.reshape(x2.size)]).T

y_true = g(xx)
y_pred, MSE = gp.predict(xx, eval_MSE=True)
sigma = np.sqrt(MSE)
y_true = y_true.reshape((res, res))
y_pred = y_pred.reshape((res, res))
sigma = sigma.reshape((res, res))
k = PHIinv(.975)

# Plot the probabilistic classification iso-values using the Gaussian property
# of the prediction
fig = pl.figure(1)
ax = fig.add_subplot(111)
ax.axes.set_aspect('equal')
pl.xticks([])
```

```
pl.yticks([])
ax.set_xticklabels([])
ax.set_yticklabels([])
pl.xlabel('$x_1$')
pl.ylabel('$x_2$')

cax = pl.imshow(np.flipud(PHI(- y_pred / sigma)), cmap=cm.gray_r, alpha=0.8, \
                extent=(- lim, lim, - lim, lim))
norm = pl.matplotlib.colors.Normalize(vmin=0., vmax=0.9)
cb = pl.colorbar(cax, ticks=[0., 0.2, 0.4, 0.6, 0.8, 1.], norm=norm)
cb.set_label('${\\rm \mathbb{P}}\left[\widehat{G}(\mathbf{x}) \leq 0\\right]$')

pl.plot(X[y <= 0, 0], X[y <= 0, 1], 'r.', markersize=12)

pl.plot(X[y > 0, 0], X[y > 0, 1], 'b.', markersize=12)

cs = pl.contour(x1, x2, y_true, [0.], colors='k', \
                linestyles='dashdot')

cs = pl.contour(x1, x2, PHI(- y_pred / sigma), [0.025], colors='b', \
                linestyles='solid')
pl.clabel(cs, fontsize=11)

cs = pl.contour(x1, x2, PHI(- y_pred / sigma), [0.5], colors='k', \
                linestyles='dashed')
pl.clabel(cs, fontsize=11)

cs = pl.contour(x1, x2, PHI(- y_pred / sigma), [0.975], colors='r', \
                linestyles='solid')
pl.clabel(cs, fontsize=11)

pl.show()
```

Gaussian Processes regression: basic introductory example

A simple one-dimensional regression exercise with a cubic correlation model whose parameters are estimated using the maximum likelihood principle.

The figure illustrates the interpolating property of the Gaussian Process model as well as its probabilistic nature in the form of a pointwise 95% confidence interval.



Python source code: `plot_gp_regression.py`

```
print __doc__

# Author: Vincent Dubourg <vincent.dubourg@gmail.com>
# License: BSD style

import numpy as np
from scikits.learn.gaussian_process import GaussianProcess
from matplotlib import pyplot as pl


def f(x):
    """The function to predict."""
    return x * np.sin(x)

# The design of experiments
X = np.atleast_2d([1., 3., 5., 6., 7., 8.]).T

# Observations
y = f(X).ravel()

# Mesh the input space for evaluations of the real function, the prediction and
# its MSE
x = np.atleast_2d(np.linspace(0, 10, 1000)).T
```

```
# Instanciate a Gaussian Process model
gp = GaussianProcess(corr='cubic', theta0=1e-2, thetaL=1e-4, thetaU=1e-1, \
                     random_start=100)

# Fit to data using Maximum Likelihood Estimation of the parameters
gp.fit(X, y)

# Make the prediction on the meshed x-axis (ask for MSE as well)
y_pred, MSE = gp.predict(x, eval_MSE=True)
sigma = np.sqrt(MSE)

# Plot the function, the prediction and the 95% confidence interval based on
# the MSE
fig = pl.figure()
pl.plot(x, f(x), 'r:', label=u'$f(x) = x\,\sin(x)$')
pl.plot(X, y, 'r.', markersize=10, label=u'Observations')
pl.plot(x, y_pred, 'b-', label=u'Prediction')
pl.fill(np.concatenate([x, x[::-1]]), \
        np.concatenate([y_pred - 1.9600 * sigma,
                        (y_pred + 1.9600 * sigma)[::-1]]), \
        alpha=.5, fc='b', ec='None', label='95% confidence interval')
pl.xlabel('$x$')
pl.ylabel('$f(x)$')
pl.ylim(-10, 20)
pl.legend(loc='upper left')

pl.show()
```

2.1.7 Generalized Linear Models

Examples concerning the *scikits.learn.linear_model* package.

Lasso regression example

Python source code: `lasso_and_elasticnet.py`

```
print __doc__

import numpy as np

################################################################################
# generate some sparse data to play with

n_samples, n_features = 50, 200
X = np.random.randn(n_samples, n_features)
coef = 3*np.random.randn(n_features)
coef[10:] = 0 # sparsify coef
y = np.dot(X, coef)

# add noise
y += 0.01*np.random.normal((n_samples,))

# Split data in train set and test set
n_samples = X.shape[0]
X_train, y_train = X[:n_samples/2], y[:n_samples/2]
X_test, y_test = X[n_samples/2:], y[n_samples/2:]
```

```
##############################################################################
# Lasso
from scikits.learn.linear_model import Lasso

alpha = 0.1
lasso = Lasso(alpha=alpha)

y_pred_lasso = lasso.fit(X_train, y_train).predict(X_test)
print lasso
print "r^2 on test data : %f" % (1 - np.linalg.norm(y_test - y_pred_lasso)**2
                                   / np.linalg.norm(y_test)**2)

##############################################################################
# ElasticNet
from scikits.learn.linear_model import ElasticNet

enet = ElasticNet(alpha=alpha, rho=0.7)

y_pred_enet = enet.fit(X_train, y_train).predict(X_test)
print enet
print "r^2 on test data : %f" % (1 - np.linalg.norm(y_test - y_pred_enet)**2
                                   / np.linalg.norm(y_test)**2)
```

Lasso on dense and sparse data

We show that linear_model.Lasso and linear_model.sparse.Lasso provide the same results and that in the case of sparse data linear_model.sparse.Lasso improves the speed.

Python source code: `lasso_dense_vs_sparse_data.py`

```
print __doc__

from time import time
import numpy as np
from scipy import sparse
from scipy import linalg

from scikits.learn.linear_model.sparse import Lasso as SparseLasso
from scikits.learn.linear_model import Lasso as DenseLasso


##############################################################################
# The two Lasso implementations on Dense data
print "--- Dense matrices"

n_samples, n_features = 200, 10000
np.random.seed(0)
y = np.random.randn(n_samples)
X = np.random.randn(n_samples, n_features)

alpha = 1
sparse_lasso = SparseLasso(alpha=alpha, fit_intercept=False)
dense_lasso = DenseLasso(alpha=alpha, fit_intercept=False)

t0 = time()
sparse_lasso.fit(X, y, max_iter=1000)
print "Sparse Lasso done in %fs" % (time() - t0)
```

```
t0 = time()
dense_lasso.fit(X, y, max_iter=1000)
print "Dense Lasso done in %fs" % (time() - t0)

print "Distance between coefficients : %s" % linalg.norm(sparse_lasso.coef_
                                                         - dense_lasso.coef_)

##############################################################################
# The two Lasso implementations on Sparse data
print "--- Sparse matrices"

Xs = X.copy()
Xs[Xs < 2.5] = 0.0
Xs = sparse.coo_matrix(Xs)
Xs = Xs.tocsc()

print "Matrix density : %s %%" % (Xs.nnz / float(X.size) * 100)

alpha = 0.1
sparse_lasso = SparseLasso(alpha=alpha, fit_intercept=False)
dense_lasso = DenseLasso(alpha=alpha, fit_intercept=False)

t0 = time()
sparse_lasso.fit(Xs, y, max_iter=1000)
print "Sparse Lasso done in %fs" % (time() - t0)

t0 = time()
dense_lasso.fit(Xs.todense(), y, max_iter=1000)
print "Dense Lasso done in %fs" % (time() - t0)

print "Distance between coefficients : %s" % linalg.norm(sparse_lasso.coef_
                                                         - dense_lasso.coef_)
```

Lasso parameter estimation with path and cross-validation

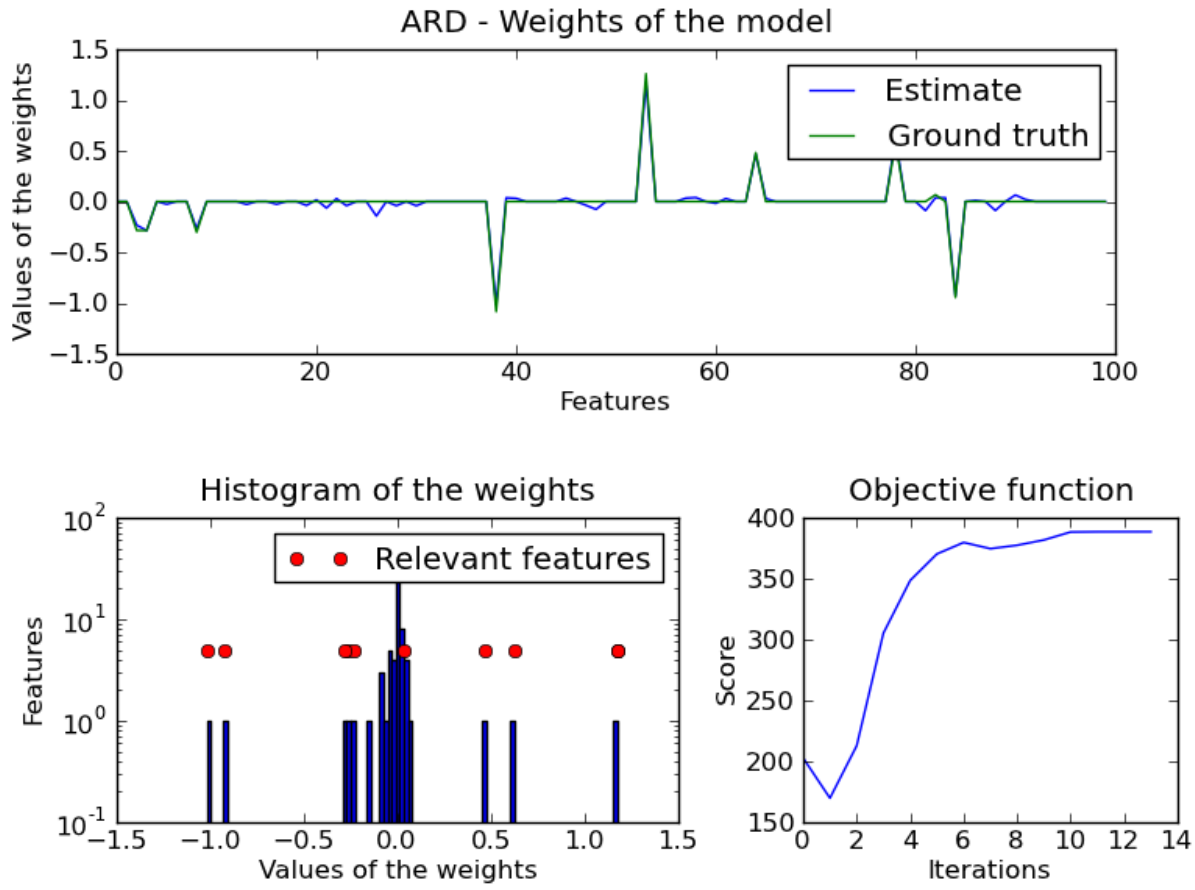
Python source code: `lasso_path_with_crossvalidation.py`

```
print __doc__

import numpy as np

##############################################################################
# generate some sparse data to play with

n_samples, n_features = 60, 100

np.random.seed(1)
X = np.random.randn(n_samples, n_features)
coef = 3*np.random.randn(n_features)
coef[10:] = 0 # sparsify coef
y = np.dot(X, coef)

# add noise
y += 0.01 * np.random.normal((n_samples,))

# Split data in train set and test set
X_train, y_train = X[:n_samples/2], y[:n_samples/2]
```

```
X_test, y_test = X[n_samples/2:], y[n_samples/2:]


##############################################################################
# Lasso with path and cross-validation using LassoCV path
from scikits.learn.linear_model import LassoCV
from scikits.learn.cross_val import KFold

cv = KFold(n_samples/2, 5)
lasso_cv = LassoCV()

# fit_params = {'max_iter':100}

y_ = lasso_cv.fit(X_train, y_train, cv=cv, max_iter=100).predict(X_test)

print "Optimal regularization parameter  = %s" % lasso_cv.alpha

# Compute explained variance on test data
print "r^2 on test data : %f" % (1 - np.linalg.norm(y_test - y_)**2
                                   / np.linalg.norm(y_test)**2)
```

Automatic Relevance Determination Regression (ARD)

Fit regression model with ARD



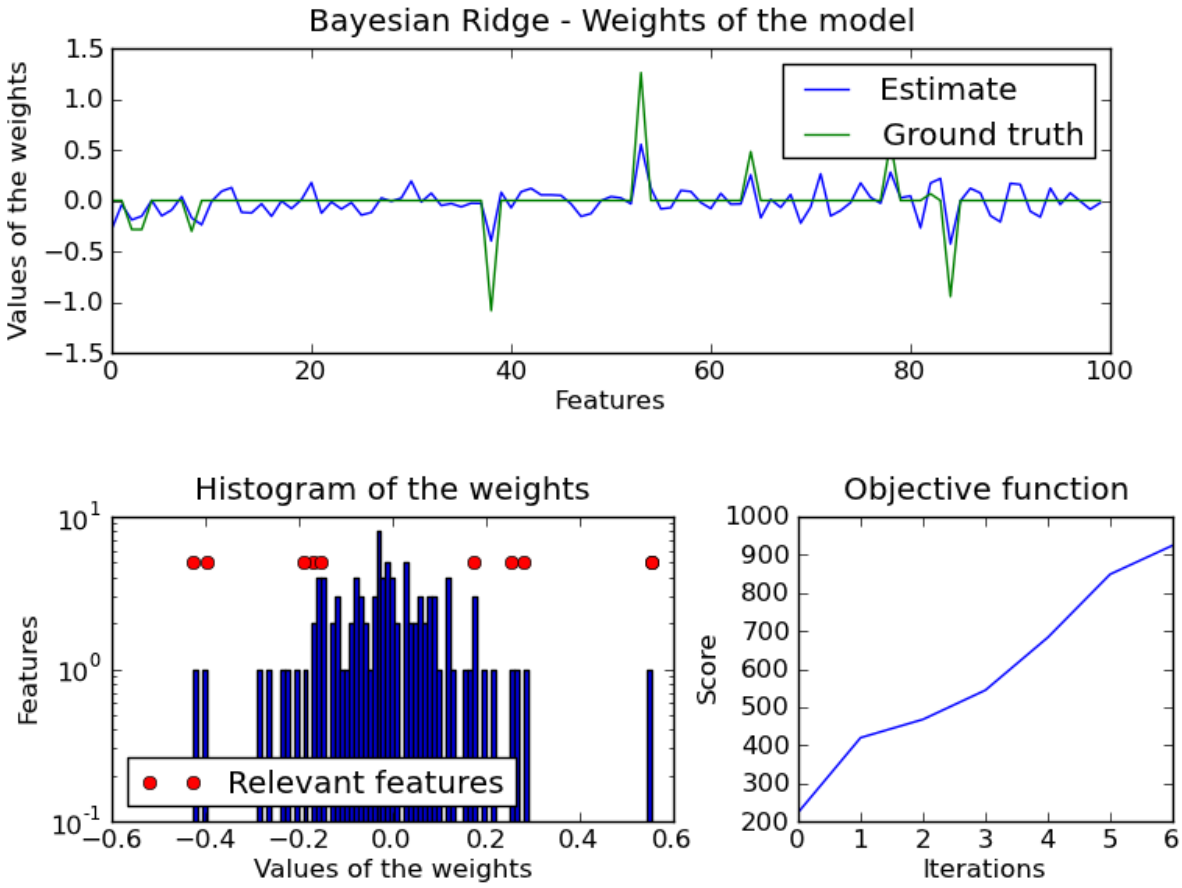
Python source code: plot_ard.py

```
print __doc__

import numpy as np
import pylab as pl
from scipy import stats

from scikits.learn.linear_model import ARDRegression

###############################################################################
# Generating simulated data with Gaussian weigthts

### Parameters of the example
np.random.seed(0)
n_samples, n_features = 50, 100
### Create gaussian data
X = np.random.randn(n_samples, n_features)
### Create weigts with a precision lambda_ of 4.
lambda_ = 4.
w = np.zeros(n_features)
### Only keep 10 weights of interest
relevant_features = np.random.randint(0, n_features, 10)
for i in relevant_features:
    w[i] = stats.norm.rvs(loc=0, scale=1. / np.sqrt(lambda_))
### Create noite with a precision alpha of 50.
alpha_ = 50.
noise =  stats.norm.rvs(loc=0, scale=1. / np.sqrt(alpha_), size=n_samples)
### Create the target
y = np.dot(X, w) + noise

###############################################################################
### Fit the ARD Regression
clf = ARDRegression(compute_score = True)
clf.fit(X, y)

###############################################################################
### Plot the true weights, the estimated weights and the histogram of the
### weights
pl.figure()
axe = pl.axes([0.1,0.6,0.8,0.325])
axe.set_title("ARD - Weights of the model")
axe.plot(clf.coef_, 'b-', label="Estimate")
axe.plot(w, 'g-', label="Ground truth")
axe.set_xlabel("Features")
axe.set_ylabel("Values of the weights")
axe.legend(loc=1)

axe = pl.axes([0.1,0.1,0.45,0.325])
axe.set_title("Histogram of the weights")
axe.hist(clf.coef_, bins=n_features, log=True)
axe.plot(clf.coef_[relevant_features],5*np.ones(len(relevant_features)),'ro',
label="Relevant features")
axe.set_ylabel("Features")
axe.set_xlabel("Values of the weights")
axe.legend(loc=1)

axe = pl.axes([0.65,0.1,0.3,0.325])
axe.set_title("Objective function")
```

```
axe.plot(clf.scores_)
axe.set_ylabel("Score")
axe.set_xlabel("Iterations")
pl.show()
```

Bayesian Ridge Regression

Computes a Bayesian Ridge Regression on a synthetic dataset



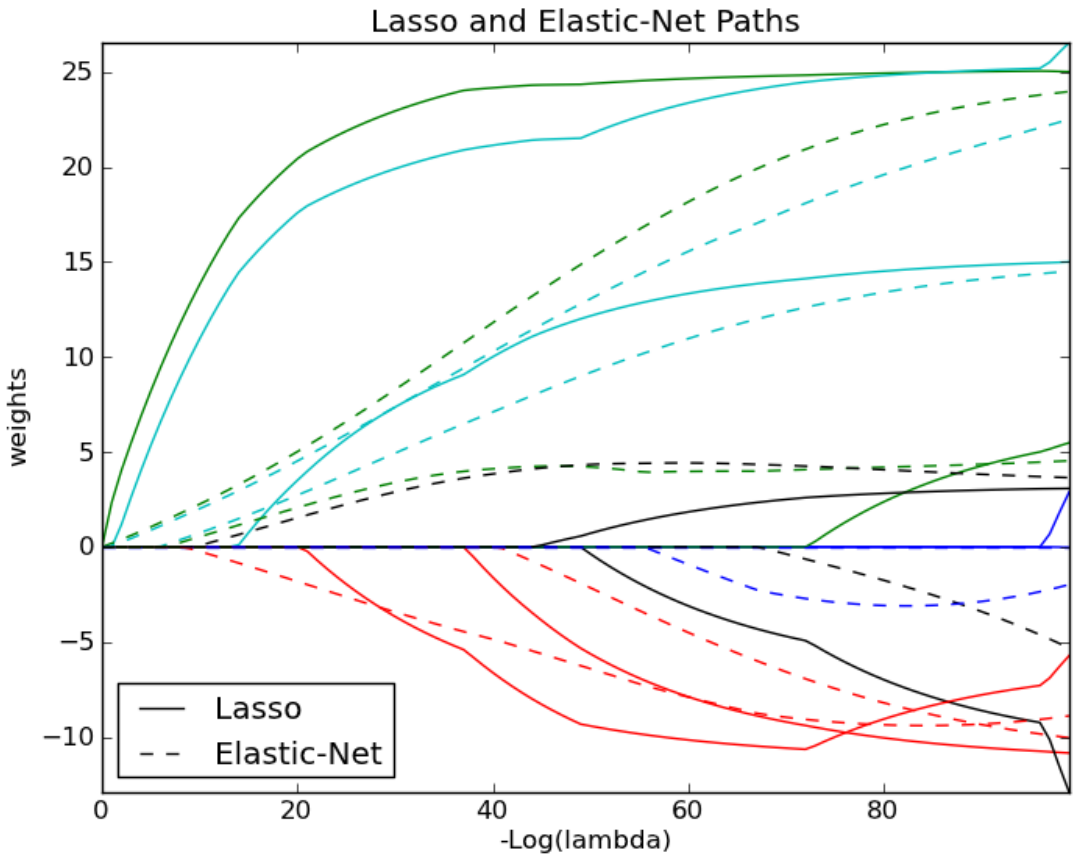
Python source code: `plot_bayesian_ridge.py`

```
print __doc__

import numpy as np
import pylab as pl
from scipy import stats

from scikits.learn.linear_model import BayesianRidge

###############################################################################
# Generating simulated data with Gaussian weigthts
np.random.seed(0)
n_samples, n_features = 50, 100
X = np.random.randn(n_samples, n_features) # Create gaussian data
```

```
# Create weigts with a precision lambda_ of 4.
lambda_ = 4.
w = np.zeros(n_features)
# Only keep 10 weights of interest
relevant_features = np.random.randint(0, n_features, 10)
for i in relevant_features:
    w[i] = stats.norm.rvs(loc = 0, scale = 1./np.sqrt(lambda_))
# Create noite with a precision alpha of 50.
alpha_ = 50.
noise =  stats.norm.rvs(loc = 0, scale = 1./np.sqrt(alpha_), size = n_samples)
# Create the target
y = np.dot(X, w) + noise

##############################################################################
# Fit the Bayesian Ridge Regression
clf = BayesianRidge(compute_score=True)
clf.fit(X, y)

##############################################################################
# Plot true weights, estimated weights and histogram of the weights
pl.figure()
axe = pl.axes([0.1,0.6,0.8,0.325])
axe.set_title("Bayesian Ridge - Weights of the model")
axe.plot(clf.coef_, 'b-', label="Estimate")
axe.plot(w, 'g-', label="Ground truth")
axe.set_xlabel("Features")
axe.set_ylabel("Values of the weights")
axe.legend(loc="upper right")

axe = pl.axes([0.1,0.1,0.45,0.325])
axe.set_title("Histogram of the weights")
axe.hist(clf.coef_, bins=n_features, log=True)
axe.plot(clf.coef_[relevant_features],5*np.ones(len(relevant_features)),'ro',
label="Relevant features")
axe.set_ylabel("Features")
axe.set_xlabel("Values of the weights")
axe.legend(loc="lower left")

axe = pl.axes([0.65,0.1,0.3,0.325])
axe.set_title("Objective function")
axe.plot(clf.scores_)
axe.set_ylabel("Score")
axe.set_xlabel("Iterations")
pl.show()
```

Lasso and Elastic Net

Lasso and elastic net (L1 and L2 penalisation) implemented using a coordinate descent.



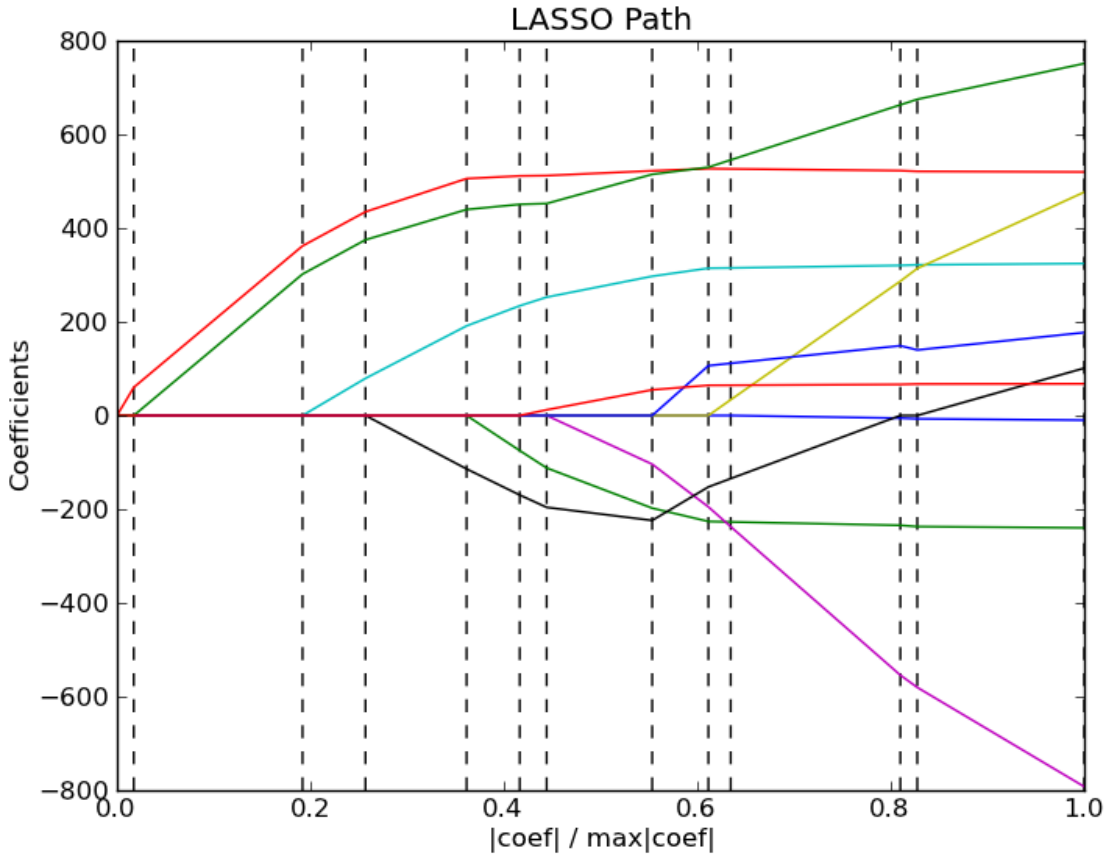
Python source code: `plot_lasso_coordinate_descent_path.py`

```
print __doc__

# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

import numpy as np
import pylab as pl

from scikits.learn.linear_model import lasso_path, enet_path
from scikits.learn import datasets

diabetes = datasets.load_diabetes()
X = diabetes.data
y = diabetes.target

X /= X.std(0) # Standardize data (easier to set the rho parameter)

##############################################################################
# Compute paths

eps = 5e-3 # the smaller it is the longer is the path

print "Computing regularization path using the lasso..."
models = lasso_path(X, y, eps=eps)
```

```
alphas_lasso = np.array([model.alpha for model in models])
coefs_lasso = np.array([model.coef_ for model in models])

print "Computing regularization path using the elastic net..."
models = enet_path(X, y, eps=eps, rho=0.8)
alphas_enet = np.array([model.alpha for model in models])
coefs_enet = np.array([model.coef_ for model in models])

##############################################################################
# Display results

ax = pl.gca()
ax.set_color_cycle(2 * ['b', 'r', 'g', 'c', 'k'])
l1 = pl.plot(coefs_lasso)
l2 = pl.plot(coefs_enet, linestyle='--')

pl.xlabel('-Log(lambda)')
pl.ylabel('weights')
pl.title('Lasso and Elastic-Net Paths')
pl.legend((l1[-1], l2[-1]), ('Lasso', 'Elastic-Net'), loc='lower left')
pl.axis('tight')
pl.show()
```

Lasso path using LARS

Computes Lasso Path along the regularization parameter using the LARS algorithm on the diabetest dataset.



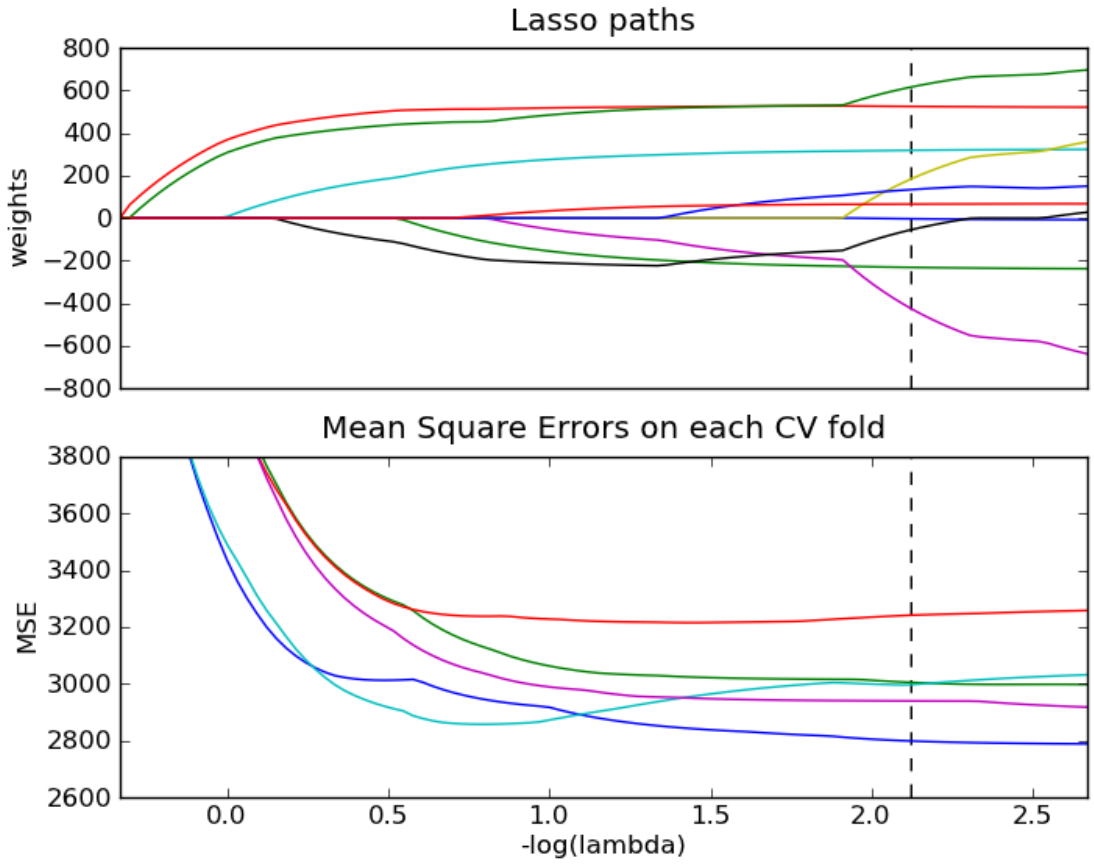
Python source code: `plot_lasso_lars.py`

```
print __doc__

# Author: Fabian Pedregosa <fabian.pedregosa@inria.fr>
#         Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

import numpy as np
import pylab as pl

from scikits.learn import linear_model
from scikits.learn import datasets

diabetes = datasets.load_diabetes()
X = diabetes.data
y = diabetes.target

print "Computing regularization path using the LARS ..."
alphas, _, coefs = linear_model.lars_path(X, y, method='lasso', verbose=True)

xx = np.sum(np.abs(coefs.T), axis=1)
xx /= xx[-1]

pl.plot(xx, coefs.T)
ymin, ymax = pl.ylim()
```

```
pl.vlines(xx, ymin, ymax, linestyle='dashed')
pl.xlabel('|coef| / max|coef|')
pl.ylabel('Coefficients')
pl.title('LASSO Path')
pl.axis('tight')
pl.show()
```

Cross validated Lasso path with coordinate descent

Compute a 5-fold cross-validated Lasso path with coordinate descent to find the optimal value of alpha.



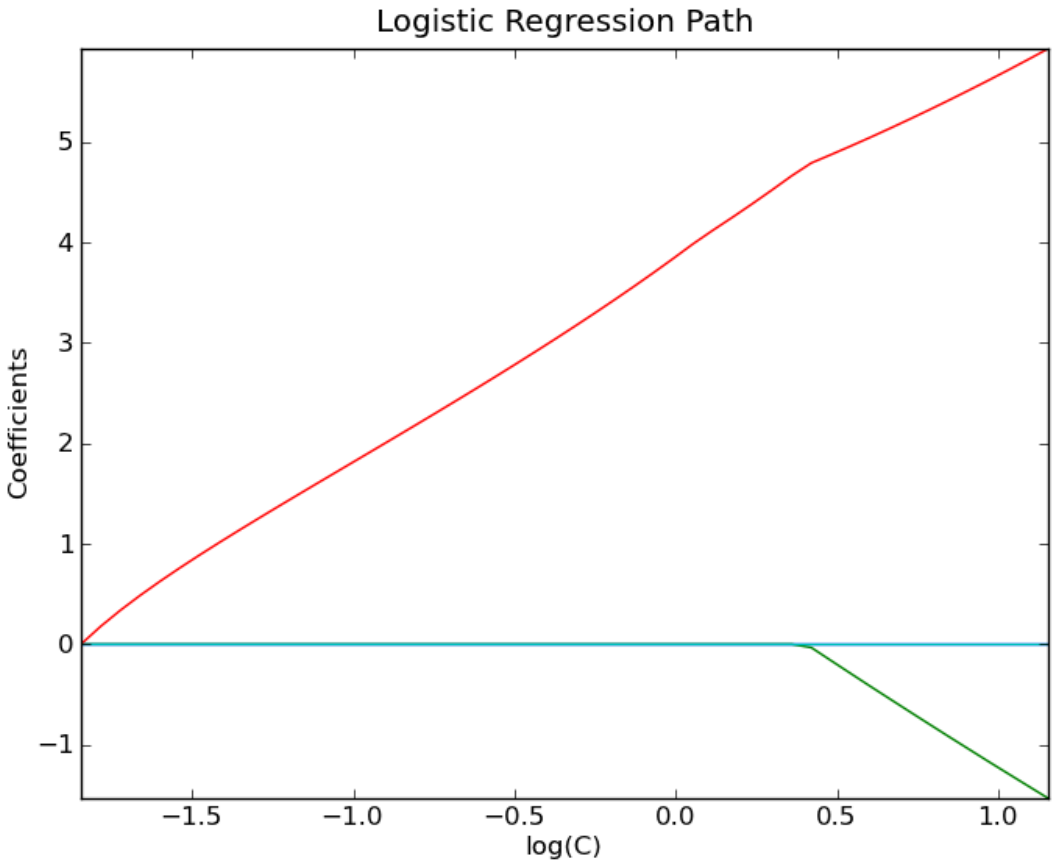
Python source code: `plot_lasso_path_crossval.py`

```
print __doc__

# Author: Olivier Grisel
# License: BSD Style.

import numpy as np
import pylab as pl

from scikits.learn.linear_model import LassoCV
from scikits.learn import datasets
```

```
diabetes = datasets.load_diabetes()
X = diabetes.data
y = diabetes.target

# normalize data as done by LARS to allow for comparison
X /= np.sqrt(np.sum(X ** 2, axis=0))

##############################################################################
# Compute paths

eps = 1e-3 # the smaller it is the longer is the path

print "Computing regularization path using the lasso..."
model = LassoCV(eps=eps).fit(X, y)

##############################################################################
# Display results
m_log_alphas = -np.log10(model.alphas)
m_log_alpha = -np.log10(model.alpha)

ax = pl.gca()
ax.set_color_cycle(2 * ['b', 'r', 'g', 'c', 'k'])
pl.subplot(2, 1, 1)
pl.plot(m_log_alphas, model.coef_path_)

ymin, ymax = pl.ylim()
pl.vlines([m_log_alpha], ymin, ymax, linestyle='dashed')

pl.xticks(())
pl.ylabel('weights')
pl.title('Lasso paths')
pl.axis('tight')

pl.subplot(2, 1, 2)
ymin, ymax = 2600, 3800
pl.plot(m_log_alphas, model.mse_path_)
pl.vlines([m_log_alpha], ymin, ymax, linestyle='dashed')

pl.xlabel('-log(lambda)')
pl.ylabel('MSE')
pl.title('Mean Square Errors on each CV fold')
pl.axis('tight')
pl.ylim(ymin, ymax)

pl.show()
```

Path with L1- Logistic Regression

Computes path on IRIS dataset.



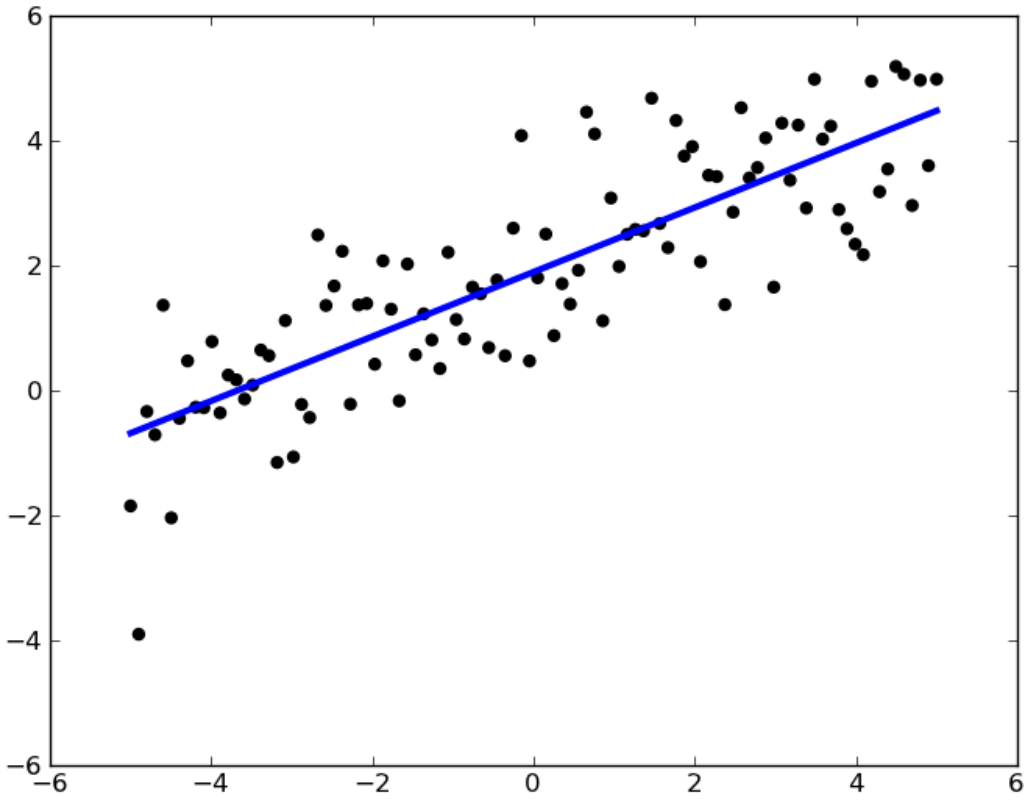
Python source code: `plot_logistic_path.py`

```
print __doc__

# Author: Alexandre Gramfort <alexandre.gramfort@inria.fr>
# License: BSD Style.

from datetime import datetime
import numpy as np
import pylab as pl

from scikits.learn import linear_model
from scikits.learn import datasets
from scikits.learn.svm import l1_min_c

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

X = X[y != 2]
y = y[y != 2]

X -= np.mean(X, 0)

################################################################################
# Demo path functions
```

```
cs = l1_min_c(X, y, loss='log') * np.logspace(0, 3)


print "Computing regularization path ..."
start = datetime.now()
clf = linear_model.LogisticRegression(C=1.0, penalty='l1', tol=1e-6)
coefs_ = [clf.fit(X, y, C=c).coef_.ravel().copy() for c in cs]
print "This took ", datetime.now() - start

coefs_ = np.array(coefs_)
pl.plot(np.log10(cs), coefs_)
ymin, ymax = pl.ylim()
pl.xlabel('log(C)')
pl.ylabel('Coefficients')
pl.title('Logistic Regression Path')
pl.axis('tight')
pl.show()
```

Ordinary Least Squares

Simple Ordinary Least Squares example, we draw the linear least squares solution for a random set of points in the plane.



Python source code: `plot_ols.py`

```
print __doc__

import numpy as np
import pylab as pl

from scikits.learn import linear_model

# this is our test set, it's just a straight line with some
# gaussian noise
xmin, xmax = -5, 5
n_samples = 100
X = [[i] for i in np.linspace(xmin, xmax, n_samples)]
Y = 2 + 0.5 * np.linspace(xmin, xmax, n_samples) \
      + np.random.randn(n_samples, 1).ravel()

# run the classifier
clf = linear_model.LinearRegression()
clf.fit(X, Y)

# and plot the result
pl.scatter(X, Y, color='black')
pl.plot(X, clf.predict(X), color='blue', linewidth=3)
pl.show()
```

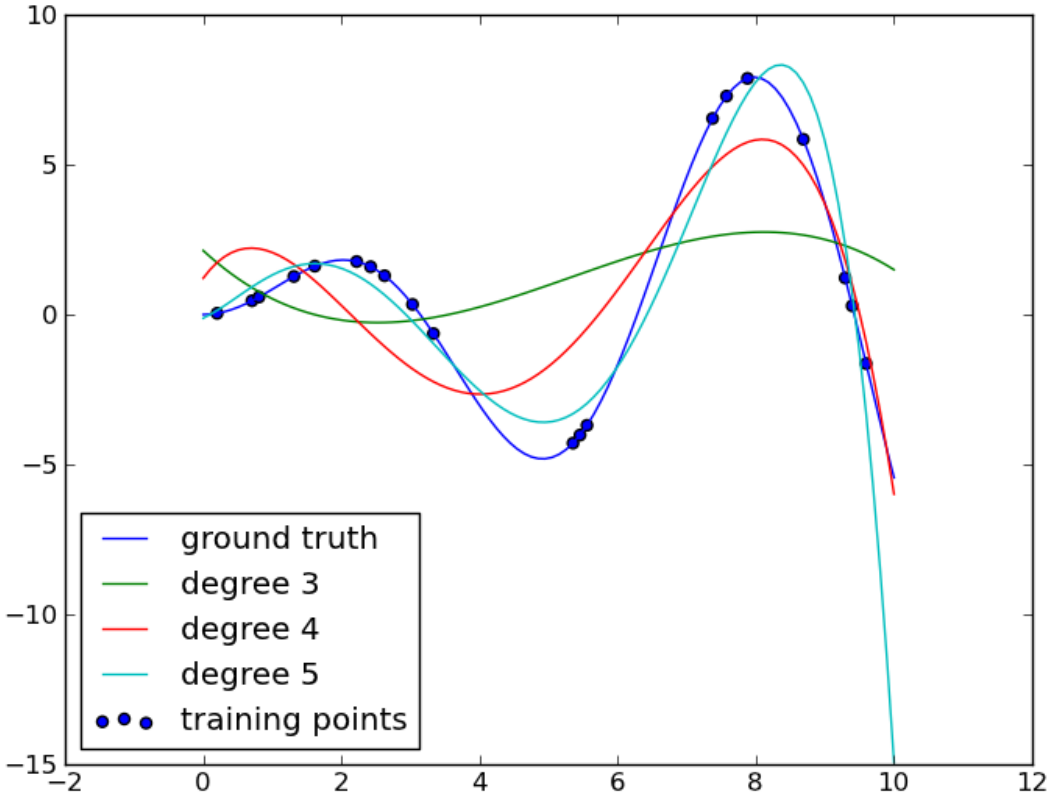
Polynomial interpolation

This example demonstrates how to approximate a function with a polynomial of degree n_degree by using ridge regression. Concretely, from n_samples 1d points, it suffices to build the Vandermonde matrix, which is n_samples x n_degree+1 and has the following form:

[[1, x_1, x_1 ** 2, x_1 ** 3, ...], [1, x_2, x_2 ** 2, x_2 ** 3, ...], ...]

Intuitively, this matrix can be interpreted as a matrix of pseudo features (the points raised to some power). The matrix is akin to (but different from) the matrix induced by a polynomial kernel.

This example shows that you can do non-linear regression with a linear model, by manually adding non-linear features. Kernel methods extend this idea and can induce very high (even infinite) dimensional feature spaces.



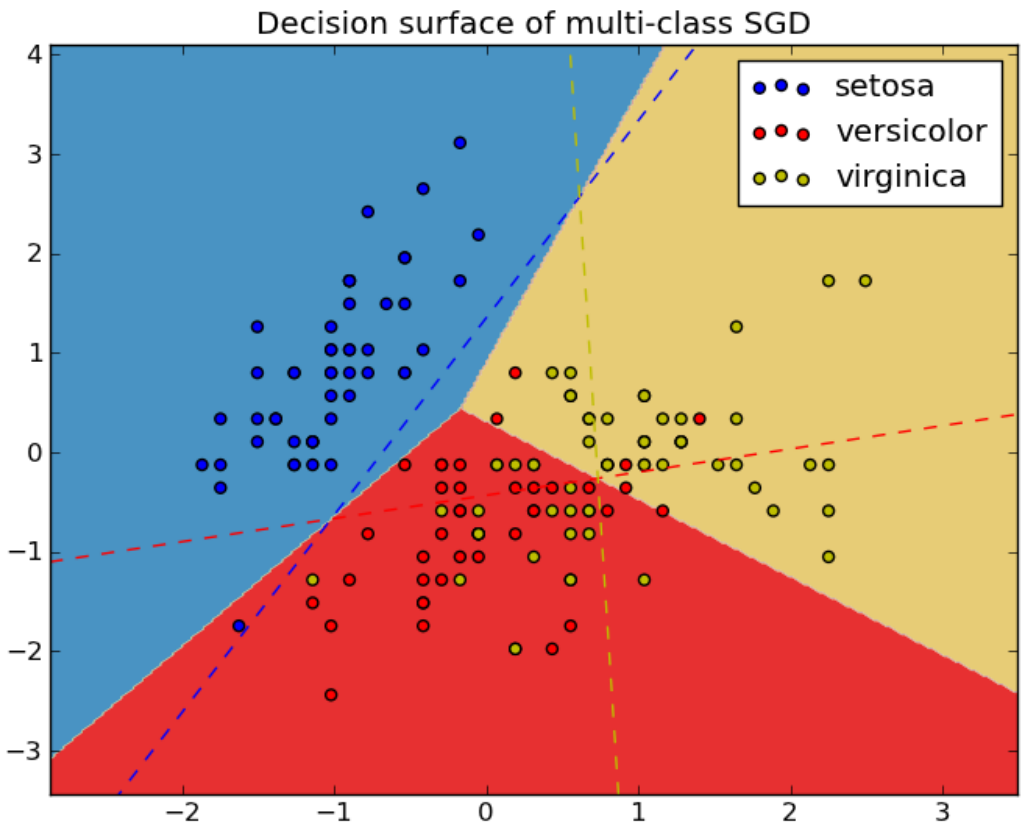
Python source code: `plot_polynomial_interpolation.py`

```
print __doc__

# Author: Mathieu Blondel
# License: BSD Style.

import numpy as np
import pylab as pl

from scikits.learn.linear_model import Ridge

np.random.seed(0)


def f(x):
    """ function to approximate by polynomial interpolation"""
    return x * np.sin(x)


# generate points used to plot
x_plot = np.linspace(0, 10, 100)

# generate points and keep a subset of them
x = np.linspace(0, 10, 100)
np.random.shuffle(x)
```

```
x = np.sort(x[:20])
y = f(x)

pl.plot(x_plot, f(x_plot), label="ground truth")
pl.scatter(x, y, label="training points")

for degree in [3, 4, 5]:
    ridge = Ridge()
    ridge.fit(np.vander(x, degree + 1), y)
    pl.plot(x_plot, ridge.predict(np.vander(x_plot, degree + 1)),
            label="degree %d" % degree)

pl.legend(loc='lower left')

pl.show()
```

Plot multi-class SGD on the iris dataset

Plot decision surface of multi-class SGD on iris dataset. The hyperplanes corresponding to the three one-versus-all (OVA) classifiers are represented by the dashed lines.



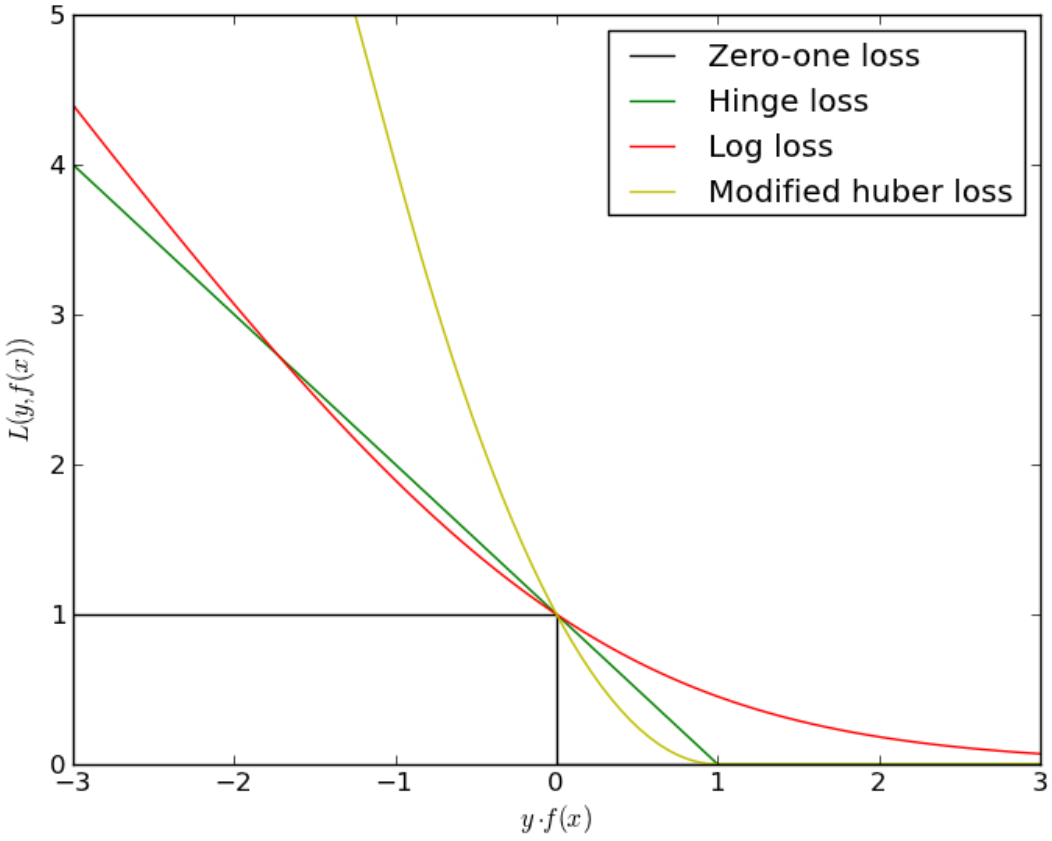
Python source code: `plot_sgd_iris.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import datasets
from scikits.learn.linear_model import SGDClassifier

# import some data to play with
iris = datasets.load_iris()
X = iris.data[:, :2]  # we only take the first two features. We could
                      # avoid this ugly slicing by using a two-dim dataset
y = iris.target
colors = "bry"

# shuffle
idx = np.arange(X.shape[0])
np.random.seed(13)
np.random.shuffle(idx)
X = X[idx]
y = y[idx]

# standardize
mean = X.mean(axis=0)
std = X.std(axis=0)
X = (X - mean) / std

h = .02  # step size in the mesh

clf = SGDClassifier(alpha=0.001, n_iter=100).fit(X, y)

# create a mesh to plot in
x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))

pl.set_cmap(pl.cm.Paired)

# Plot the decision boundary. For that, we will asign a color to each
# point in the mesh [x_min, m_max]x[y_min, y_max].
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
# Put the result into a color plot
Z = Z.reshape(xx.shape)
pl.set_cmap(pl.cm.Paired)
cs = pl.contourf(xx, yy, Z)
pl.axis('tight')

# Plot also the training points
for i, color in zip(clf.classes, colors):
    idx = np.where(y == i)
    pl.scatter(X[idx, 0], X[idx, 1], c=color, label=iris.target_names[i])
pl.title("Decision surface of multi-class SGD")
pl.axis('tight')

# Plot the three one-against-all classifiers
xmin, xmax = pl.xlim()
ymin, ymax = pl.ylim()
coef = clf.coef_
```

```
intercept = clf.intercept_


def plot_hyperplane(c, color):
    def line(x0):
        return (-(x0 * coef[c, 0]) - intercept[c]) / coef[c, 1]

    pl.plot([xmin, xmax], [line(xmin), line(xmax)],
            ls="--", color=color)

for i, color in zip(clf.classes, colors):
    plot_hyperplane(i, color)
pl.legend()
pl.show()
```

SGD: Convex Loss Functions

Plot the convex loss functions supported by *scikits.learn.linear_model.stochastic_gradient*.



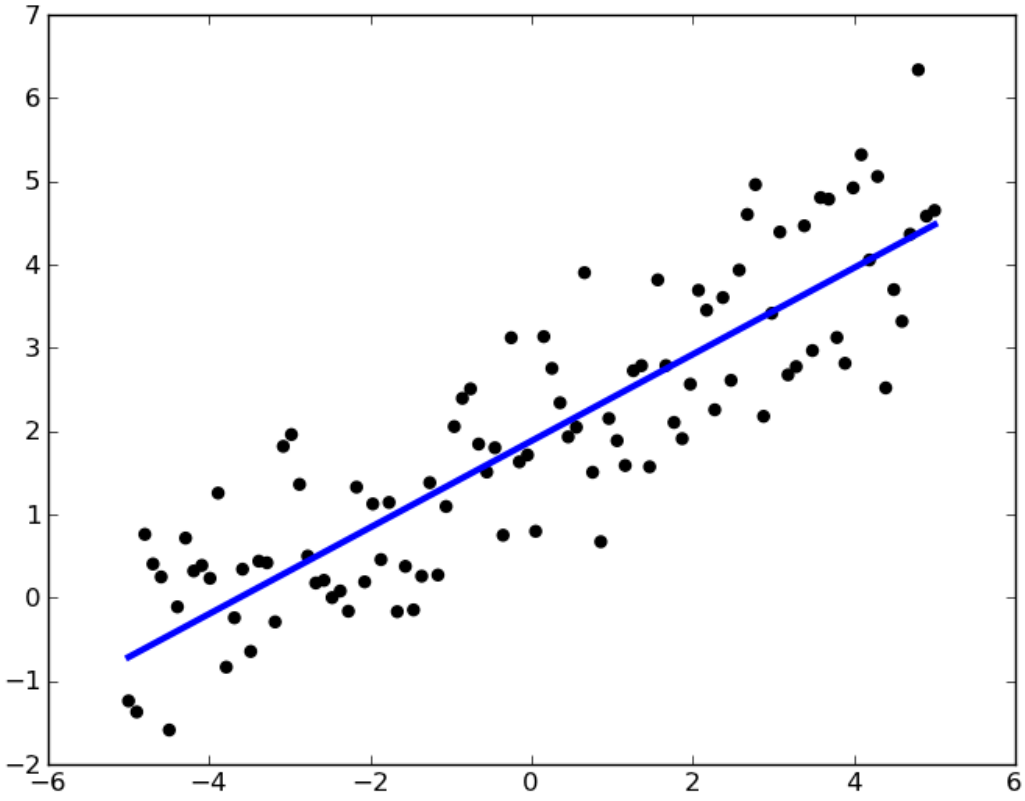
Python source code: `plot_sgd_loss_functions.py`

```
print __doc__

import numpy as np
```

```
import pylab as pl
from scikits.learn.linear_model.sgd_fast import Hinge, \
     ModifiedHuber, SquaredLoss

################################################################################
# Define loss funcitons
xmin, xmax = -3, 3
hinge = Hinge()
log_loss = lambda z, p: np.log2(1.0 + np.exp(-z))
modified_huber = ModifiedHuber()
squared_loss = SquaredLoss()

################################################################################
# Plot loss funcitons
xx = np.linspace(xmin, xmax, 100)
pl.plot([xmin, 0, 0, xmax], [1, 1, 0, 0], 'k-',
        label="Zero-one loss")
pl.plot(xx, [hinge.loss(x,1) for x in xx], 'g-',
        label="Hinge loss")
pl.plot(xx, [log_loss(x,1) for x in xx], 'r-',
        label="Log loss")
pl.plot(xx, [modified_huber.loss(x,1) for x in xx], 'y-',
        label="Modified huber loss")
#pl.plot(xx, [2.0*squared_loss.loss(x,1) for x in xx], 'c-',
#        label="Squared loss")
pl.ylim((0, 5))
pl.legend(loc="upper right")
pl.xlabel(r"$y \cdot f(x)$")
pl.ylabel("$L(y, f(x))$")
pl.show()
```

Ordinary Least Squares with SGD

Simple Ordinary Least Squares example with stochastic gradient descent, we draw the linear least squares solution for a random set of points in the plane.

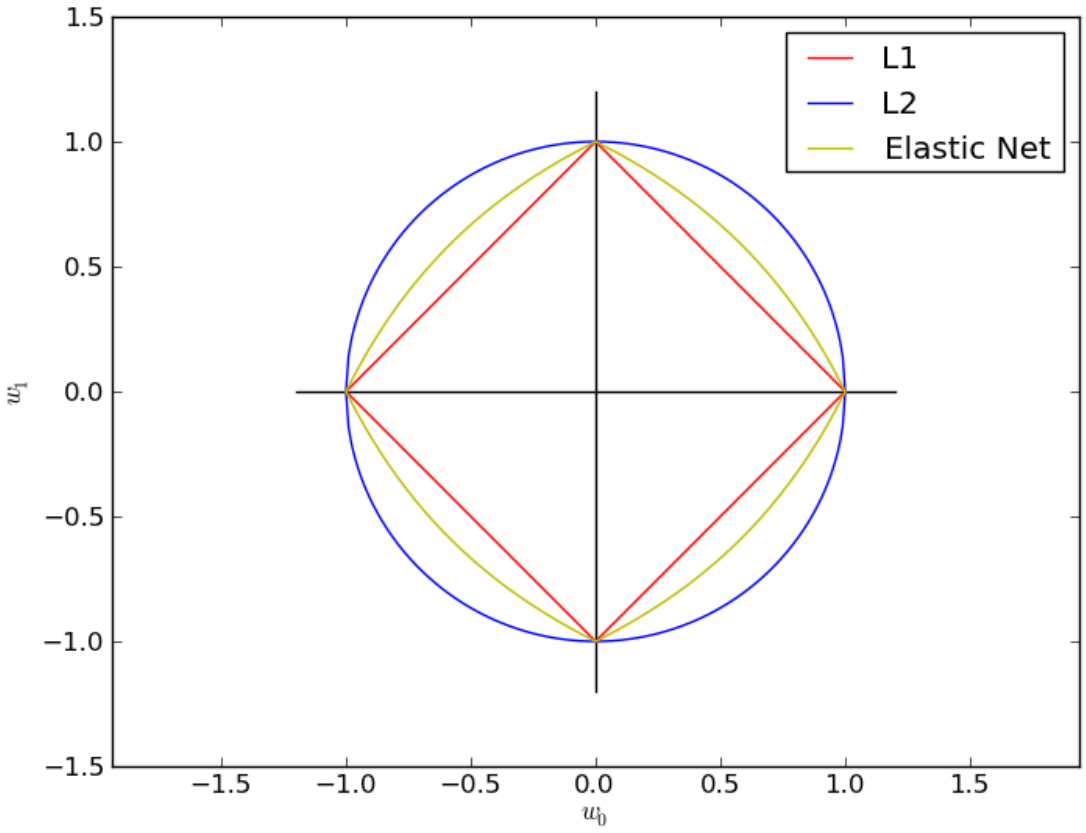


Python source code: `plot_sgd_ols.py`

```
print __doc__

import numpy as np
import pylab as pl

from scikits.learn.linear_model import SGDRegressor

# this is our test set, it's just a straight line with some
# gaussian noise
xmin, xmax = -5, 5
n_samples = 100
X = [[i] for i in np.linspace(xmin, xmax, n_samples)]
Y = 2 + 0.5 * np.linspace(xmin, xmax, n_samples) \
      + np.random.randn(n_samples, 1).ravel()

# run the classifier
clf = SGDRegressor(alpha=0.1, n_iter=20)
clf.fit(X, Y)

# and plot the result
pl.scatter(X, Y, color='black')
pl.plot(X, clf.predict(X), color='blue', linewidth=3)
pl.show()
```

SGD: Penalties

Plot the contours of the three penalties supported by *scikits.learn.linear_model.stochastic_gradient*.



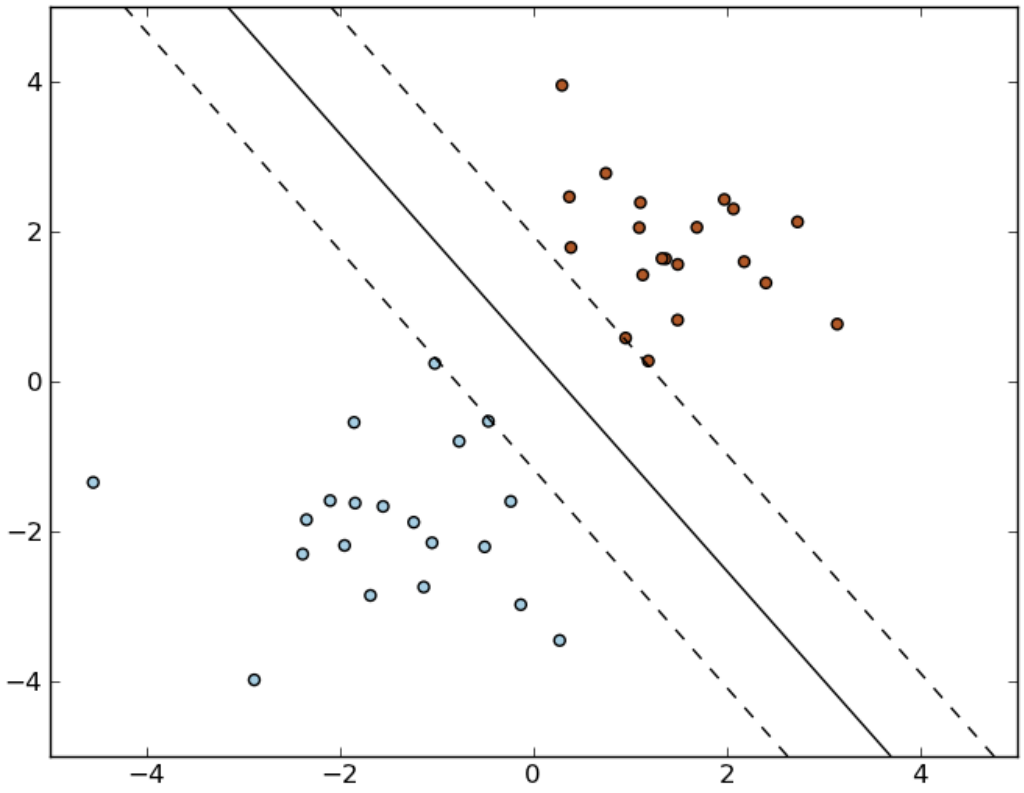
Python source code: `plot_sgd_penalties.py`

```
from __future__ import division
print __doc__

import numpy as np
import pylab as pl

def l1(xs): return np.array([np.sqrt((1 - np.sqrt(x**2.0))**2.0) for x in xs])

def l2(xs): return np.array([np.sqrt(1.0-x**2.0) for x in xs])

def el(xs, z):
    return np.array([(2 - 2*x - 2*z + 4*x*z -
                      (4*z**2 - 8*x*z**2 + 8*x**2*z**2 -
                       16*x**2*z**3 + 8*x*z**3 + 4*x**2*z**4)**(1/2) -
                      2*x*z**2)/(2 - 4*z) for x in xs])

def cross(ext):
    pl.plot([-ext,ext],[0,0], "k-")
    pl.plot([0,0], [-ext,ext], "k-")
```

```
xs = np.linspace(0, 1, 100)

alpha = 0.501 # 0.5 division throuh zero

cross(1.2)

pl.plot(xs, l1(xs), "r-", label="L1")
pl.plot(xs, -1.0*l1(xs), "r-")
pl.plot(-1*xs, l1(xs), "r-")
pl.plot(-1*xs, -1.0*l1(xs), "r-")

pl.plot(xs, l2(xs), "b-", label="L2")
pl.plot(xs, -1.0 * l2(xs), "b-")
pl.plot(-1*xs, l2(xs), "b-")
pl.plot(-1*xs, -1.0 * l2(xs), "b-")

pl.plot(xs, el(xs, alpha), "y-", label="Elastic Net")
pl.plot(xs, -1.0 * el(xs, alpha), "y-")
pl.plot(-1*xs, el(xs, alpha), "y-")
pl.plot(-1*xs, -1.0 * el(xs, alpha), "y-")

pl.xlabel(r"$w_0$")
pl.ylabel(r"$w_1$")
pl.legend()

pl.axis("equal")
pl.show()
```

SGD: Maximum margin separating hyperplane

Plot the maximum margin separating hyperplane within a two-class separable dataset using a linear Support Vector Machines classifier trained using SGD.



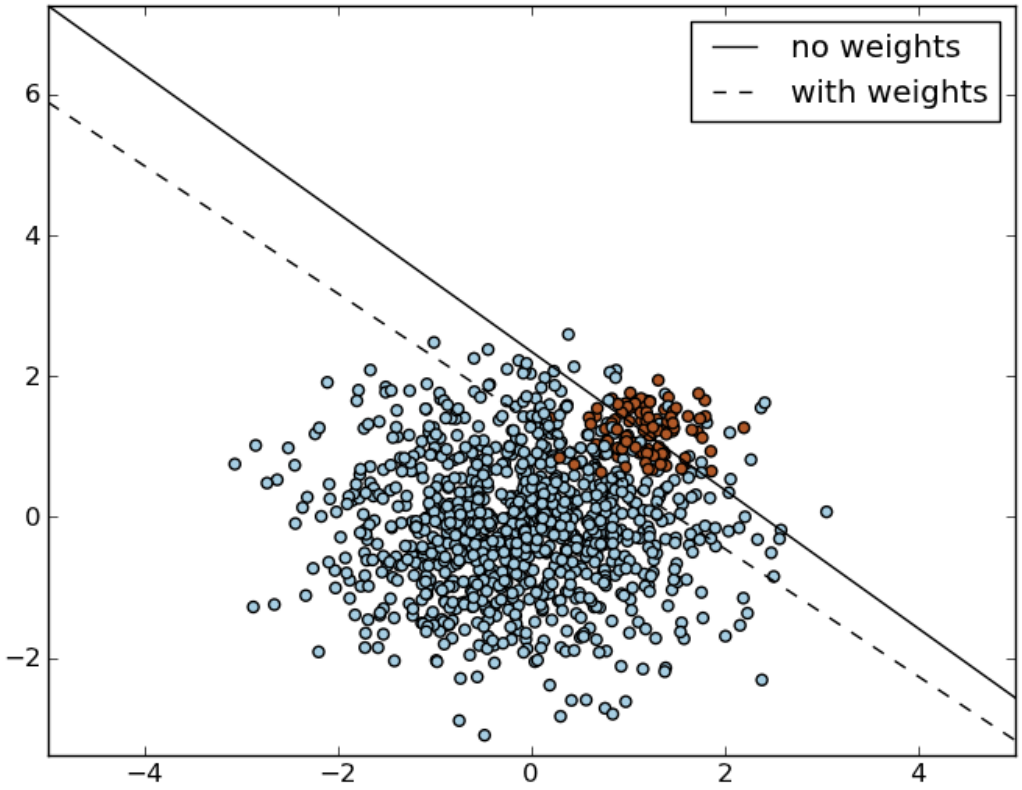
Python source code: `plot_sgd_separating_hyperplane.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn.linear_model import SGDClassifier

# we create 40 separable points
np.random.seed(0)
X = np.r_[np.random.randn(20, 2) - [2,2], np.random.randn(20, 2) + [2, 2]]
Y = [0]*20 + [1]*20

# fit the model
clf = SGDClassifier(loss="hinge", alpha = 0.01, n_iter=50,
                    fit_intercept=True)
clf.fit(X, Y)

# plot the line, the points, and the nearest vectors to the plane
xx = np.linspace(-5, 5, 10)
yy = np.linspace(-5, 5, 10)
X1, X2 = np.meshgrid(xx, yy)
Z = np.empty(X1.shape)
for (i,j), val in np.ndenumerate(X1):
    x1 = val
    x2 = X2[i,j]
```

```
    p = clf.decision_function([x1, x2])
    Z[i,j] = p[0]
levels = [-1.0, 0.0, 1.0]
linestyles = ['dashed','solid', 'dashed']
colors = 'k'
pl.set_cmap(pl.cm.Paired)
pl.contour(X1, X2, Z, levels, colors=colors, linestyles=linestyles)
pl.scatter(X[:,0], X[:,1], c=Y)

pl.axis('tight')
pl.show()
```

SGD: Separating hyperplane with weighted classes

Fit linear SVMs with and without class weighting. Allows to handle problems with unbalanced classes.



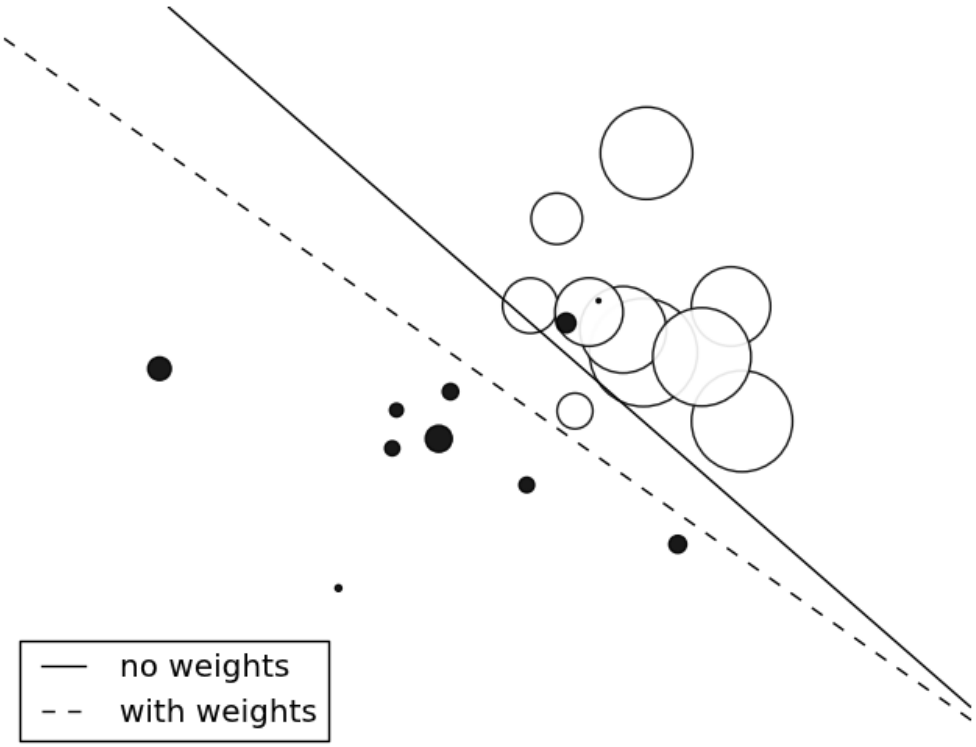
Python source code: `plot_sgd_weighted_classes.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn.linear_model import SGDClassifier
```

```
# we create 40 separable points
np.random.seed(0)
n_samples_1 = 1000
n_samples_2 = 100
X = np.r_[1.5*np.random.randn(n_samples_1, 2),
          0.5*np.random.randn(n_samples_2, 2) + [2, 2]]
y = np.array([0]*(n_samples_1) + [1]*(n_samples_2), dtype=np.float64)
idx = np.arange(y.shape[0])
np.random.shuffle(idx)
X = X[idx]
y = y[idx]
mean = X.mean(axis=0)
std = X.std(axis=0)
X = (X - mean) / std

# fit the model and get the separating hyperplane
clf = SGDClassifier(n_iter=100, alpha=0.01)
clf.fit(X, y)

w = clf.coef_.ravel()
a = -w[0] / w[1]
xx = np.linspace(-5, 5)
yy = a * xx - clf.intercept_ / w[1]


# get the separating hyperplane using weighted classes
wclf = SGDClassifier(n_iter=100, alpha=0.01)
wclf.fit(X, y, class_weight={1: 10})

ww = wclf.coef_.ravel()
wa = -ww[0] / ww[1]
wyy = wa * xx - wclf.intercept_ / ww[1]

# plot separating hyperplanes and samples
pl.set_cmap(pl.cm.Paired)
h0 = pl.plot(xx, yy, 'k-')
h1 = pl.plot(xx, wyy, 'k--')
pl.scatter(X[:,0], X[:,1], c=y)
pl.legend((h0, h1), ('no weights', 'with weights'))

pl.axis('tight')
pl.show()
```

SGD: Weighted samples

Plot decision function of a weighted dataset, where the size of points is proportional to its weight.



Python source code: `plot_sgd_weighted_samples.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import linear_model

# we create 20 points
np.random.seed(0)
X = np.r_[np.random.randn(10, 2) + [1, 1], np.random.randn(10, 2)]
y = [1]*10 + [-1]*10
sample_weight = 100 * np.abs(np.random.randn(20))
# and assign a bigger weight to the last 10 samples
sample_weight[:10] *= 10

# plot the weighted data points
xx, yy = np.meshgrid(np.linspace(-4, 5, 500), np.linspace(-4, 5, 500))
pl.set_cmap(pl.cm.bone)
pl.scatter(X[:, 0], X[:, 1], c=y, s=sample_weight, alpha=0.9)

## fit the unweighted model
clf = linear_model.SGDClassifier(alpha=0.01, n_iter=100)
clf.fit(X, y)
Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
```

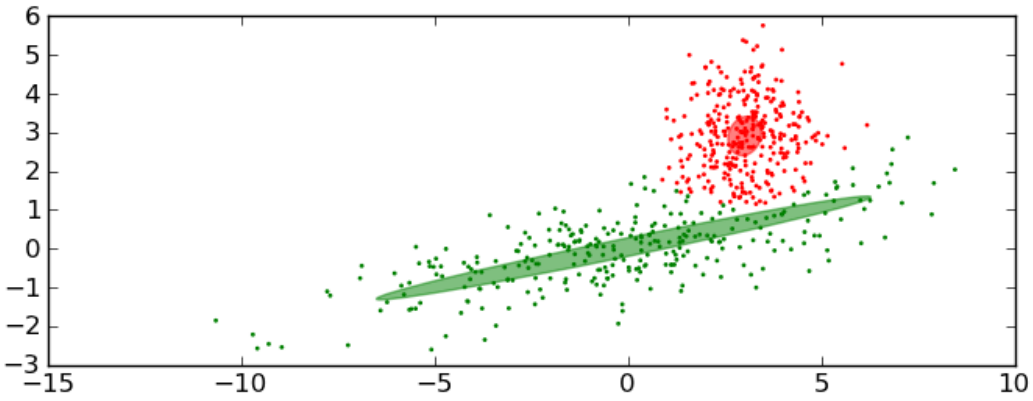
```
pl.contour(xx, yy, Z, levels=[0], linestyles=['solid'])

## fit the weighted model
clf = linear_model.SGDClassifier(alpha=0.01, n_iter=100)
clf.fit(X, y, sample_weight=sample_weight)
Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
pl.contour(xx, yy, Z, levels=[0], linestyles=['dashed'])

pl.legend(["no weights", "with weights"],
          loc="lower left")

pl.axis('off')
pl.show()
```

2.1.8 Gaussian Mixture Models

Examples concerning the *scikits.learn.mixture* package.

Gaussian Mixture Model Ellipsoids

Plot the confidence ellipsoids of a mixture of two gaussians.



Python source code: `plot_gmm.py`

```
import numpy as np
from scikits.learn import mixture
import itertools

import pylab as pl
import matplotlib as mpl

n, m = 300, 2

# generate random sample, two components
np.random.seed(0)
C = np.array([[0., -0.7], [3.5, .7]])
X = np.r_[np.dot(np.random.randn(n, 2), C),
          np.random.randn(n, 2) + np.array([3, 3])]

clf = mixture.GMM(n_states=2, cvtype='full')
clf.fit(X)

splot = pl.subplot(111, aspect='equal')
color_iter = itertools.cycle (['r', 'g', 'b', 'c'])

Y_ = clf.predict(X)

for i, (mean, covar, color) in enumerate(zip(clf.means, clf.covars, color_iter)):
    v, w = np.linalg.eigh(covar)
    u = w[0] / np.linalg.norm(w[0])
    pl.scatter(X[Y_==i, 0], X[Y_==i, 1], .8, color=color)
    angle = np.arctan(u[1]/u[0])
    angle = 180 * angle / np.pi # convert to degrees
    ell = mpl.patches.Ellipse (mean, v[0], v[1], 180 + angle, color=color)
    ell.set_clip_box(splot.bbox)
    ell.set_alpha(0.5)
    splot.add_artist(ell)

pl.show()
```

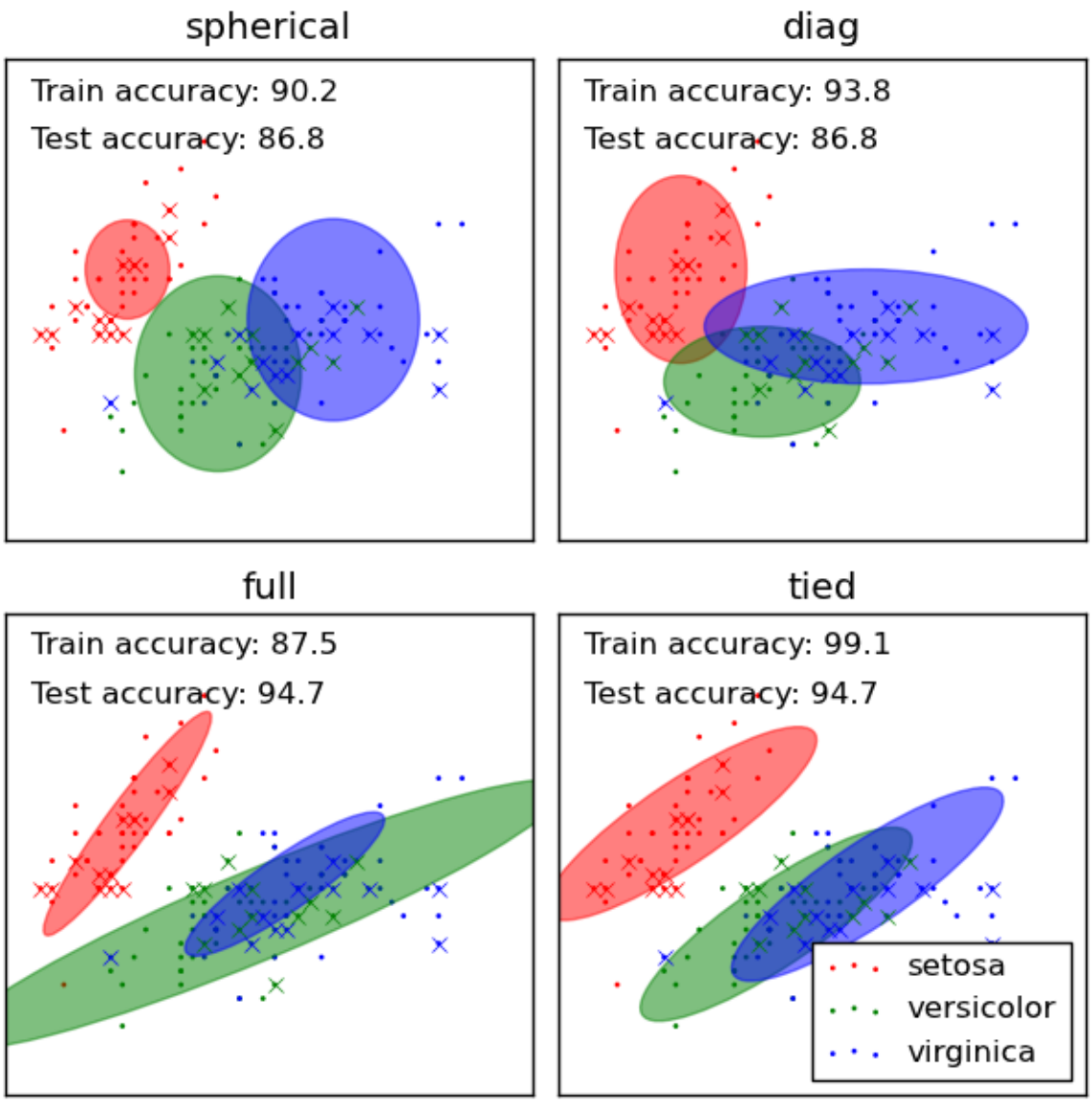
GMM classification

Demonstration of *gmm* for classification.

Plots predicted labels on both training and held out test data using a variety of GMM classifiers on the iris dataset.

Compares GMMs with spherical, diagonal, full, and tied covariance matrices in increasing order of performance. Although one would expect full covariance to perform best in general, it is prone to overfitting on small datasets and does not generalize well to held out test data.

On the plots, train data is shown as dots, while test data is shown as crosses. The iris dataset is four-dimensional. Only the first two dimensions are shown here, and thus some points are separated in other dimensions.



Python source code: `plot_gmm_classifier.py`

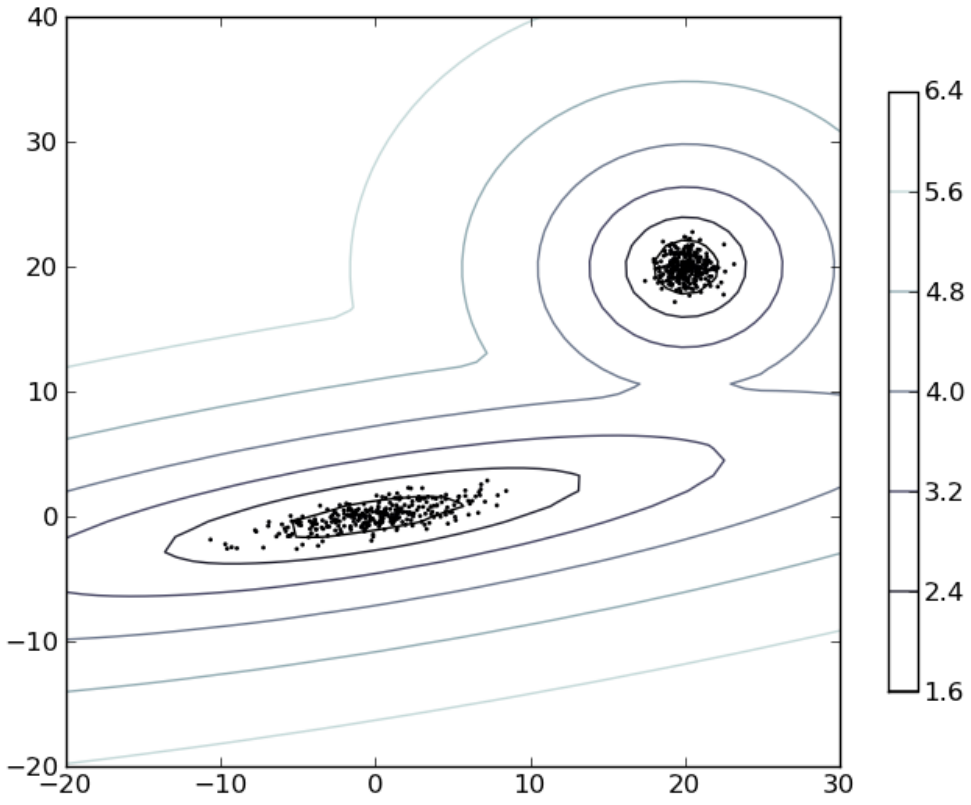
```
print __doc__

# Author: Ron Weiss <ronweiss@gmail.com>, Gael Varoquaux
# License: BSD Style.

# $Id$

import pylab as pl
import matplotlib as mpl
import numpy as np

from scikits.learn import datasets
from scikits.learn.cross_val import StratifiedKFold
from scikits.learn.mixture import GMM

def make_ellipses(gmm, ax):
    for n, color in enumerate('rgb'):
```

```
        v, w = np.linalg.eigh(gmm.covars[n][:2, :2])
        u = w[0] / np.linalg.norm(w[0])
        angle = np.arctan(u[1]/u[0])
        angle = 180 * angle / np.pi # convert to degrees
        v *= 9
        ell = mpl.patches.Ellipse(gmm.means[n, :2], v[0], v[1], 180 + angle,
                                  color=color)
        ell.set_clip_box(ax.bbox)
        ell.set_alpha(0.5)
        ax.add_artist(ell)

iris = datasets.load_iris()

# Break up the dataset into non-overlapping training (75%) and testing
# (25%) sets.
skf = StratifiedKFold(iris.target, k=4)
# Only take the first fold.
train_index, test_index = skf.__iter__().next()


X_train = iris.data[train_index]
y_train = iris.target[train_index]
X_test = iris.data[test_index]
y_test = iris.target[test_index]

n_classes = len(np.unique(y_train))

# Try GMMs using different types of covariances.
classifiers = dict((x, GMM(n_states=n_classes, cvtype=x))
                   for x in ['spherical', 'diag', 'tied', 'full'])

n_classifiers = len(classifiers)

pl.figure(figsize=(3*n_classifiers/2, 6))
pl.subplots_adjust(bottom=.01, top=0.95, hspace=.15, wspace=.05,
                   left=.01, right=.99)


for index, (name, classifier) in enumerate(classifiers.iteritems()):
    # Since we have class labels for the training data, we can
    # initialize the GMM parameters in a supervised manner.
    classifier.means = [X_train[y_train == i, :].mean(axis=0)
                        for i in xrange(n_classes)]

    # Train the other parameters using the EM algorithm.
    classifier.fit(X_train, init_params='wc', n_iter=20)

    h = pl.subplot(2, n_classifiers/2, index + 1)
    make_ellipses(classifier, h)

    for n, color in enumerate('rgb'):
        data = iris.data[iris.target == n]
        pl.scatter(data[:,0], data[:, 1], 0.8, color=color,
                   label=iris.target_names[n])
    # Plot the test data with crosses
    for n, color in enumerate('rgb'):
        data = X_test[y_test == n]
        pl.plot(data[:, 0], data[:, 1], 'x', color=color)
```

```
    y_train_pred = classifier.predict(X_train)
    train_accuracy  = np.mean(y_train_pred.ravel() == y_train.ravel()) * 100
    pl.text(0.05, 0.9, 'Train accuracy: %.1f' % train_accuracy,
                    transform=h.transAxes)

    y_test_pred = classifier.predict(X_test)
    test_accuracy  = np.mean(y_test_pred.ravel() == y_test.ravel()) * 100
    pl.text(0.05, 0.8, 'Test accuracy: %.1f' % test_accuracy,
                    transform=h.transAxes)

    pl.xticks(())
    pl.yticks(())
    pl.title(name)

pl.legend(loc='lower right', prop=dict(size=12))


pl.show()
```

Density Estimation for a mixture of Gaussians

Plot the density estimation of a mixture of two gaussians. Data is generated from two gaussians with different centers and covariance matrices.



Python source code: `plot_gmm_pdf.py`

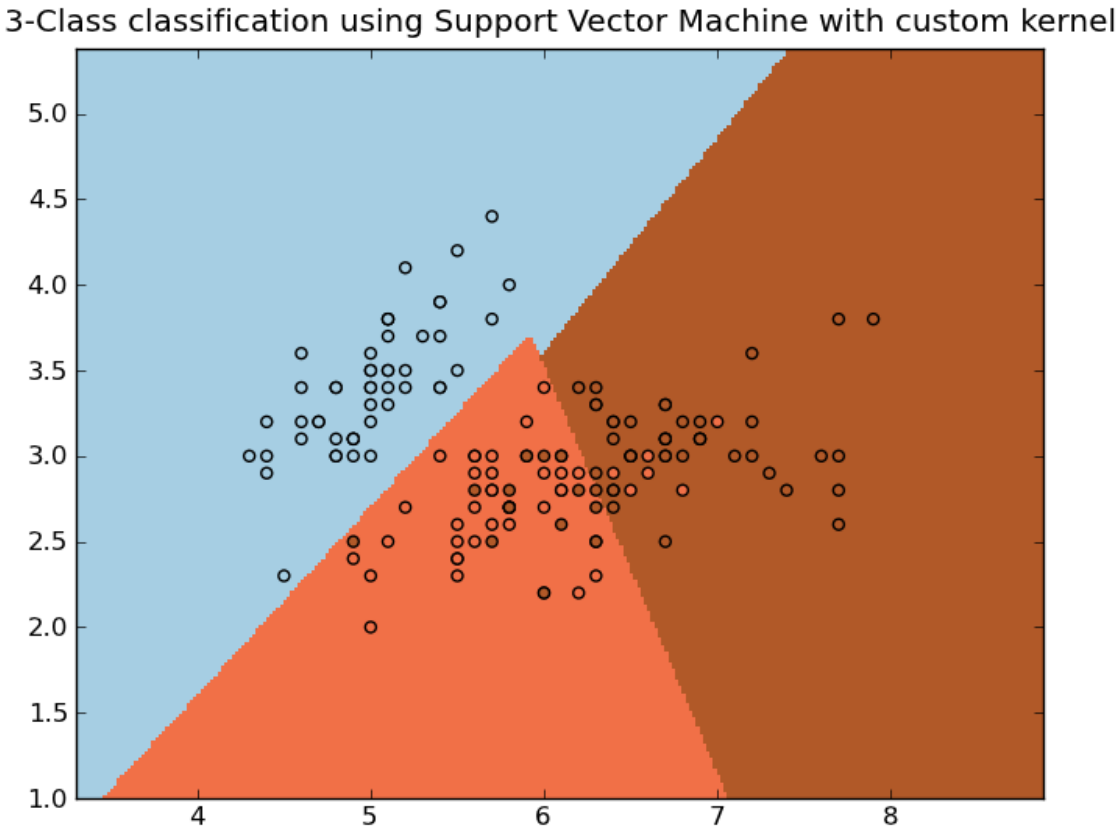
```
import numpy as np
import pylab as pl
from scikits.learn import mixture

n_samples = 300

# generate random sample, two components
np.random.seed(0)
C = np.array([[0., -0.7], [3.5, .7]])
X_train = np.r_[np.dot(np.random.randn(n_samples, 2), C),
          np.random.randn(n_samples, 2) + np.array([20, 20])]

clf = mixture.GMM(n_states=2, cvtype='full')
clf.fit(X_train)

x = np.linspace(-20.0, 30.0)
y = np.linspace(-20.0, 40.0)
X, Y = np.meshgrid(x, y)
XX = np.c_[X.ravel(), Y.ravel()]
Z =  np.log(-clf.eval(XX)[0])
Z = Z.reshape(X.shape)

CS = pl.contour(X, Y, Z)
CB = pl.colorbar(CS, shrink=0.8, extend='both')
pl.scatter(X_train[:, 0], X_train[:, 1], .8)

pl.axis('tight')
pl.show()
```

2.1.9 Support Vector Machines

Examples concerning the *scikits.learn.svm* package.

SVM with custom kernel

Simple usage of Support Vector Machines to classify a sample. It will plot the decision surface and the support vectors.



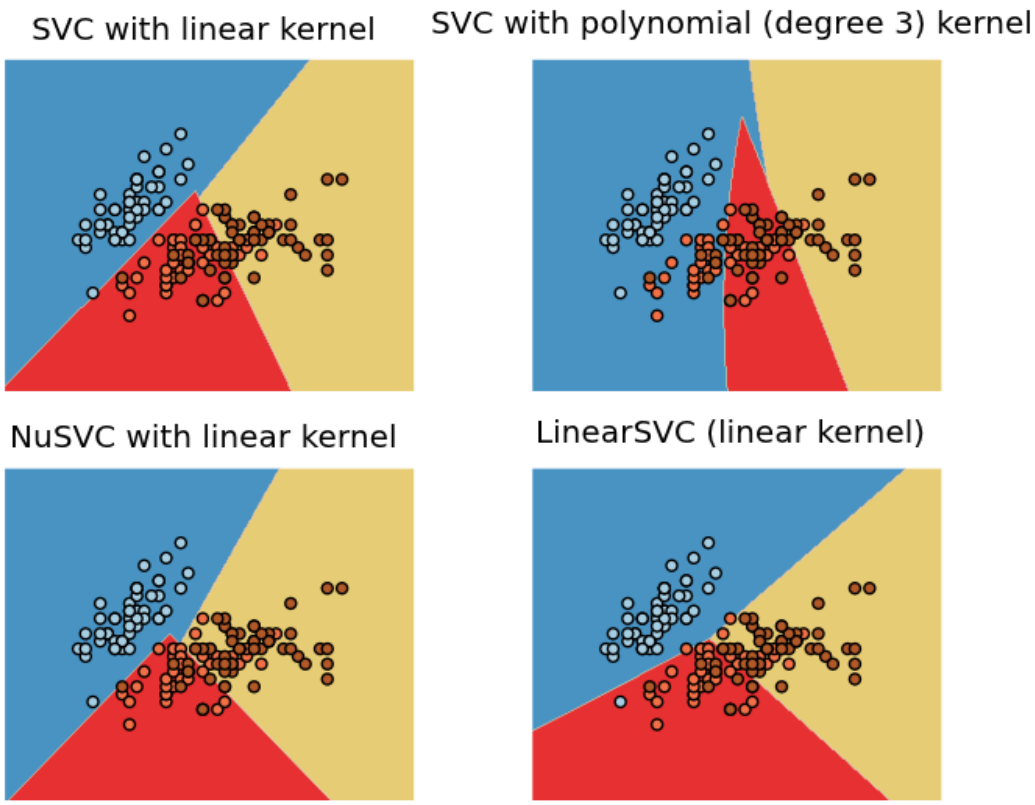
Python source code: `plot_custom_kernel.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm, datasets

# import some data to play with
iris = datasets.load_iris()
X = iris.data[:, :2] # we only take the first two features. We could
                     # avoid this ugly slicing by using a two-dim dataset
Y = iris.target


def my_kernel(x, y):
    """
    We create a custom kernel:

                 (2  0)
    k(x, y) = x  (    ) y.T
                 (0  1)
    """
    M = np.array([[2, 0], [0, 1.0]])
    return np.dot(np.dot(x, M), y.T)
```

```
h=.02 # step size in the mesh

# we create an instance of SVM and fit out data.
clf = svm.SVC(kernel=my_kernel)
clf.fit(X, Y)

# Plot the decision boundary. For that, we will asign a color to each
# point in the mesh [x_min, m_max]x[y_min, y_max].
x_min, x_max = X[:,0].min()-1, X[:,0].max()+1
y_min, y_max = X[:,1].min()-1, X[:,1].max()+1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])

# Put the result into a color plot
Z = Z.reshape(xx.shape)
pl.set_cmap(pl.cm.Paired)
pl.pcolormesh(xx, yy, Z)

# Plot also the training points
pl.scatter(X[:,0], X[:,1], c=Y)
pl.title('3-Class classification using Support Vector Machine with custom kernel')
pl.axis('tight')
pl.show()
```

Plot different SVM classifiers in the iris dataset

Comparison of different linear SVM classifiers on the iris dataset. It will plot the decision surface for four different SVM classifiers.



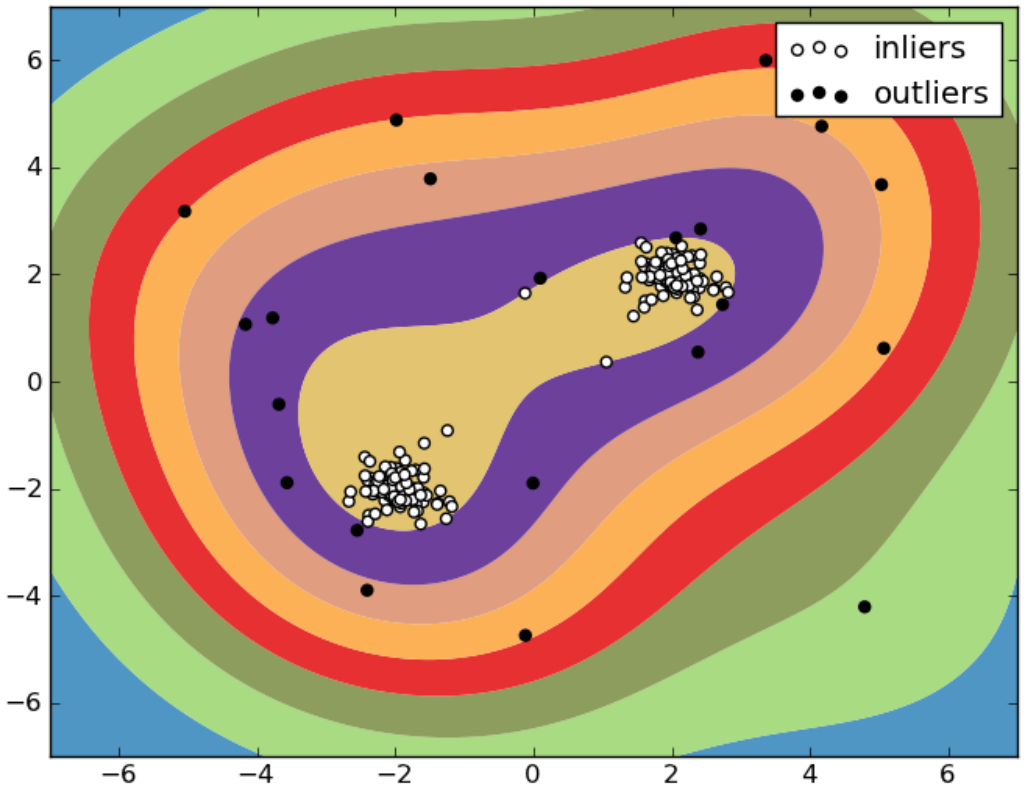
Python source code: `plot_iris.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm, datasets

# import some data to play with
iris = datasets.load_iris()
X = iris.data[:, :2] # we only take the first two features. We could
                     # avoid this ugly slicing by using a two-dim dataset
Y = iris.target

h=.02 # step size in the mesh

# we create an instance of SVM and fit out data. We do not scale our
# data since we want to plot the support vectors
svc     = svm.SVC(kernel='linear').fit(X, Y)
rbf_svc = svm.SVC(kernel='poly').fit(X, Y)
nu_svc  = svm.NuSVC(kernel='linear').fit(X,Y)
lin_svc = svm.LinearSVC().fit(X, Y)

# create a mesh to plot in
x_min, x_max = X[:,0].min()-1, X[:,0].max()+1
y_min, y_max = X[:,1].min()-1, X[:,1].max()+1
```

```
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))

# title for the plots
titles = ['SVC with linear kernel',
          'SVC with polynomial (degree 3) kernel',
          'NuSVC with linear kernel',
          'LinearSVC (linear kernel)']


pl.set_cmap(pl.cm.Paired)

for i, clf in enumerate((svc, rbf_svc, nu_svc, lin_svc)):
    # Plot the decision boundary. For that, we will asign a color to each
    # point in the mesh [x_min, m_max]x[y_min, y_max].
    pl.subplot(2, 2, i+1)
    Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])

    # Put the result into a color plot
    Z = Z.reshape(xx.shape)
    pl.set_cmap(pl.cm.Paired)
    pl.contourf(xx, yy, Z)
    pl.axis('off')

    # Plot also the training points
    pl.scatter(X[:,0], X[:,1], c=Y)

    pl.title(titles[i])

pl.show()
```

One-class SVM with non-linear kernel (RBF)

One-class SVM is an unsupervised algorithm that estimates outliers in a dataset.



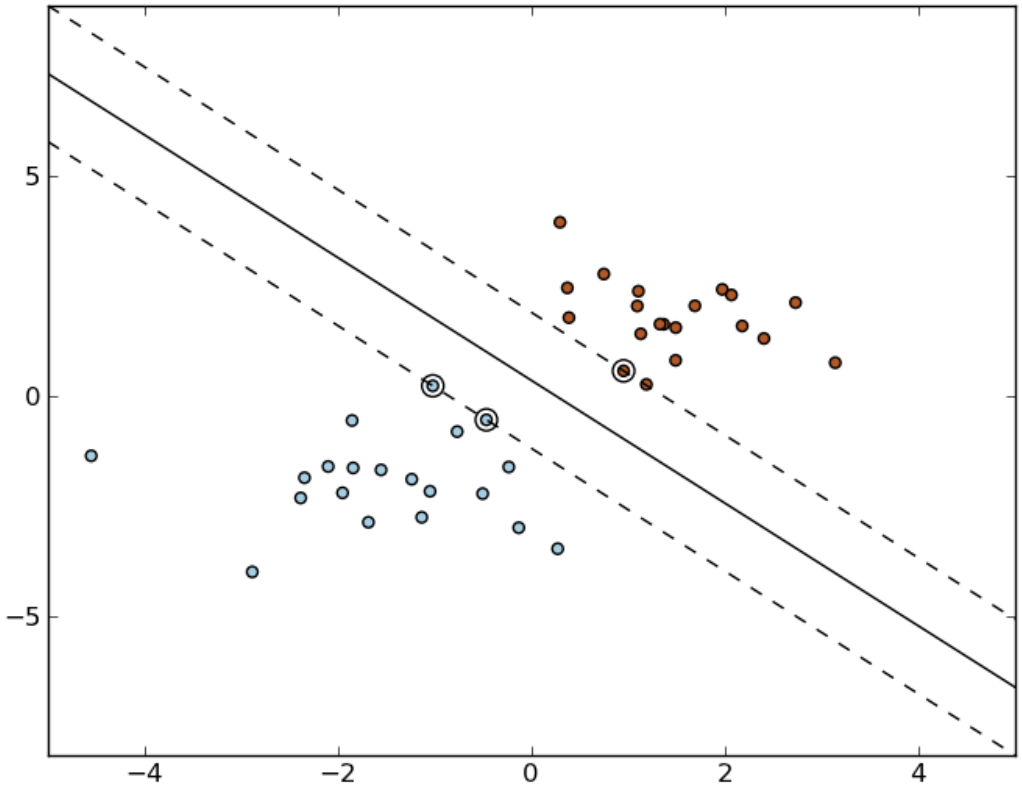
Python source code: `plot_oneclass.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm

xx, yy = np.meshgrid(np.linspace(-7, 7, 500), np.linspace(-7, 7, 500))
X = 0.3 * np.random.randn(100, 2)
X = np.r_[X + 2, X - 2]

# Add 10 % of outliers (leads to nu=0.1)
X = np.r_[X, np.random.uniform(low=-6, high=6, size=(20, 2))]

# fit the model
clf = svm.OneClassSVM(nu=0.1, kernel="rbf", gamma=0.1)
clf.fit(X)

# plot the line, the points, and the nearest vectors to the plane
Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
y_pred = clf.predict(X)

pl.set_cmap(pl.cm.Paired)
pl.contourf(xx, yy, Z)
```

```
pl.scatter(X[y_pred>0,0], X[y_pred>0,1], c='white', label='inliers')
pl.scatter(X[y_pred<=0,0], X[y_pred<=0,1], c='black', label='outliers')
pl.axis('tight')
pl.legend()
pl.show()
```

SVM: Maximum margin separating hyperplane

Plot the maximum margin separating hyperplane within a two-class separable dataset using a Support Vector Machines classifier with linear kernel.



Python source code: `plot_separating_hyperplane.py`

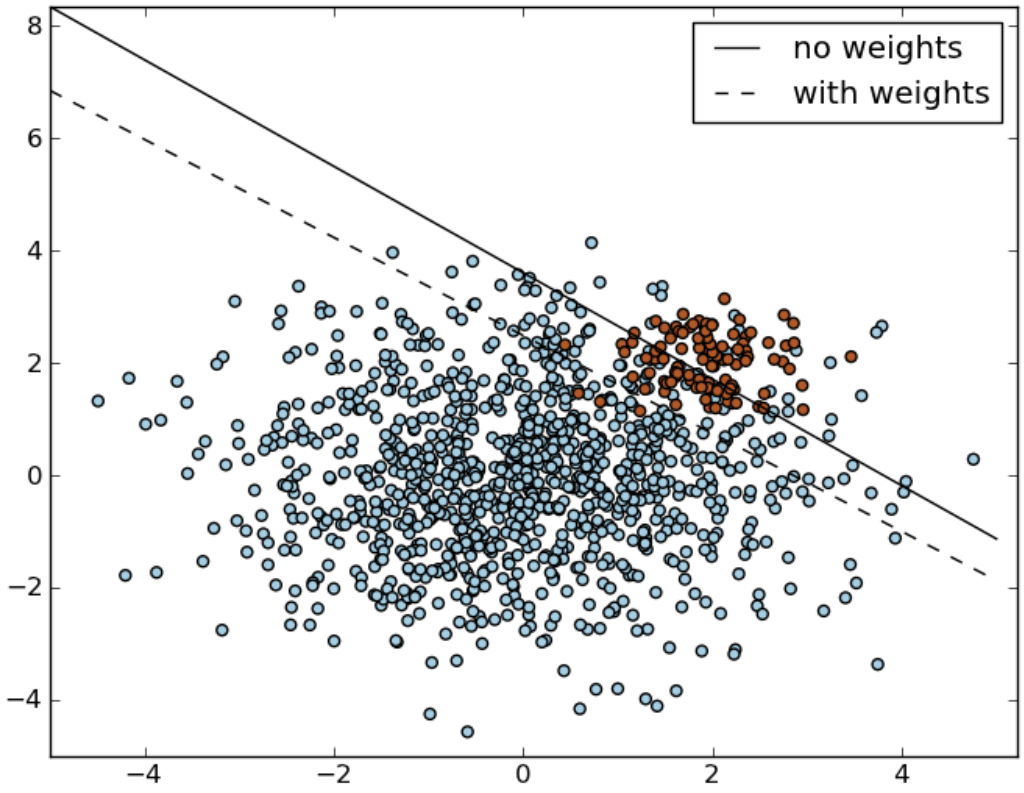
```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm

# we create 40 separable points
np.random.seed(0)
X = np.r_[np.random.randn(20, 2) - [2,2], np.random.randn(20, 2) + [2, 2]]
Y = [0]*20 + [1]*20

# fit the model
```

```
clf = svm.SVC(kernel='linear')
clf.fit(X, Y)

# get the separating hyperplane
w =  clf.coef_[0]
a = -w[0]/w[1]
xx = np.linspace(-5, 5)
yy = a*xx - (clf.intercept_[0])/w[1]

# plot the parallels to the separating hyperplane that pass through the
# support vectors
b = clf.support_vectors_[0]
yy_down = a*xx + (b[1] - a*b[0])
b = clf.support_vectors_[-1]
yy_up = a*xx + (b[1] - a*b[0])

# plot the line, the points, and the nearest vectors to the plane
pl.set_cmap(pl.cm.Paired)
pl.plot(xx, yy, 'k-')
pl.plot(xx, yy_down, 'k--')
pl.plot(xx, yy_up, 'k--')

pl.scatter(clf.support_vectors_[:, 0], clf.support_vectors_[:, 1],
           s=80, facecolors='none')
pl.scatter(X[:,0], X[:,1], c=Y)

pl.axis('tight')
pl.show()
```

SVM: Separating hyperplane for unbalanced classes

Find the optimal separating hyperplane using an SVC for classes that are unbalanced.

We first find the separating plane with a plain SVC and then plot (dashed) the separating hyperplane with automatically correction for unbalanced classes.



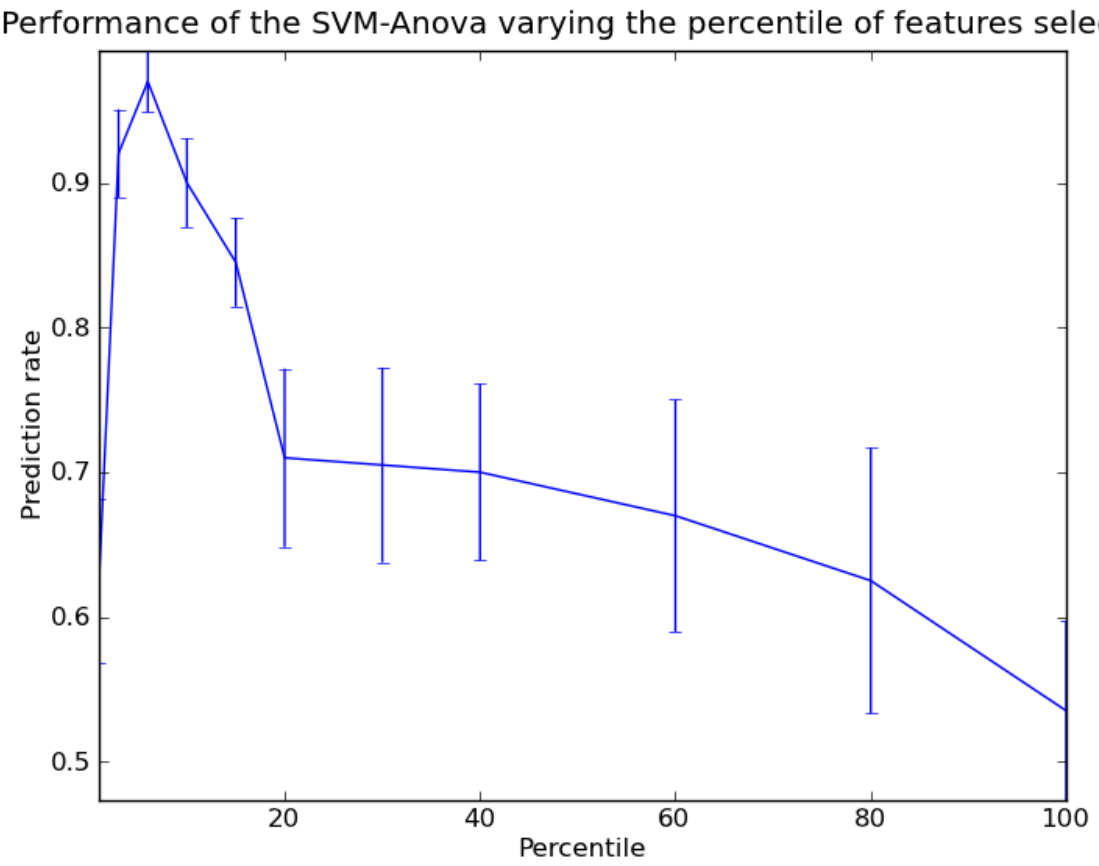
Python source code: `plot_separating_hyperplane_unbalanced.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm

# we create 40 separable points
np.random.seed(0)
n_samples_1 = 1000
n_samples_2 = 100
X = np.r_[1.5*np.random.randn(n_samples_1, 2),
          0.5*np.random.randn(n_samples_2, 2) + [2, 2]]
y = [0]*(n_samples_1) + [1]*(n_samples_2)

# fit the model and get the separating hyperplane
clf = svm.SVC(kernel='linear')
clf.fit(X, y)

w = clf.coef_[0]
a = -w[0] / w[1]
xx = np.linspace(-5, 5)
yy = a * xx - clf.intercept_[0] / w[1]
```

```
# get the separating hyperplane using weighted classes
wclf = svm.SVC(kernel='linear')
wclf.fit(X, y, class_weight={1: 10})

ww = wclf.coef_[0]
wa = -ww[0] / ww[1]
wyy = wa * xx - wclf.intercept_[0] / ww[1]

# plot separating hyperplanes and samples
pl.set_cmap(pl.cm.Paired)
h0 = pl.plot(xx, yy, 'k-')
h1 = pl.plot(xx, wyy, 'k--')
pl.scatter(X[:,0], X[:,1], c=y)
pl.legend((h0, h1), ('no weights', 'with weights'))

pl.axis('tight')
pl.show()
```

SVM-Anova: SVM with univariate feature selection

This example shows how to perform univariate feature before running a SVC (support vector classifier) to improve the classification scores.

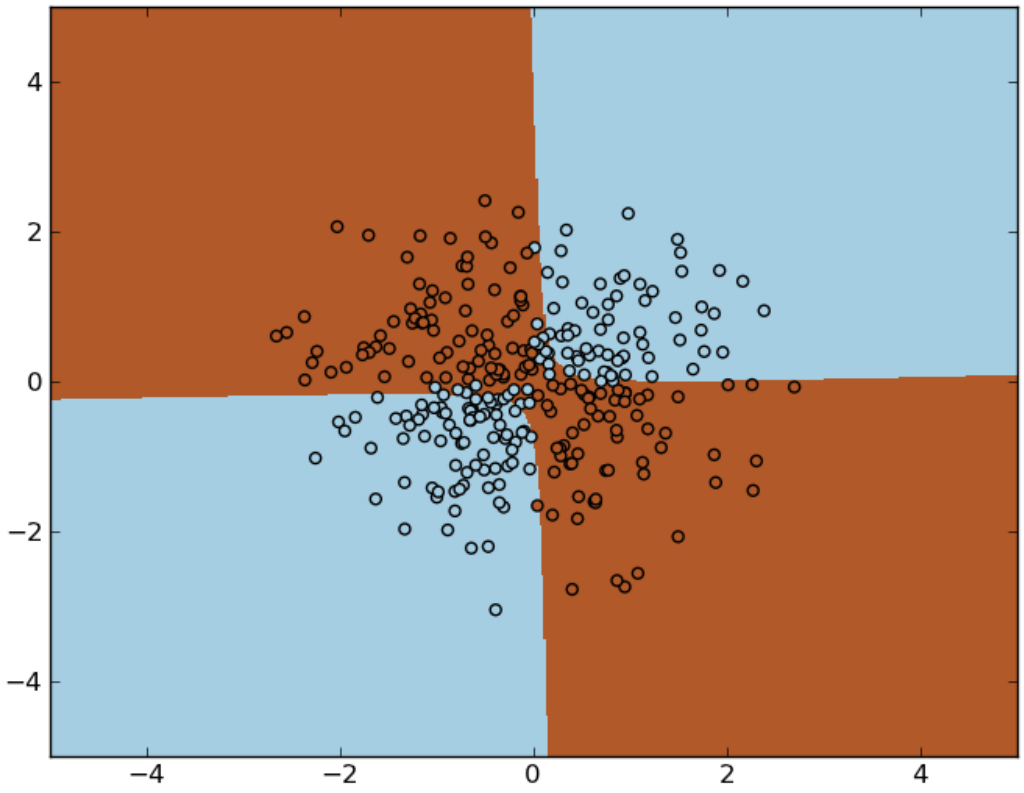


Python source code: `plot_svm_anova.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm, datasets, feature_selection, cross_val
from scikits.learn.pipeline import Pipeline

###############################################################################
# Import some data to play with
digits = datasets.load_digits()
y = digits.target
# Throw away data, to be in the curse of dimension settings
y = y[:200]
X = digits.data[:200]
n_samples = len(y)
X = X.reshape((n_samples, -1))
# add 200 non-informative features
X = np.hstack((X, 2*np.random.random((n_samples, 200))))

###############################################################################
# Create a feature-selection transform and an instance of SVM that we
# combine together to have an full-blown estimator

transform = feature_selection.SelectPercentile(feature_selection.f_classif)

clf = Pipeline([('anova', transform), ('svc', svm.SVC())])

###############################################################################
# Plot the cross-validation score as a function of percentile of features
score_means = list()
score_stds  = list()
percentiles = (1, 3, 6, 10, 15, 20, 30, 40, 60, 80, 100)

for percentile in percentiles:
    clf._set_params(anova__percentile=percentile)
    # Compute cross-validation score using all CPUs
    this_scores = cross_val.cross_val_score(clf, X, y, n_jobs=1)
    score_means.append(this_scores.mean())
    score_stds.append(this_scores.std())

pl.errorbar(percentiles, score_means, np.array(score_stds))

pl.title(
    'Performance of the SVM-Anova varying the percentile of features selected')
pl.xlabel('Percentile')
pl.ylabel('Prediction rate')

pl.axis('tight')
pl.show()
```

Non-linear SVM

Perform binary classification using non-linear SVC with RBF kernel. The target to predict is a XOR of the inputs.



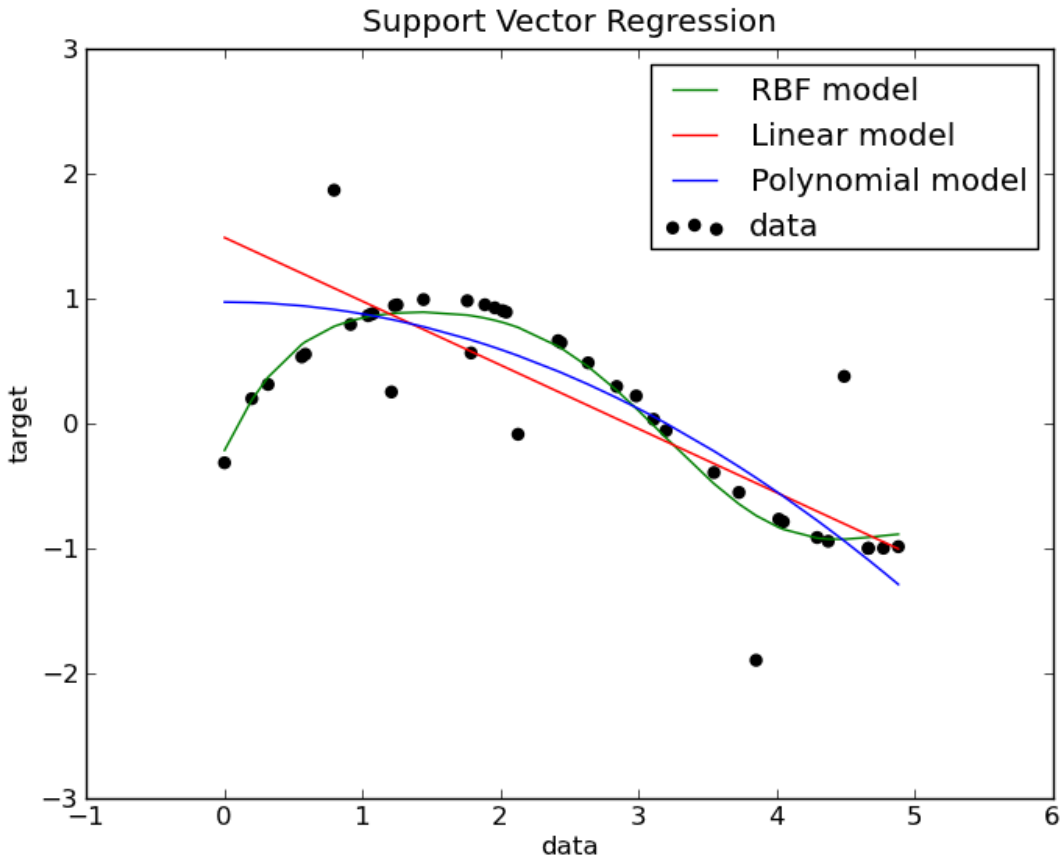
Python source code: `plot_svm_nonlinear.py`

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm

xx, yy = np.meshgrid(np.linspace(-5, 5, 500), np.linspace(-5, 5, 500))
np.random.seed(0)
X = np.random.randn(300, 2)
Y = np.logical_xor(X[:,0]>0, X[:,1]>0)

# fit the model
clf = svm.NuSVC()
clf.fit(X, Y)

# plot the line, the points, and the nearest vectors to the plane
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

pl.set_cmap(pl.cm.Paired)
pl.pcolormesh(xx, yy, Z)
pl.scatter(X[:,0], X[:,1], c=Y)

pl.axis('tight')
```

```
pl.show()
```

Support Vector Regression (SVR) using linear and non-linear kernels

Toy example of 1D regression using linear, polynominial and RBF kernels.



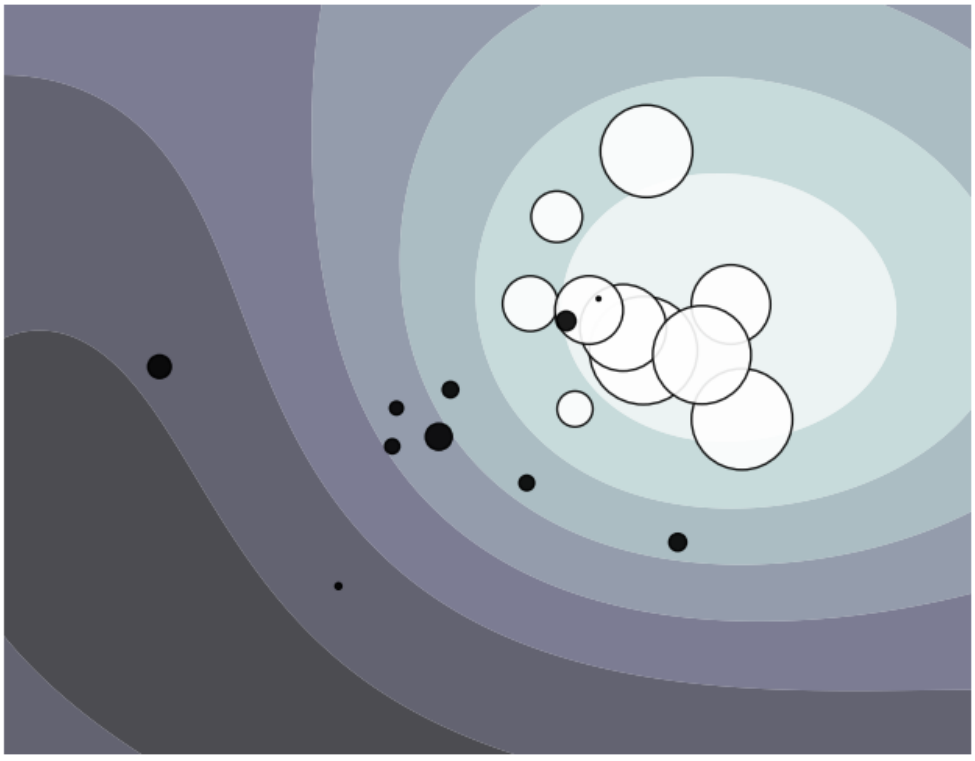
Python source code: `plot_svm_regression.py`

```
print __doc__

###############################################################################
# Generate sample data
import numpy as np

X = np.sort(5*np.random.rand(40, 1), axis=0)
y = np.sin(X).ravel()

###############################################################################
# Add noise to targets
y[::5] += 3*(0.5 - np.random.rand(8))

###############################################################################
# Fit regression model
from scikits.learn.svm import SVR
```

```
svr_rbf = SVR(kernel='rbf', C=1e4, gamma=0.1)
svr_lin = SVR(kernel='linear', C=1e4)
svr_poly = SVR(kernel='poly', C=1e4, degree=2)
y_rbf = svr_rbf.fit(X, y).predict(X)
y_lin = svr_lin.fit(X, y).predict(X)
y_poly = svr_poly.fit(X, y).predict(X)

##############################################################################
# look at the results
import pylab as pl
pl.scatter(X, y, c='k', label='data')
pl.hold('on')
pl.plot(X, y_rbf, c='g', label='RBF model')
pl.plot(X, y_lin, c='r', label='Linear model')
pl.plot(X, y_poly, c='b', label='Polynomial model')
pl.xlabel('data')
pl.ylabel('target')
pl.title('Support Vector Regression')
pl.legend()
pl.show()
```

SVM: Weighted samples

Plot decision function of a weighted dataset, where the size of points is proportional to its weight.



Python source code: plot_weighted_samples.py

```
print __doc__

import numpy as np
import pylab as pl
from scikits.learn import svm

# we create 20 points
np.random.seed(0)
X = np.r_[np.random.randn(10, 2) + [1, 1], np.random.randn(10, 2)]
Y = [1]*10 + [-1]*10
sample_weight = 100 * np.abs(np.random.randn(20))
# and assign a bigger weight to the last 10 samples
sample_weight[:10] *= 10

# # fit the model
clf = svm.SVC()
clf.fit(X, Y, sample_weight=sample_weight)

# plot the decision function
xx, yy = np.meshgrid(np.linspace(-4, 5, 500), np.linspace(-4, 5, 500))

Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

# plot the line, the points, and the nearest vectors to the plane
pl.set_cmap(pl.cm.bone)
pl.contourf(xx, yy, Z, alpha=0.75)
pl.scatter(X[:, 0], X[:, 1], c=Y, s=sample_weight, alpha=0.9)

pl.axis('off')
pl.show()
```

CHAPTER

THREE

DEVELOPMENT

3.1 Contributing

This project is a community effort, and everyone is welcomed to contribute.

The project is hosted on http://github.com/scikit-learn/scikit-learn

3.1.1 Submitting a bug report

In case you experience difficulties using the package, do not hesitate to submit a ticket to the Bug Tracker.

You are also welcomed to post there feature requests and patches.

3.1.2 Retrieving the latest code

You can check the latest sources with the command:

```
git clone git://github.com/scikit-learn/scikit-learn.git
```

or if you have write privileges:

```
git clone git@github.com:scikit-learn/scikit-learn.git
```

If you run the development version, it is cumbersome to re-install the package each time you update the sources. It is thus preferred that you add the scikit-directory to your `PYTHONPATH` and build the extension in place:

```
python setup.py build_ext --inplace
```

On Unix you can simply type `make` in the top-level folder to build in-place and launch all the tests. Have a look at the `Makefile` for additional utilities.

3.1.3 Contributing code

How to contribute

The prefered way to contribute to *scikit-learn* is to fork the main repository on github:

1. Create an account on github if you don't have one already.
2. Fork the scikit-learn repo: click on the 'Fork' button, at the top, center of the page. This creates a copy of the code on the github server where you can work.

3. Clone this copy to your local disk (you need the *git* program to do this):

```
$ git clone git@github.com:YourLogin/scikit-learn.git
```

4. Work on this copy, on your computer, using git to do the version control:

```
$ git add modified_files
$ git commit
$ git push origin master
```

   and so on.

If your changes are not just trivial fixes, it is better to directly work in a branch with the name of the feature your are working on. In this case, replace step 4 by step 5:

5. Create a branch to host your changes and publish it on your public repo:

```
$ git checkout -b my-feature
$ gid add modified_files
$ git commit
$ git push origin my-feature
```

When you are ready, and you have pushed your changes on your github repo, go the web page of the repo, and click on 'Pull request' to send us a pull request. Send us a mail with your pull request, and we can look at your changes, and integrate them.

Before asking for a pull or a review, please check that your contribution complies with the following rules:

- Follow the coding-guidelines (see below).
- All public methods should have informative docstrings with sample usage presented as doctests when appropriate.
- Code with a good unittest coverage (at least 80%), check with:

```
$ pip install nose coverage
$ nosetests --with-coverage path/to/tests_for_package
```

- All other tests pass when everything is rebuilt from scrath, under Unix, check with (from the toplevel source folder):

```
$ make
```

- No pyflakes warnings, check with:

```
$ pip install pyflakes
$ pyflakes path/to/module.py
```

- No PEP8 warnings, check with:

```
$ pip install pep8
$ pep8 path/to/module.py
```

- At least one example script in the `examples/` folder. Have a look at other examples for reference. Example should demonstrate why this method is useful in practice and if possible compare it to other methods available in the scikit.
- At least one paragraph of narrative documentation with links to references in the literature (with PDF links when possible) and the example.

  The documentation should also include expected time and space complexity of the algorithm and scalablity, e.g. "this algorithm can scale to a large number of samples > 100000, but does not scale in dimensionality: n_features is expected to be lower than 100".

To build the documentation see documentation below.

Bonus points for contributions that include a performance analysis with a benchmark script and profiling output (please report on the mailing list or on the github wiki).

Also check out the following guide on *How to optimize for speed* for more details on profiling and cython optimizations.

Note: The current state of the scikit-learn code base is not compliant with all of those guidelines but we expect that enforcing those constraints on all new contributions will get the overall code base quality in the right direction.

EasyFix Issues

The best way to get your feet wet is to pick up an issue from the issue tracker that are labeled as EasyFix. This means that the knowledge needed to solve the issue is low, but still you are helping the project and letting more experienced developers concentrate on other issues.

Documentation

We are glad to accept any sort of documentation: function docstrings, rst docs (like this one), tutorials, etc. Rst docs live in the source code repository, under directory doc/.

You can edit them using any text editor and generate the html docs by typing from the doc/ directory `make html` (or `make html-noplot`, see README in that directory for more info). That should create a directory _build/html/ with html files that are viewable in a web browser.

For building the documentation, you will need sphinx and matplotlib.

> **Warning: Sphinx version**
> While we do our best to have the documentation build under as many version of Sphinx as possible, the different versions tend to behave slightly differently. To get the best results, you should use version 1.0.

Developers web site

More information can be found at the developer's wiki.

3.1.4 Other ways to contribute

Code is not the only way to contribute to this project. For instance, documentation is also a very important part of the project and ofter doesn't get as much attention as it deserves. If you find a typo in the documentation, or have made improvements, don't hesitate to send an email to the mailing list or a github pull request. Full documentation can be found under directory doc/.

It also helps us if you spread the word: reference it from your blog, articles, link to us from your website, or simply by saying "I use it":

3.1.5 Coding guidelines

The following are some guidelines on how new code should be written. Of course, there are special cases and there will be exceptions to these rules. However, following these rules when submitting new code makes the review easier so new code can be integrated in less time.

Uniformly formatted code makes it easier to share code ownership. The scikit learn tries to follow closely the official Python guidelines detailed in PEP8 that details how code should be formatted, and indented. Please read it and follow it.

In addition, we add the following guidelines:

- Use underscores to separate words in non class names: `n_samples` rather than `nsamples`.
- Avoid multiple statements on one line. Prefer a line return after a control flow statement (`if`/`for`).
- Use relative imports for references inside scikits.learn.
- **Please don't use 'import *' in any case**. It is considered harmful by the official Python recommendations. It makes the code harder to read as the origin of symbols is no longer explicitly referenced, but most important, it prevents using a static analysis tool like pyflakes to automatically find bugs in scikit.
- Use the numpy docstring standard in all your docstrings.

A good example of code that we like can be found here.

3.1.6 APIs of scikit learn objects

To have a uniform API, we try to have a common basic API for all the objects. In addition, to avoid the proliferation of framework code, we try to adopt simple conventions and limit to a minimum the number of methods an object has to implement.

Different objects

The main objects of the scikit learn are (one class can implement multiple interfaces):

Estimator The base object, implements:

```
estimator = obj.fit(data)
```

Predictor For supervised learning, or some unsupervised problems, implements:

```
prediction = obj.predict(data)
```

Transformer For filtering or modifying the data, in a supervised or unsupervised way, implements:

```
new_data = obj.transform(data)
```

When fitting and transforming can be performed much more efficiently together than separately, implements:

```
new_data = obj.fit_transform(data)
```

Model A model that can give a goodness of fit or a likelihood of unseen data, implements (higher is better):

```
score = obj.score(data)
```

Estimators

The API has one predominant object: the estimator. A estimator is an object that fits a model based on some training data and is capable of inferring some properties on new data. It can be for instance a classifier or a regressor. All estimators implement the fit method:

```
estimator.fit(X, y)
```

Instantiation

This concerns the object creation. The object's __init__ method might accept as arguments constants that determine the estimator behavior (like the C constant in SVMs).

It should not, however, take the actual training data as argument, as this is left to the `fit()` method:

```
clf2 = SVC(C=2.3)
clf3 = SVC([[1, 2], [2, 3]], [-1, 1]) # WRONG!
```

The arguments that go in the __init__ should all be keyword arguments with a default value. In other words, a user should be able to instanciate an estimator without passing to it any arguments.

The arguments in given at instanciation of an estimator should all correspond to hyper parameters describing the model or the optimisation problem that estimator tries to solve. They should however not be parameters of the estimation routine: these are passed directly to the `fit` method.

In addition, **every keyword argument given to the ''__init__'' should correspond to an attribute on the instance**. The scikit relies on this to find what are the relevent attributes to set on an estimator when doing model selection.

All estimators should inherit from `scikit.learn.base.BaseEstimator`.

Fitting

The next thing you'll probably want to do is to estimate some parameters in the model. This is implemented in the .fit() method.

The fit method takes as argument the training data, which can be one array in the case of unsupervised learning, or two arrays in the case of supervised learning.

Note that the model is fitted using X and y but the object holds no reference to X, y. There are however some exceptions to this, as in the case of precomputed kernels where you need to store access these data in the predict method.

Parameters	
X	array-like, with shape = [N, D], where N is the number of samples and D is the number of features.
Y	array, with shape = [N], where N is the number of samples.
args, kwargs	Parameters can also be set in the fit method.

X.shape[0] should be the same as Y.shape[0]. If this requisite is not met, an exception should be raised.

Y might be dropped in the case of unsupervised learning.

The method should return the object (`self`).

Python tuples

In addition to numpy arrays, all methods should be able to accept Python tuples as arguments. In practice, this means you should call `numpy.asanyarray` at the beginning at each public method that accepts arrays.

Optional Arguments

In iterative algorithms, number of iterations should be specified by an int called `n_iter`.

Unresolved API issues

Some things are must still be decided:

- what should happen when predict is called before than fit() ?
- which exception should be raised when arrays' shape do not match in fit() ?

Working notes

For unresolved issues, TODOs, remarks on ongoing work, developers are adviced to maintain notes on the github wiki: https://github.com/scikit-learn/scikit-learn/wiki

Specific models

In linear models, coefficients are stored in an array called `coef_`, and independent term is stored in `intercept_`.

3.2 How to optimize for speed

The following gives some practical guidelines to help you write efficient code for the scikit-learn project.

Note: While it is always useful to profile your code so as to **check performance assumptions**, it is also highly recommended to **review the literature** to ensure that the implemented algorithm is the state of the art for the task before investing into costly implementation optimization.

Times and times, hours of efforts invested in optimizing complicated implementation details have been rended irrelevant by the late discovery of simple **algorithmic tricks**, or by using another algorithm altogether that is better suited to the problem.

The section *A sample algorithmic trick: warm restarts for cross validation* gives an example of such a trick.

3.2.1 Python, Cython or C/C++?

In general, the scikit-learn project emphasizes the **readability** of the source code to make it easy for the project users to dive into the source code so as to understand how the algorithm behaves on their data but also for ease of maintanability (by the developers).

When implementing a new algorithm is thus recommended to **start implementing it in Python using Numpy and Scipy** by taking care of avoiding looping code using the vectorized idioms of those libraries. In practice this means trying to **replace any nested for loops by calls to equivalent Numpy array methods**. The goal is to avoid the CPU wasting time in the Python interpreter rather than crunching numbers to fit your statistical model.

Sometimes however an algorithm cannot be expressed efficiently in simple vectorized Numpy code. In this case, the recommended strategy is the following:

1. **Profile** the Python implementation to find the main bottleneck and isolate it in a **dedicated module level function**. This function will be reimplemented as a compiled extension module.
2. If there exists a well maintained BSD or MIT **C/C++** implementation of the same algorithm that is not too big, you can write a **Cython wrapper** for it and include a copy of the source code of the library in the scikit-learn source tree: this strategy is used for the classes `svm.LinearSVC`, `svm.SVC` and `linear_model.LogisticRegression` (wrappers for liblinear and libsvm).

3. Otherwise, write an optimized version of your Python function using **Cython** directly. This strategy is used for the `linear_model.ElasticNet` and `linear_model.SGDClassifier` classes for instance.
4. **Move the Python version of the function in the tests** and use it to check that the results of the compiled extension are consistent with the gold standard, easy to debug Python version.
5. Once the code is optimized (not simple bottleneck spottable by profiling), check whether it is possible to have **coarse grained parallelism** that is amenable to **multi-processing** by using the `joblib.Parallel` class.

When using Cython, include the generated C source code alongside with the Cython source code. The goal is to make it possible to install the scikit on any machine with Python, Numpy, Scipy and C/C++ compiler.

3.2.2 Profiling Python code

In order to profile Python code we recommend to write a script that loads and prepare you data and then use the IPython integrated profiler for interactively exploring the relevant part for the code.

Suppose we want to profile the Non Negative Matrix Factorization module of the scikit. Let us setup a new IPython session and load the digits dataset and as in the *NMF for digits feature extraction* example:

```
In [1]: from scikits.learn.decomposition import NMF

In [2]: from scikits.learn.datasets import load_digits

In [3]: X = load_digits().data
```

Before starting the profiling session and engaging in tentative optimization iterations, it is important to measure the total execution time of the function we want to optimize without any kind of profiler overhead and save it somewhere for later reference:

```
In [4]: %timeit NMF(n_components=16, tol=1e-2).fit(X)
1 loops, best of 3: 1.7 s per loop
```

To have have a look at the overall performance profile using the `%prun` magic command:

```
In [5]: %prun -l nmf.py NMF(n_components=16, tol=1e-2).fit(X)
         14496 function calls in 1.682 CPU seconds

   Ordered by: internal time
   List reduced from 90 to 9 due to restriction <'nmf.py'>

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
       36    0.609    0.017    1.499    0.042 nmf.py:151(_nls_subproblem)
     1263    0.157    0.000    0.157    0.000 nmf.py:18(_pos)
        1    0.053    0.053    1.681    1.681 nmf.py:352(fit_transform)
      673    0.008    0.000    0.057    0.000 nmf.py:28(norm)
        1    0.006    0.006    0.047    0.047 nmf.py:42(_initialize_nmf)
       36    0.001    0.000    0.010    0.000 nmf.py:36(_sparseness)
       30    0.001    0.000    0.001    0.000 nmf.py:23(_neg)
        1    0.000    0.000    0.000    0.000 nmf.py:337(__init__)
        1    0.000    0.000    1.681    1.681 nmf.py:461(fit)
```

The `totime` columns is the most interesting: it gives to total time spent executing the code of a given function ignoring the time spent in executing the sub-functions. The real total time (local code + sub-function calls) is given by the `cumtime` column.

Note the use of the `-l nmf.py` that restricts the output to lines that contains the "nmf.py" string. This is useful to have a quick look at the hotspot of the nmf Python module it-self ignoring anything else.

Here is the begining of the output of the same command without the `-l nmf.py` filter:

```
In [5] %prun NMF(n_components=16, tol=1e-2).fit(X)
         16159 function calls in 1.840 CPU seconds

   Ordered by: internal time

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
     2833    0.653    0.000    0.653    0.000 {numpy.core._dotblas.dot}
       46    0.651    0.014    1.636    0.036 nmf.py:151(_nls_subproblem)
     1397    0.171    0.000    0.171    0.000 nmf.py:18(_pos)
     2780    0.167    0.000    0.167    0.000 {method 'sum' of 'numpy.ndarray' objects}
        1    0.064    0.064    1.840    1.840 nmf.py:352(fit_transform)
     1542    0.043    0.000    0.043    0.000 {method 'flatten' of 'numpy.ndarray' objects}
      337    0.019    0.000    0.019    0.000 {method 'all' of 'numpy.ndarray' objects}
     2734    0.011    0.000    0.181    0.000 fromnumeric.py:1185(sum)
        2    0.010    0.005    0.010    0.005 {numpy.linalg.lapack_lite.dgesdd}
      748    0.009    0.000    0.065    0.000 nmf.py:28(norm)
...
```

The above results show that the execution is largely dominated by dot products operations (delegated to blas). Hence there is probably no huge gain to expect by rewriting this code in Cython or C/C++: in this case out of the 1.7s total execution time, almost 0.7s are spent in compiled code we can consider optimal. By rewriting the rest of the Python code and assuming we could achieve a 1000% boost on this portion (which is highly unlikely given the shallowness of the Python loops), we would not gain more than a 2.4x speed-up globally.

Hence major improvements can only be achieved by **algorithmic improvements** in this particular example (e.g. trying to find operation that are both costly and useless to avoid computing then rather than trying to optimize their implementation).

It is however still interesting to check what's happening inside the `_nls_subproblem` function which is the hotspot if we only consider Python code: it takes around 100% of the cumulated time of the module. In order to better understand the profile of this specific function, let us install `line-prof` and wire it to IPython:

```
$ pip install line-profiler
$ vim ~/.ipython/ipy_user_conf.py
```

Ensure the following lines are present:

```
import IPython.ipapi
ip = IPython.ipapi.get()
```

Towards the end of the file, define the `%lprun` magic:

```
import line_profiler
ip.expose_magic('lprun', line_profiler.magic_lprun)
```

Now restart IPython and let us use this new toy:

```
In [1]: from scikits.learn.datasets import load_digits

In [2]: from scikits.learn.decomposition.nmf import _nls_subproblem, NMF

In [3]: X = load_digits().data

In [4]: %lprun -f _nls_subproblem NMF(n_components=16, tol=1e-2).fit(X)
Timer unit: 1e-06 s

File: scikits/learn/decomposition/nmf.py
Function: _nls_subproblem at line 137
Total time: 1.73153 s
```

```
Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
   137                                           def _nls_subproblem(V, W, H_init, tol, max_iter):
   138                                               """Non-negative least square solver
   ...
   170                                               """
   171        48         5863    122.1      0.3      if (H_init < 0).any():
   172                                                     raise ValueError("Negative values in H_init
   173
   174        48          139      2.9      0.0      H = H_init
   175        48       112141   2336.3      5.8      WtV = np.dot(W.T, V)
   176        48        16144    336.3      0.8      WtW = np.dot(W.T, W)
   177
   178                                               # values justified in the paper
   179        48          144      3.0      0.0      alpha = 1
   180        48          113      2.4      0.0      beta = 0.1
   181       638         1880      2.9      0.1      for n_iter in xrange(1, max_iter + 1):
   182       638       195133    305.9     10.2          grad = np.dot(WtW, H) - WtV
   183       638       495761    777.1     25.9          proj_gradient = norm(grad[np.logical_or(grac
   184       638         2449      3.8      0.1          if proj_gradient < tol:
   185        48          130      2.7      0.0              break
   186
   187      1474         4474      3.0      0.2          for inner_iter in xrange(1, 20):
   188      1474        83833     56.9      4.4              Hn = H - alpha * grad
   189                                                       # Hn = np.where(Hn > 0, Hn, 0)
   190      1474       194239    131.8     10.1              Hn = _pos(Hn)
   191      1474        48858     33.1      2.5              d = Hn - H
   192      1474       150407    102.0      7.8              gradd = np.sum(grad * d)
   193      1474       515390    349.7     26.9              dQd = np.sum(np.dot(WtW, d) * d)
   ...
```

By looking at the top values of the `% Time` column it is really easy to pin-point the most expensive expressions that would deserve additional care.

3.2.3 Performance tips for the Cython developer

If the profiling of the python code reveals that the python interpreter overhead is larger by one order of magnitude or more than the cost of the actual numerical computation (e.g. `for` loops over vector components, nested evaluation of conditional expression, scalar arithmetics...), it is probably adequate to extract the hotspot portion of the code as a standalone function in a `.pyx` file and add static type declarations and then use **cython_** to generate a C program suitable to be compiled as a Python extension module.

The official documentation available http://docs.cython.org/ contains tutorial and reference guide for developing such a module. In the following we will just highlight a couple of tricks that we found important in practice on the existing cython codebase in the scikit-learn project.

TODO: html report, type declarations, bound checks, division by zero checks, memory alignement, direct blas calls...

- http://www.euroscipy.org/file/3696?vid=download
- http://conference.scipy.org/proceedings/SciPy2009/paper_1/
- http://conference.scipy.org/proceedings/SciPy2009/paper_2/

3.2.4 Profiling compiled extensions

When working with compiled extensions (written in C/C++ with a wrapper or directly as Cython extension), the default Python profiler is useless: we need a dedicated tool to instrospect what's happening inside the compiled extension itself.

In order to profile compiled Python extensions one could use `gprof` after having recompiled the project with `gcc -pg` and using the `python-dbg` variant of the interpreter on debian / ubuntu: however this approach requires to also have `numpy` and `scipy` recompiled with `-pg` which is rather complicated to get working.

Fortunately there exist two alternative profilers that don't require you to recompile everything.

Using google-perftools

TODO

- https://github.com/fabianp/yep
- http://fseoane.net/blog/2011/a-profiler-for-python-extensions/

Note: google-perftools provides a nice 'line by line' report mode that can be triggered with the `--lines` option. However this does not seem to work correctly at the time of writing. This issue can be tracked on the project issue tracker.

Using valgrind / callgrind / kcachegrind

TODO

3.2.5 Multi-core parallelism using `joblib.Parallel`

TODO: give a simple teaser example here.

Checkout the official joblib documentation:

- http://packages.python.org/joblib/

3.2.6 A sample algorithmic trick: warm restarts for cross validation

TODO: demonstrate the warm restart tricks for cross validation of linear regression with Coordinate Descent.

3.3 About us

This is a community effort, and as such many people have contributed to it over the years.

3.3.1 History

This project was started in 2007 as a Google Summer of Code project by David Cournapeau. Later that year, Matthieu Brucher started work on this project as part of his thesis.

In 2010 Fabian Pedregosa, Gael Varoquaux, Alexandre Gramfort and Vincent Michel took leadership of the project and made the first public release, February the 1st 2010. Since then, several releases have appeard following a ~3 month cycle.

3.3.2 People

- David Cournapeau, 2007-2009
- Fred Mailhot, 2008, Artificial Neural Networks (ann) module.
- David Cooke
- David Huard
- Dave Morrill
- Ed Schofield
- Eric Jones, 2008, Genetic Algorithms (ga) module. No longer part of scikits.learn.
- Jarrod Millman
- Matthieu Brucher contributed the manifold module. It is not currently part of the scikit, althouth it is planned to be newly included in the upcoming 0.7 release.
- Travis Oliphant
- Pearu Peterson
- Fabian Pedregosa joined the project in January 2010 and is the current maintainer.
- Gael Varoquaux
- Jake VanderPlas contributed the BallTree module in February 2010.
- Alexandre Gramfort
- Olivier Grisel
- Bertrand Thirion, contributed the hierarchical clustering module together with Gael Varoquaux, Alexandre Gramfort and Vincent Michel.
- Vincent Michel.
- Chris Filo Gorgolewski
- Angel Soler Gollonet contributed the official logo and web page layout.
- Yaroslav Halchenko is the maintainer for Debian OS and has contributed several fixes.
- Ron Weiss joined the project in July 2010 and contributed both the mixture and hmm module.
- Virgile Fritsch. Bug fixes.
- Mathieu Blondel joined the project in September 2010 and has worked since on the sparse matrix support, Ridge generalized crossval, text feature extraction and general bug fixes.
- Peter Prettenhofer joined the project in October 2010 and contributed the *Stochastic Gradient Descent* module as well as several examples and fixes.
- Vincent Dubourg joined the project in November 2010 and contributed the *Gaussian Processes* module.
- Alexandre Passos joined the project in November 2010 contributed the fast SVD variant.
- Vlad Niculae joined the project in March 2011 and contributed the non-negative matrix factorization module.

- Thouis (Ray) Jones joined the project in contributed the Cython bindings

for the BallTree class.

If I forgot anyone, do not hesitate to send me an email to fabian.pedregosa@inria.fr and I'll include you in the list.

3.3.3 Funding

INRIA actively supports this project. It has provided funding for Fabian Pedregosa to work on this project full time in the period 2010-2012. It also hosts coding sprints and other events.

Google sponsored David Cournapeau with a Summer of Code Scolarship in the summer of 2007. If you would like to participate in the next Google Summer of code program, please see this page

The NeuroDebian project providing Debian packaging and contributions is supported by Dr. James V. Haxby (Dartmouth College).

PYTHON MODULE INDEX

S

PYTHON MODULE INDEX

S

INDEX

F

S