ML101-evaluated

October 13, 2016

1 Some Python Data Science Resources

1.1 Python

Use a scientific Python distribution `Anaconda` (I use Python 2.7 version) which comes together with lots of libraries, jupyter notebook.. The distribution can be installed locally in the home directory..

1.1.1 General libraries

- `numpy` : **fast array library**
- `scipy` : various higher level scientific routines
- `matplotlib` : a plotting library

1.1.2 More specialized libraries

- `scikit-learn` : **machine learning library - lots of implemented machine learning algorithms**
- `pandas` : R-like concepts like `data.frame`
- `scikit-image` : various computer vision algorithms
- `opencv` : bindings to a powerful C++ computer vision library
- ...

1.1.3 Neural networks

- `keras` : **very easy to use and flexible**
- `lasagne`
- `caffe`
- `mxnet` : fast and efficient

1.1.4 Other

- `xgboost` : **very good and fast gradient boosted trees**
- `rpy2` : do computations using R from Python...
- `mne-python` : library for analyzing/plotting EEG/MEG data
- `pyeeg` : some utilities for analyzing (EEG) time-series data
- ...

2 scikit-learn examples

`scikit-learn` implements a bewildering number of algorithms. It has a very good user manual but it is very easy to get lost which algorithms to use...

Fortunately it is enough to use just a basic few:

classification: Logistic Regression, Support Vector Machine, Nearest Neighbour, Random Forest, Gradient Boosted Trees

regression: Ridge, regression versions of the above

unsupervised: RandomizedPCA, FastICA, K-Means (clustering)

For neural networks and gradient boosted trees for large datasets its better to use other libraries (`keras`, `xgboost`)

2.1 Example: recognizing handwritten digits

Load necessary libraries:

```
In [1]: %matplotlib inline
        from numpy import *
        import matplotlib.pyplot as plt
        from sklearn import datasets
```

Load a toy version of handwritten digits: only 8x8

```
In [2]: digits = datasets.load_digits()
        print digits.images.shape
```

```
(1797, 8, 8)
```

```
In [3]: for i in range(40):
            plt.subplot(4,10,i+1)
            plt.axis('off')
            plt.imshow(digits.images[i],cmap=plt.cm.gray_r)
        plt.show()
```

```
In [4]: print digits.target[:40]
```

```
[0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 9 5 5 6 5 0
 9 8 9]
```

2.1.1 Prepare data

It may be good to shuffle the data...

```
In [5]: random.seed(555)
        random.shuffle(digits.images)
        random.seed(555)
        random.shuffle(digits.target)
```

```
In [6]: for i in range(40):
            plt.subplot(4,10,i+1)
            plt.axis('off')
            plt.imshow(digits.images[i],cmap=plt.cm.gray_r)
        plt.show()
        print digits.target[:40]
```

```
[4 3 5 2 0 3 7 3 1 4 4 5 2 6 8 5 9 9 3 6 1 6 8 0 0 2 3 2 0 2 1 6 0 3 7 5 8
 2 8 0]
```

Most classifiers require vectors of numbers - transform images to 64 element vectors

Note: in this way we loose geometrical information which pixels are neighbouring.. (this is only recovered in Convolutional Neural Networks - see later)

```
In [7]: data=digits.images.reshape((len(digits.images),-1))
        print data.shape
        n=len(data)
```

```
(1797, 64)
```

Check the range of data

```
In [8]: print amin(data), amax(data)
```

```
0.0 16.0
```

Normalize to the interval [0,1]

```
In [9]: data[:,:]=data/16.0
        print amin(data), amax(data)
```

```
0.0 1.0
```

2.1.2 Create training and test data

Never test your model on the same data that you used to train it - split the whole dataset into a separate train and test set. The best way to do it is to use say 5-fold cross-validation (CV): split data into 5 chunks and then make 5 splits into train/test datasets.

Then choose classifier and its parameters based on its performance on all the 5 splits..

```
In [10]: from sklearn.cross_validation import KFold
         kf=KFold(20, n_folds=5)
         for tr, tst in kf:
             print 'train:', tr, 'test:', tst
```

```
train: [ 4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19] test: [0 1 2 3]
train: [ 0  1  2  3  8  9 10 11 12 13 14 15 16 17 18 19] test: [4 5 6 7]
train: [ 0  1  2  3  4  5  6  7 12 13 14 15 16 17 18 19] test: [ 8  9 10 11]
train: [ 0  1  2  3  4  5  6  7  8  9 10 11 16 17 18 19] test: [12 13 14 15]
train: [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15] test: [16 17 18 19]
```

There is a more refined version which tries to keep the proportions of the classes same in each fold (`KStratifiedFold`).

Here for simplicity we will make just a single split...

```
In [11]: nn=2*n/3
         X=data[:nn]
         y=digits.target[:nn]
         Xt=data[nn:]
         yt=digits.target[nn:]
```

2.2 Linear models

The first thing to try is the simplest linear model - for classification this is `LogisticRegression`, for regression this is `Ridge`.

- it will be a baseline for more advanced models
- for (noisy) data with lots of features it works remarkably well
- there is only a single parameter to tune (the amount of *regularization* to control overfitting/dependence on outliers)
- for regularization to work one should have all features to have a comparable numerical range
- then the magnitudes of linear coefficients indicate something about the features importance [**note:** there are much more sophisticated ways for analyzing that]

```
In [12]: from sklearn.linear_model import *
         from sklearn.metrics import *
```

```
In [13]: clf=LogisticRegression()
         clf.fit(X,y)
```

Out[13]: LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
                  intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1,
                  penalty='l2', random_state=None, solver='liblinear', tol=0.0001,
                  verbose=0, warm_start=False)

```
In [14]: preds=clf.predict(Xt)
```

```
In [15]: print accuracy_score(yt,preds)
```

```
0.961602671119
```

```
In [16]: print preds[10:30], yt[10:30]
```

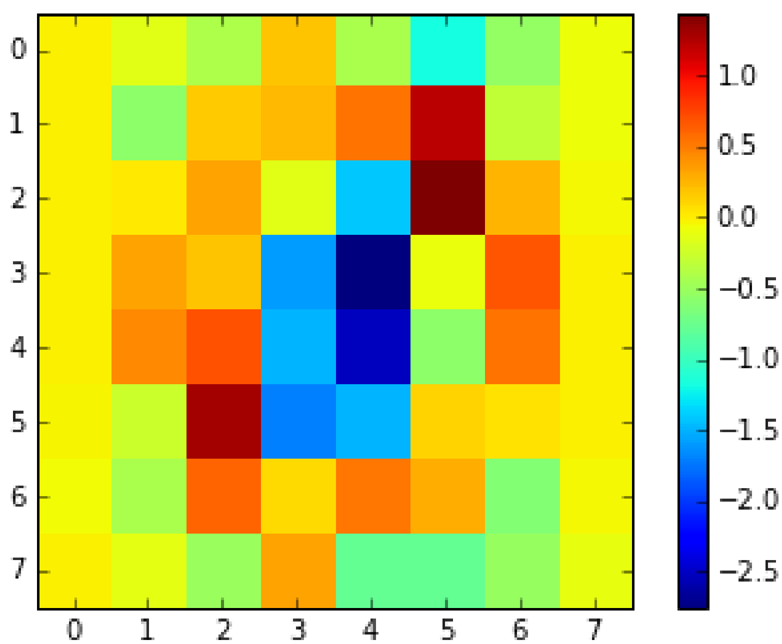
```
[3 9 5 7 1 0 5 9 3 3 9 4 3 3 6 9 4 6 1 8] [3 9 5 7 1 0 5 9 3 3 9 4 3 3 6 9 4 6 3 8]
```

```
In [17]: print confusion_matrix(yt,preds)
```

```
[[50  0  0  0  0  0  0  0  0  0]
 [ 0 63  2  0  0  0  1  0  0  0]
 [ 0  0 48  0  0  0  0  0  0  0]
 [ 0  1  1 49  0  0  0  2  0  0]
 [ 0  1  0  0 67  0  0  0  1  1]
 [ 0  0  0  0  0 65  0  0  0  0]
 [ 0  1  0  0  0  0 58  0  0  0]
 [ 0  0  0  0  0  0  0 63  1  1]
 [ 0  3  0  0  0  0  2  0 50  0]
 [ 0  1  0  1  0  1  0  0  2 63]]
```

rows: true classes; columns: predicted classes
We can examine the coefficients corresponding to the class of 0

```
In [18]: cfs0=clf.coef_[0].reshape((8,8))
         plt.imshow(cfs0,interpolation="nearest")
         plt.colorbar()
         plt.show()
```



```
In [19]: clf=LogisticRegressionCV()
         clf.fit(X,y)
         preds=clf.predict(Xt)
```

```
In [20]: print accuracy_score(yt,preds)
```

```
0.966611018364
```

```
In [21]: clf.C_
```

```
Out[21]: array([   2.7825594 ,   21.5443469 ,   21.5443469 ,    2.7825594 ,
                  21.5443469 ,    2.7825594 ,   21.5443469 ,  166.81005372,
                   2.7825594 ,   21.5443469 ])
```

2.3 Support Vector Machines

These can be either linear or nonlinear - here the default is nonlinear and the nonlinearity is parametrized by a gaussian *kernel* (kernel=`rbf` - radial basis functions). One has to set two parameters: regularization parameter `C` and the width of the gaussian

```
In [34]: from sklearn.svm import SVC
         clf = SVC(C=100,gamma=0.01)
         clf.fit(X,y)
         preds=clf.predict(Xt)
```

```
In [35]: print accuracy_score(yt,preds)
```

```
0.986644407346
```

```
In [36]: print confusion_matrix(yt,preds)
```

```
[[50  0  0  0  0  0  0  0  0  0]
 [ 0 66  0  0  0  0  0  0  0  0]
 [ 0  0 48  0  0  0  0  0  0  0]
 [ 0  0  0 52  0  0  0  0  1  0]
 [ 0  0  0  0 70  0  0  0  0  0]
 [ 0  0  0  0  0 64  0  0  0  1]
 [ 0  1  0  0  0  0 58  0  0  0]
 [ 0  0  0  0  0  0  0 64  0  1]
 [ 0  1  0  0  1  0  0  0 53  0]
 [ 0  0  0  1  0  1  0  0  0 66]]
```

Default parameters:

```
In [24]: clf = SVC()
         clf.fit(X,y)
         preds=clf.predict(Xt)
         print accuracy_score(yt,preds)
```

```
0.954924874791
```

2.4 Random Forest

Very good strictly nonlinear classifier, essentially one key parameter `n_estimators` (number of trees) - the more the better...

```
In [25]: from sklearn.ensemble import RandomForestClassifier as RFC
```

```
In [26]: clf=RFC(n_estimators=500)
         clf.fit(X,y)
         preds=clf.predict(Xt)
         print accuracy_score(yt,preds)
```

```
0.976627712855
```

2.5 Gradient Boosted Trees

Very good nonlinear classifier (often better than Random Forest) - more parameters to tune: number of trees, learning rate, size of the trees.

For more complex datasets often *much* better than linear models...

```
In [27]: from sklearn.ensemble import GradientBoostingClassifier as GBC
```

```
In [28]: clf=GBC(n_estimators=500)
         clf.fit(X,y)
         preds=clf.predict(Xt)
         print accuracy_score(yt,preds)
```

```
0.964941569282
```

A very good implementation (fast and multithreaded for large datasets) is `xgboost`

```
In [29]: from xgboost import XGBClassifier
```

```
In [30]: clf=XGBClassifier(max_depth=3, n_estimators=500)
         clf.fit(X,y)
         preds=clf.predict(Xt)
         print accuracy_score(yt,preds)
```

```
0.964941569282
```

2.6 Nearest neighbours

Makes classification according to k nearest neighbours.

Note: Problems for high dimensional data: * The curse of dimensionality *

```
In [31]: from sklearn.neighbors import KNeighborsClassifier
```

```
In [32]: clf=KNeighborsClassifier()
         clf.fit(X,y)
         preds=clf.predict(Xt)
         print accuracy_score(yt,preds)
```

```
0.986644407346
```

```
In [33]: print confusion_matrix(yt,preds)
```

```
[[50  0  0  0  0  0  0  0  0  0]
 [ 0 66  0  0  0  0  0  0  0  0]
 [ 0  0 48  0  0  0  0  0  0  0]
 [ 0  0  0 52  0  0  0  1  0  0]
 [ 0  0  0  0 69  0  0  1  0  0]
 [ 0  0  0  0  0 65  0  0  0  0]
 [ 0  0  0  0  0  0 59  0  0  0]
 [ 0  0  0  0  0  0  0 64  0  1]
 [ 0  3  1  0  0  0  0  0 51  0]
 [ 0  1  0  0  0  0  0  0  0 67]]
```

3 Neural networks

`keras` - a very good neural network library

- very easy to use
- can use graphic card GPU's (NVIDIA only!) for computation - **crucial** for larger convolutional networks
- can produce more involved network topologies (multiple inputs/outputs, merges between various layers) - so called Functional API
- includes all basic layer types including convolutional, recurrent
- based either on `Theano` or `TensorFlow` low-level backend

There exist other possibilities: `caffe`, `lasagne`, `mxnet`,...

```
In [37]: from keras.models import Sequential
         from keras.layers.core import Dense, Dropout, Activation
         from keras.optimizers import SGD, Adam, RMSprop
         from keras.layers.advanced_activations import *
```

```
Using Theano backend.
```

```
In [39]: model = Sequential()
         model.add(Dense(64, input_dim=X.shape[1], activation='relu'))
         model.add(Dense(64, activation='relu'))
         model.add(Dense(10))
         model.add(Activation('softmax'))
```

```
In [40]: model.compile(optimizer='adam',
                       loss='sparse_categorical_crossentropy',
                       metrics=['accuracy'])
```

```
In [41]: from keras.utils.np_utils import to_categorical
         ys=to_categorical(y)
```

```
In [42]: print y[1], ys[1]
```

```
3 [ 0.  0.  0.  1.  0.  0.  0.  0.  0.  0.]
```

```
In [43]: model.fit(X, y, nb_epoch=30, batch_size=128, validation_data=(Xt,yt))
```

```
Train on 1198 samples, validate on 599 samples
Epoch 1/30
1198/1198 [==============================] - 0s - loss: 2.2499 - acc: 0.1878 - val_loss: 2.1526 - val_ac
Epoch 2/30
1198/1198 [==============================] - 0s - loss: 2.0808 - acc: 0.4249 - val_loss: 1.9894 - val_ac
```

```
Epoch 3/30
1198/1198 [==============================] - 0s - loss: 1.8953 - acc: 0.6110 - val_loss: 1.7899 - val_ac
Epoch 4/30
1198/1198 [==============================] - 0s - loss: 1.6721 - acc: 0.6953 - val_loss: 1.5535 - val_ac
Epoch 5/30
1198/1198 [==============================] - 0s - loss: 1.4208 - acc: 0.7588 - val_loss: 1.2931 - val_ac
Epoch 6/30
1198/1198 [==============================] - 0s - loss: 1.1607 - acc: 0.7880 - val_loss: 1.0398 - val_ac
Epoch 7/30
1198/1198 [==============================] - 0s - loss: 0.9181 - acc: 0.8239 - val_loss: 0.8147 - val_ac
Epoch 8/30
1198/1198 [==============================] - 0s - loss: 0.7195 - acc: 0.8806 - val_loss: 0.6434 - val_ac
Epoch 9/30
1198/1198 [==============================] - 0s - loss: 0.5689 - acc: 0.8973 - val_loss: 0.5195 - val_ac
Epoch 10/30
1198/1198 [==============================] - 0s - loss: 0.4625 - acc: 0.9098 - val_loss: 0.4342 - val_ac
Epoch 11/30
1198/1198 [==============================] - 0s - loss: 0.3880 - acc: 0.9157 - val_loss: 0.3752 - val_ac
Epoch 12/30
1198/1198 [==============================] - 0s - loss: 0.3307 - acc: 0.9307 - val_loss: 0.3273 - val_ac
Epoch 13/30
1198/1198 [==============================] - 0s - loss: 0.2851 - acc: 0.9424 - val_loss: 0.2967 - val_ac
Epoch 14/30
1198/1198 [==============================] - 0s - loss: 0.2525 - acc: 0.9474 - val_loss: 0.2709 - val_ac
Epoch 15/30
1198/1198 [==============================] - 0s - loss: 0.2269 - acc: 0.9583 - val_loss: 0.2471 - val_ac
Epoch 16/30
1198/1198 [==============================] - 0s - loss: 0.2050 - acc: 0.9583 - val_loss: 0.2360 - val_ac
Epoch 17/30
1198/1198 [==============================] - 0s - loss: 0.1924 - acc: 0.9574 - val_loss: 0.2186 - val_ac
Epoch 18/30
1198/1198 [==============================] - 0s - loss: 0.1735 - acc: 0.9674 - val_loss: 0.2077 - val_ac
Epoch 19/30
1198/1198 [==============================] - 0s - loss: 0.1607 - acc: 0.9691 - val_loss: 0.1963 - val_ac
Epoch 20/30
1198/1198 [==============================] - 0s - loss: 0.1488 - acc: 0.9725 - val_loss: 0.1900 - val_ac
Epoch 21/30
1198/1198 [==============================] - 0s - loss: 0.1401 - acc: 0.9725 - val_loss: 0.1804 - val_ac
Epoch 22/30
1198/1198 [==============================] - 0s - loss: 0.1304 - acc: 0.9783 - val_loss: 0.1760 - val_ac
Epoch 23/30
1198/1198 [==============================] - 0s - loss: 0.1239 - acc: 0.9775 - val_loss: 0.1697 - val_ac
Epoch 24/30
1198/1198 [==============================] - 0s - loss: 0.1189 - acc: 0.9775 - val_loss: 0.1644 - val_ac
Epoch 25/30
1198/1198 [==============================] - 0s - loss: 0.1129 - acc: 0.9800 - val_loss: 0.1605 - val_ac
Epoch 26/30
1198/1198 [==============================] - 0s - loss: 0.1048 - acc: 0.9825 - val_loss: 0.1537 - val_ac
Epoch 27/30
1198/1198 [==============================] - 0s - loss: 0.0998 - acc: 0.9833 - val_loss: 0.1490 - val_ac
Epoch 28/30
1198/1198 [==============================] - 0s - loss: 0.0954 - acc: 0.9825 - val_loss: 0.1452 - val_ac
Epoch 29/30
1198/1198 [==============================] - 0s - loss: 0.0900 - acc: 0.9808 - val_loss: 0.1446 - val_ac
```

```
Epoch 30/30
1198/1198 [==============================] - 0s - loss: 0.0859 - acc: 0.9858 - val_loss: 0.1370 - val_ac
```

Out[43]: `<keras.callbacks.History at 0x7f1f416f4210>`

In [44]:
```
preds=model.predict_classes(Xt)
print
print accuracy_score(yt,preds)
```

```
599/599 [==============================] - 0s

0.9632721202
```

3.0.1 Comments

- this dataset is very simple and small
- therefore simpler models work as well or better than more complex ones
- for various kinds of datasets various algorithms are best - there is no single best one