ch06

November 11, 2022

Python Machine Learning 3rd Edition by Sebastian Raschka, Packt Publishing Ltd. 2019

Code Repository: https://github.com/rasbt/python-machine-learning-book-3rd-edition

Code License: MIT License

1 Python Machine Learning - Code Examples

2 Chapter 6 - Learning Best Practices for Model Evaluation and Hyperparameter Tuning

Note that the optional watermark extension is a small IPython notebook plugin that I developed to make the code reproducible. You can just skip the following line(s).

[ ]:
```
%load_ext watermark
%watermark -a "Sebastian Raschka" -u -d -v -p numpy,pandas,matplotlib,sklearn
```

```
Sebastian Raschka
last updated: 2020-03-04

CPython 3.7.1
IPython 7.12.0

numpy 1.18.1
pandas 1.0.1
matplotlib 3.1.0
sklearn 0.22
```

The use of `watermark` is optional. You can install this Jupyter extension via

```
conda install watermark -c conda-forge
```

or

```
pip install watermark
```

For more information, please see: https://github.com/rasbt/watermark.

2.0.1 Overview

- Streamlining workflows with pipelines
  - Loading the Breast Cancer Wisconsin dataset

[ ]:
```
from IPython.display import Image
%matplotlib inline
```

3 Streamlining workflows with pipelines

…

3.1 Loading the Breast Cancer Wisconsin dataset

[ ]:
```
import pandas as pd

df = pd.read_csv('https://archive.ics.uci.edu/ml/'
                 'machine-learning-databases'
                 '/breast-cancer-wisconsin/wdbc.data', header=None)

# if the Breast Cancer dataset is temporarily unavailable from the
# UCI machine learning repository, un-comment the following line
# of code to load the dataset from a local path:

# df = pd.read_csv('wdbc.data', header=None)

df.head()
```

[ ]:
```
          0  1      2      3       4       5        6        7       8  \
0    842302  M  17.99  10.38  122.80  1001.0  0.11840  0.27760  0.3001
1    842517  M  20.57  17.77  132.90  1326.0  0.08474  0.07864  0.0869
2  84300903  M  19.69  21.25  130.00  1203.0  0.10960  0.15990  0.1974
3  84348301  M  11.42  20.38   77.58   386.1  0.14250  0.28390  0.2414
4  84358402  M  20.29  14.34  135.10  1297.0  0.10030  0.13280  0.1980
```

```
         9  ...     22     23      24      25      26      27      28      29  \
0  0.14710  ...  25.38  17.33  184.60  2019.0  0.1622  0.6656  0.7119  0.2654
1  0.07017  ...  24.99  23.41  158.80  1956.0  0.1238  0.1866  0.2416  0.1860
2  0.12790  ...  23.57  25.53  152.50  1709.0  0.1444  0.4245  0.4504  0.2430
3  0.10520  ...  14.91  26.50   98.87   567.7  0.2098  0.8663  0.6869  0.2575
4  0.10430  ...  22.54  16.67  152.20  1575.0  0.1374  0.2050  0.4000  0.1625

       30       31
0  0.4601  0.11890
1  0.2750  0.08902
2  0.3613  0.08758
3  0.6638  0.17300
4  0.2364  0.07678

[5 rows x 32 columns]
```

[ ]:
```
df.shape
```

[ ]:
```
(569, 32)
```

[ ]:
```
from sklearn.preprocessing import LabelEncoder

X = df.loc[:, 2:].values
y = df.loc[:, 1].values
le = LabelEncoder()
y = le.fit_transform(y)
le.classes_
```

[ ]:
```
array(['B', 'M'], dtype=object)
```

[ ]:
```
le.transform(['M', 'B'])
```

[ ]:
```
array([1, 0])
```

[ ]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = \
    train_test_split(X, y,
                     test_size=0.20,
                     stratify=y,
                     random_state=1)
```

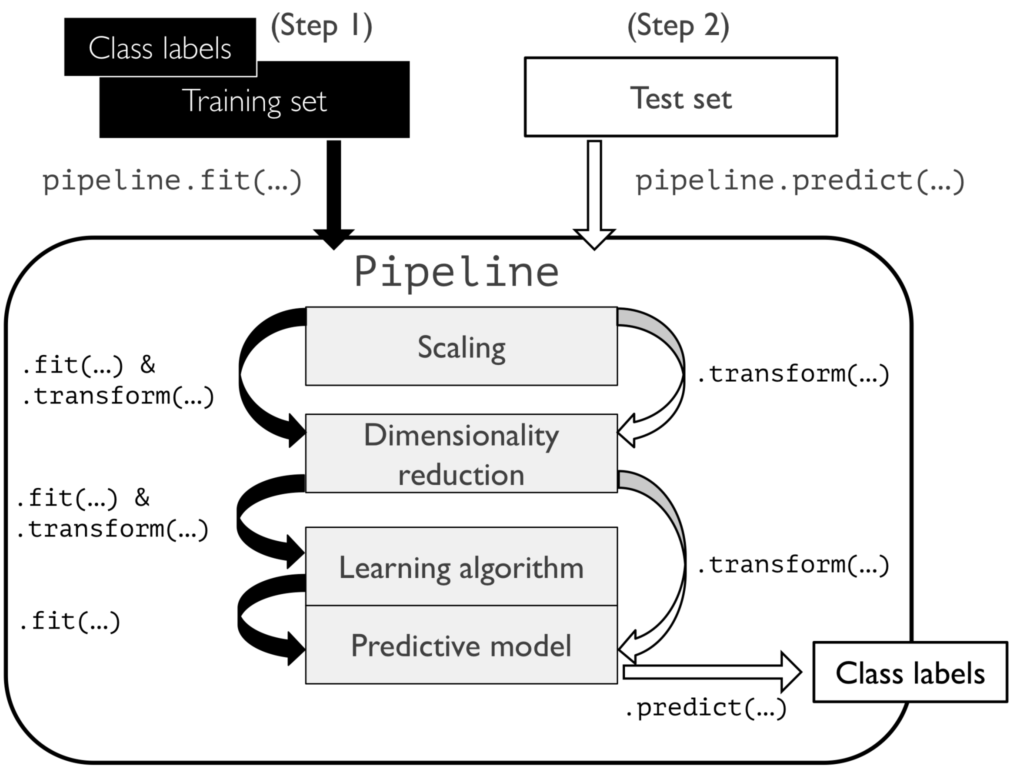
3.2 Combining transformers and estimators in a pipeline

[ ]:
```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import make_pipeline

pipe_lr = make_pipeline(StandardScaler(),
                        PCA(n_components=2),
                        LogisticRegression(random_state=1, solver='lbfgs'))

pipe_lr.fit(X_train, y_train)
y_pred = pipe_lr.predict(X_test)
print('Test Accuracy: %.3f' % pipe_lr.score(X_test, y_test))
```

```
Test Accuracy: 0.956
```

[ ]:
```
Image(filename='images/06_01.png', width=500)
```

[ ]:



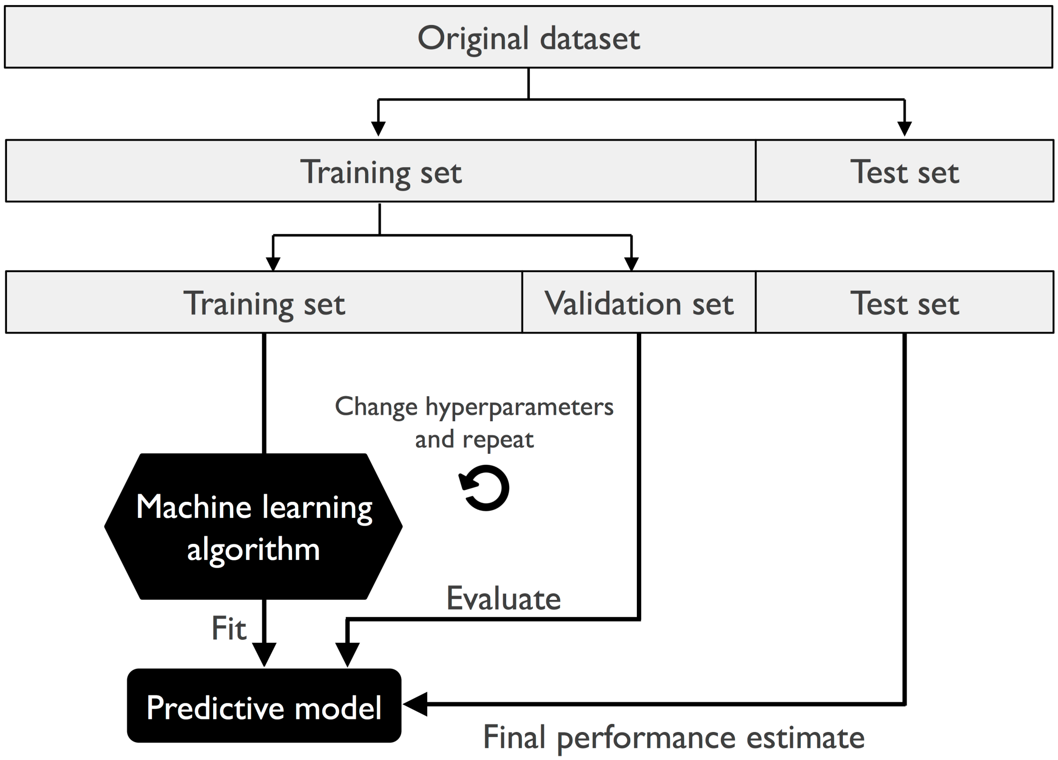
4 Using k-fold cross validation to assess model performance

…

4.1 The holdout method

[ ]:
```
Image(filename='images/06_02.png', width=500)
```

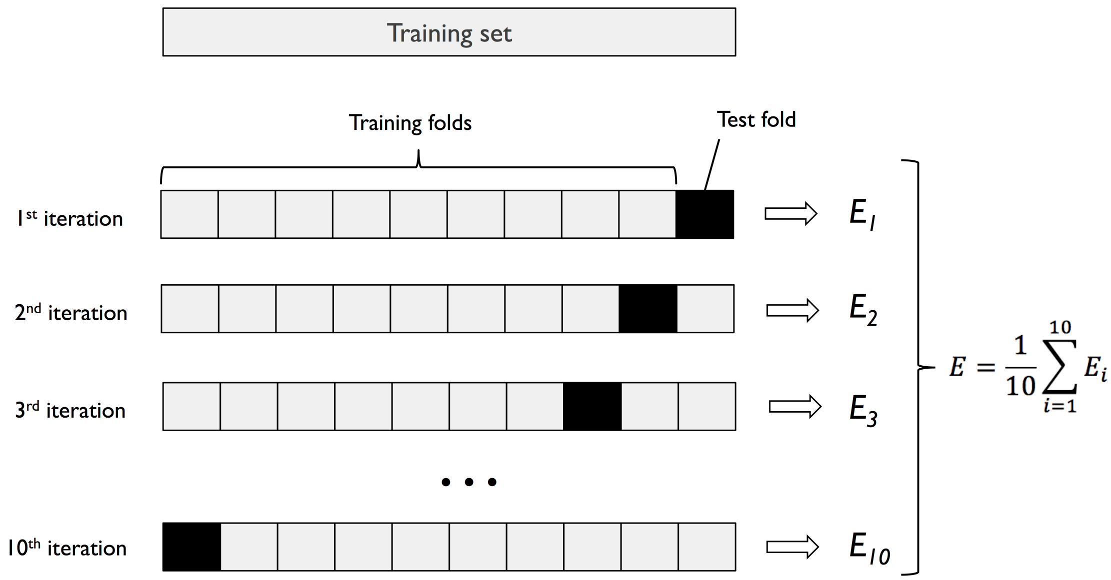
[ ]:



4.2 K-fold cross-validation

[ ]:
```
Image(filename='images/06_03.png', width=500)
```

[ ]:



[ ]:
```python
import numpy as np
from sklearn.model_selection import StratifiedKFold


kfold = StratifiedKFold(n_splits=10).split(X_train, y_train)

scores = []
for k, (train, test) in enumerate(kfold):
    pipe_lr.fit(X_train[train], y_train[train])
    score = pipe_lr.score(X_train[test], y_train[test])
    scores.append(score)
    print('Fold: %2d, Class dist.: %s, Acc: %.3f' % (k+1,
          np.bincount(y_train[train]), score))

print('\nCV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
```

```
Fold:  1, Class dist.: [256 153], Acc: 0.935
Fold:  2, Class dist.: [256 153], Acc: 0.935
Fold:  3, Class dist.: [256 153], Acc: 0.957
Fold:  4, Class dist.: [256 153], Acc: 0.957
Fold:  5, Class dist.: [256 153], Acc: 0.935
Fold:  6, Class dist.: [257 153], Acc: 0.956
Fold:  7, Class dist.: [257 153], Acc: 0.978
Fold:  8, Class dist.: [257 153], Acc: 0.933
Fold:  9, Class dist.: [257 153], Acc: 0.956
Fold: 10, Class dist.: [257 153], Acc: 0.956
```

```
CV accuracy: 0.950 +/- 0.014
```

[ ]:
```
from sklearn.model_selection import cross_val_score

scores = cross_val_score(estimator=pipe_lr,
                         X=X_train,
                         y=y_train,
                         cv=10,
                         n_jobs=1)
print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
```

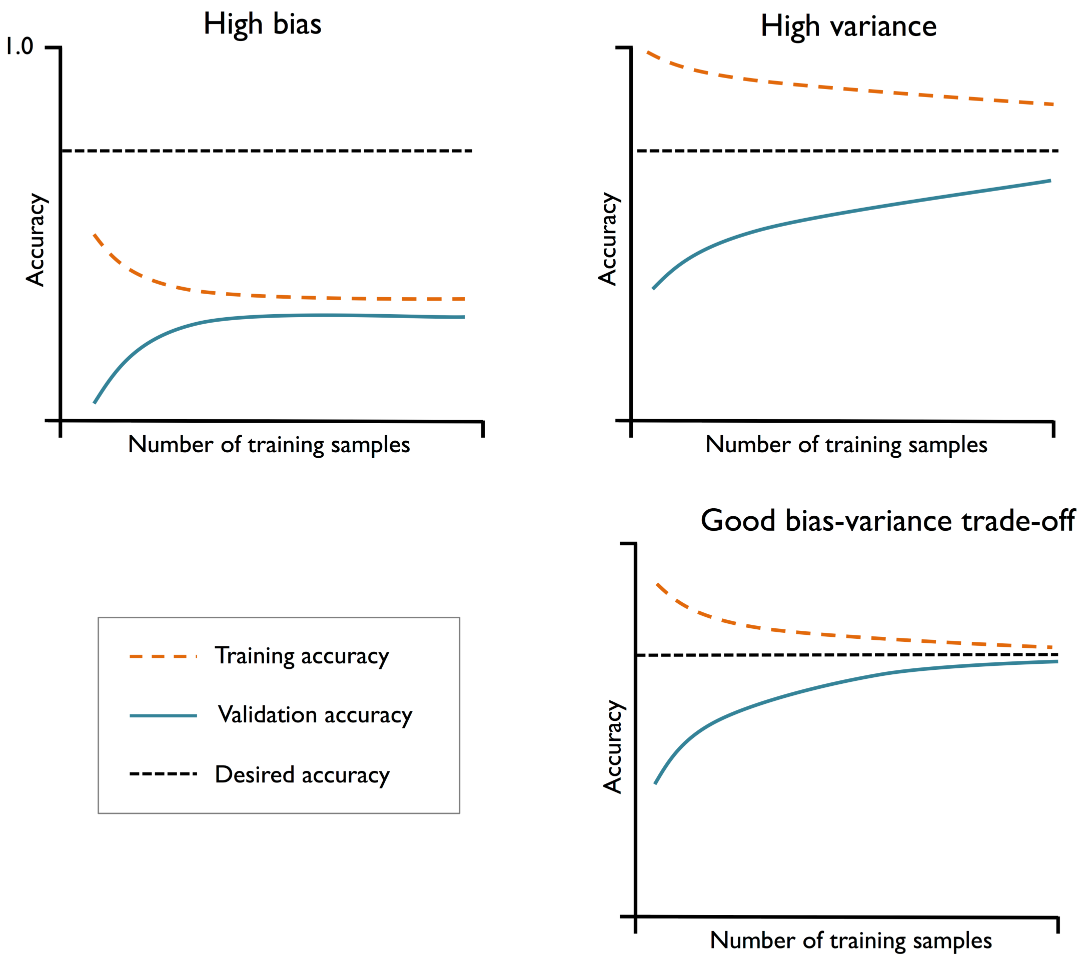
```
CV accuracy scores: [0.93478261 0.93478261 0.95652174 0.95652174 0.93478261
0.95555556
 0.97777778 0.93333333 0.95555556 0.95555556]
CV accuracy: 0.950 +/- 0.014
```

5 Debugging algorithms with learning curves

5.1 Diagnosing bias and variance problems with learning curves

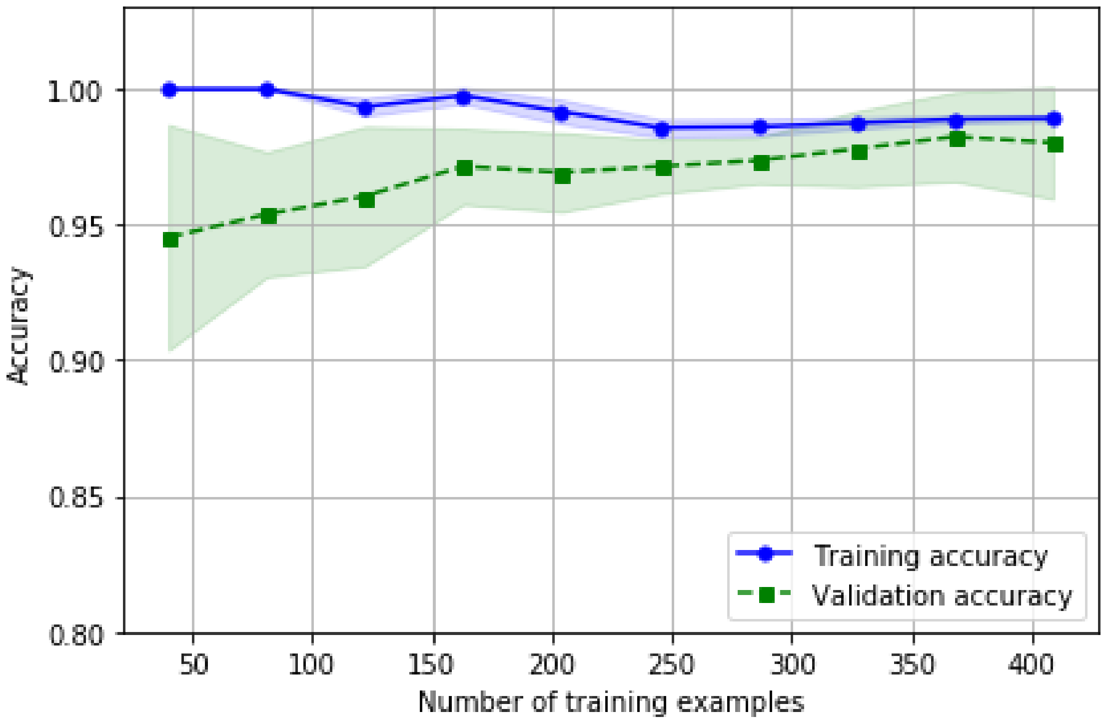
[ ]:
```
Image(filename='images/06_04.png', width=600)
```

[ ]:



[ ]:
```
import matplotlib.pyplot as plt
from sklearn.model_selection import learning_curve


pipe_lr = make_pipeline(StandardScaler(),
                        LogisticRegression(penalty='l2', random_state=1,
                                           solver='lbfgs', max_iter=10000))

train_sizes, train_scores, test_scores =\
                learning_curve(estimator=pipe_lr,
                               X=X_train,
                               y=y_train,
                               train_sizes=np.linspace(0.1, 1.0, 10),
                               cv=10,
                               n_jobs=1)

train_mean = np.mean(train_scores, axis=1)
```

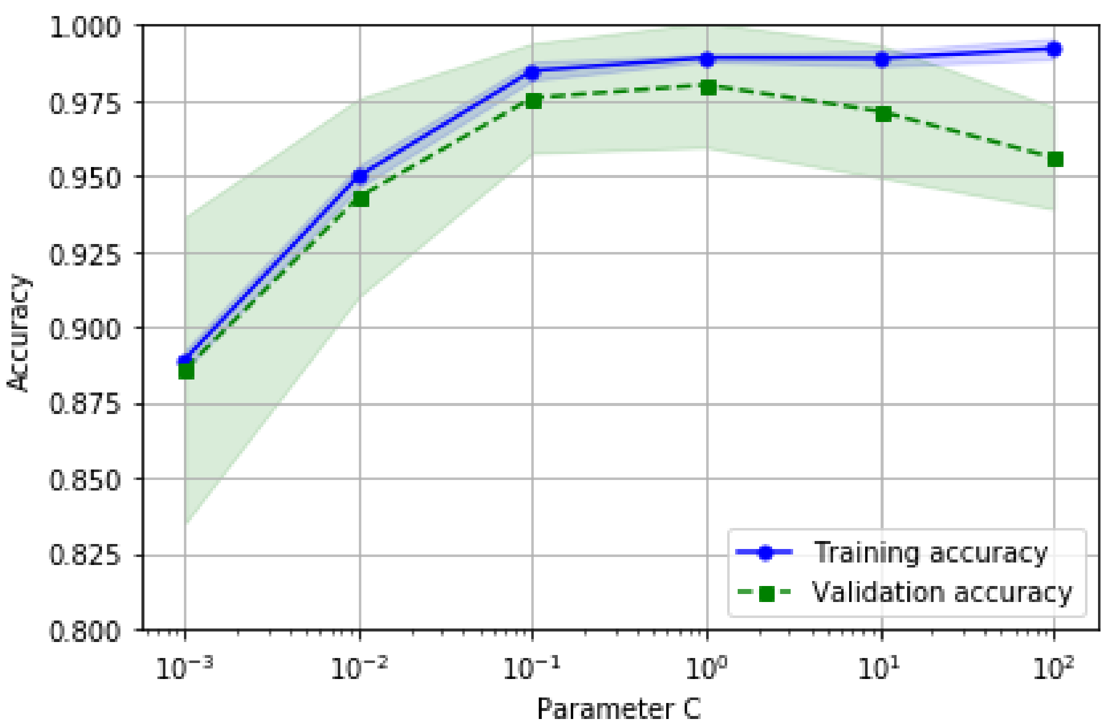
```
train_std = np.std(train_scores, axis=1)
test_mean = np.mean(test_scores, axis=1)
test_std = np.std(test_scores, axis=1)

plt.plot(train_sizes, train_mean,
         color='blue', marker='o',
         markersize=5, label='Training accuracy')

plt.fill_between(train_sizes,
                 train_mean + train_std,
                 train_mean - train_std,
                 alpha=0.15, color='blue')

plt.plot(train_sizes, test_mean,
         color='green', linestyle='--',
         marker='s', markersize=5,
         label='Validation accuracy')

plt.fill_between(train_sizes,
                 test_mean + test_std,
                 test_mean - test_std,
                 alpha=0.15, color='green')

plt.grid()
plt.xlabel('Number of training examples')
plt.ylabel('Accuracy')
plt.legend(loc='lower right')
plt.ylim([0.8, 1.03])
plt.tight_layout()
# plt.savefig('images/06_05.png', dpi=300)
plt.show()
```



5.2 Addressing over- and underfitting with validation curves

[ ]:
```
from sklearn.model_selection import validation_curve


param_range = [0.001, 0.01, 0.1, 1.0, 10.0, 100.0]
train_scores, test_scores = validation_curve(
                estimator=pipe_lr,
                X=X_train,
                y=y_train,
                param_name='logisticregression__C',
                param_range=param_range,
                cv=10)

train_mean = np.mean(train_scores, axis=1)
train_std = np.std(train_scores, axis=1)
test_mean = np.mean(test_scores, axis=1)
test_std = np.std(test_scores, axis=1)

plt.plot(param_range, train_mean,
         color='blue', marker='o',
         markersize=5, label='Training accuracy')
```

```python
plt.fill_between(param_range, train_mean + train_std,
                 train_mean - train_std, alpha=0.15,
                 color='blue')

plt.plot(param_range, test_mean,
         color='green', linestyle='--',
         marker='s', markersize=5,
         label='Validation accuracy')

plt.fill_between(param_range,
                 test_mean + test_std,
                 test_mean - test_std,
                 alpha=0.15, color='green')

plt.grid()
plt.xscale('log')
plt.legend(loc='lower right')
plt.xlabel('Parameter C')
plt.ylabel('Accuracy')
plt.ylim([0.8, 1.0])
plt.tight_layout()
# plt.savefig('images/06_06.png', dpi=300)
plt.show()
```



6 Fine-tuning machine learning models via grid search

6.1 Tuning hyperparameters via grid search

[ ]:
```
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

pipe_svc = make_pipeline(StandardScaler(),
                         SVC(random_state=1))

param_range = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0, 1000.0]

param_grid = [{'svc__C': param_range,
               'svc__kernel': ['linear']},
              {'svc__C': param_range,
               'svc__gamma': param_range,
               'svc__kernel': ['rbf']}]

gs = GridSearchCV(estimator=pipe_svc,
                  param_grid=param_grid,
                  scoring='accuracy',
                  refit=True,
                  cv=10,
                  n_jobs=-1)
gs = gs.fit(X_train, y_train)
print(gs.best_score_)
print(gs.best_params_)
```

```
0.9846859903381642
{'svc__C': 100.0, 'svc__gamma': 0.001, 'svc__kernel': 'rbf'}
```

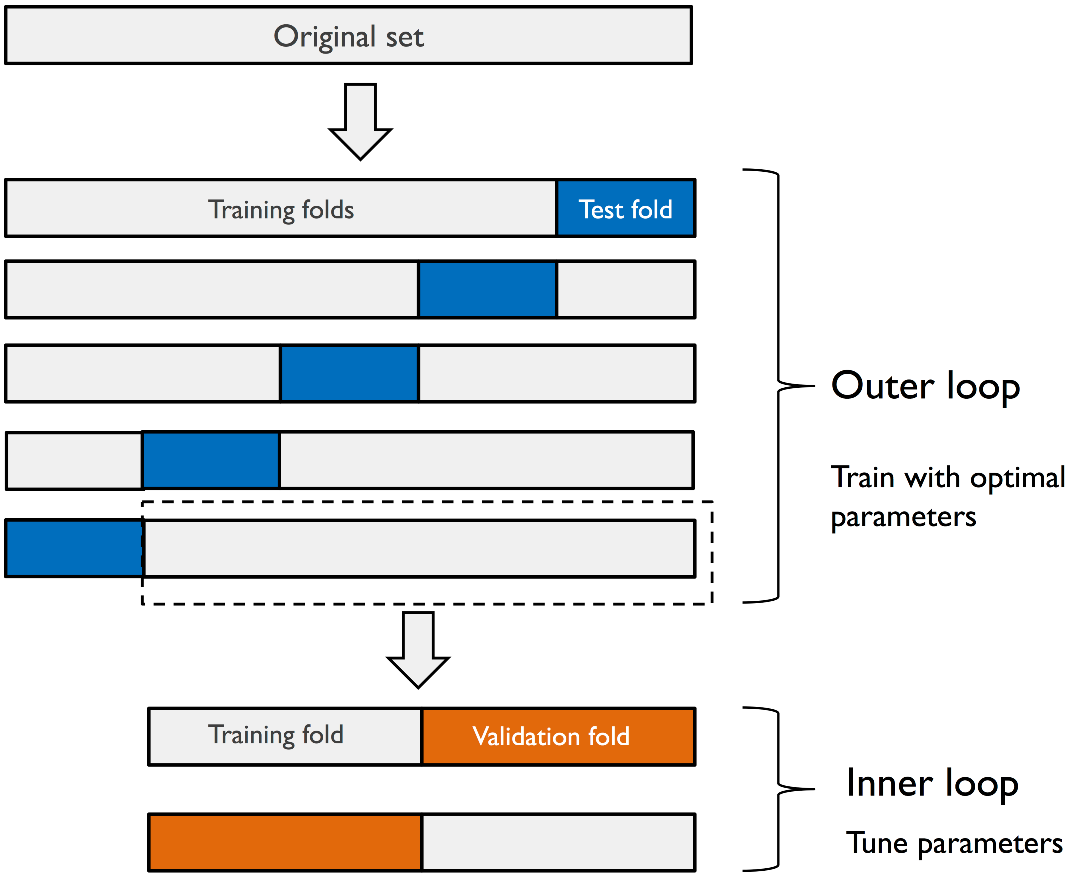
[ ]:
```
clf = gs.best_estimator_

# clf.fit(X_train, y_train)
# note that we do not need to refit the classifier
# because this is done automatically via refit=True.

print('Test accuracy: %.3f' % clf.score(X_test, y_test))
```

```
Test accuracy: 0.974
```

6.2 Algorithm selection with nested cross-validation

[ ]:
```
Image(filename='images/06_07.png', width=500)
```

[ ]:




```
[ ]: gs = GridSearchCV(estimator=pipe_svc,
                       param_grid=param_grid,
                       scoring='accuracy',
                       cv=2)

     scores = cross_val_score(gs, X_train, y_train,
                              scoring='accuracy', cv=5)
     print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores),
                                           np.std(scores)))
```

```
CV accuracy: 0.974 +/- 0.015
```

```
[ ]: from sklearn.tree import DecisionTreeClassifier

     gs = GridSearchCV(estimator=DecisionTreeClassifier(random_state=0),
                       param_grid=[{'max_depth': [1, 2, 3, 4, 5, 6, 7, None]}],
                       scoring='accuracy',
```

```
                 cv=2)

scores = cross_val_score(gs, X_train, y_train,
                         scoring='accuracy', cv=5)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores),
                                      np.std(scores)))
```

```
CV accuracy: 0.934 +/- 0.016
```

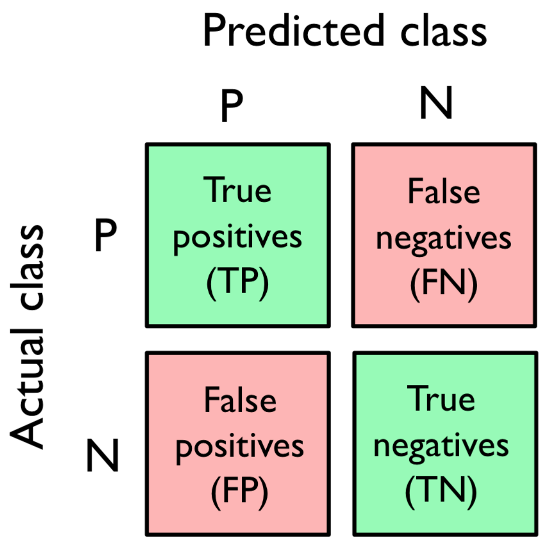
7 Looking at different performance evaluation metrics

…

7.1 Reading a confusion matrix

[ ]:
```
Image(filename='images/06_08.png', width=300)
```

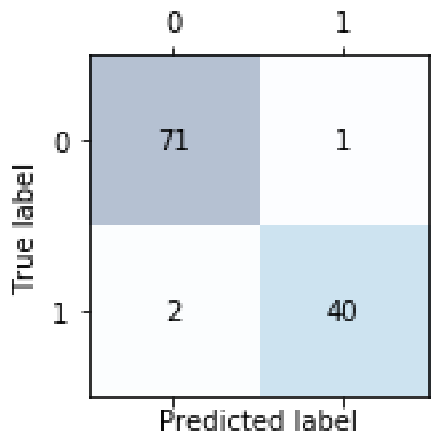
[ ]:



[ ]:
```
from sklearn.metrics import confusion_matrix

pipe_svc.fit(X_train, y_train)
y_pred = pipe_svc.predict(X_test)
confmat = confusion_matrix(y_true=y_test, y_pred=y_pred)
print(confmat)
```

```
[[71  1]
 [ 2 40]]
```

[ ]:
```
fig, ax = plt.subplots(figsize=(2.5, 2.5))
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
for i in range(confmat.shape[0]):
    for j in range(confmat.shape[1]):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.tight_layout()
#plt.savefig('images/06_09.png', dpi=300)
plt.show()
```



7.1.1 Additional Note

Remember that we previously encoded the class labels so that *malignant* examples are the "postive" class (1), and *benign* examples are the "negative" class (0):

[ ]:
```
le.transform(['M', 'B'])
```

[ ]:
```
array([1, 0])
```

[ ]:
```
confmat = confusion_matrix(y_true=y_test, y_pred=y_pred)
print(confmat)
```

```
[[71  1]
 [ 2 40]]
```

Next, we printed the confusion matrix like so:

[ ]:
```
confmat = confusion_matrix(y_true=y_test, y_pred=y_pred)
print(confmat)
```

```
[[71  1]
 [ 2 40]]
```

Note that the (true) class 0 examples that are correctly predicted as class 0 (true negatives) are now in the upper left corner of the matrix (index 0, 0). In order to change the ordering so that the true negatives are in the lower right corner (index 1,1) and the true positves are in the upper left, we can use the `labels` argument like shown below:

```
[ ]: confmat = confusion_matrix(y_true=y_test, y_pred=y_pred, labels=[1, 0])
     print(confmat)
```

```
[[40  2]
 [ 1 71]]
```

We conclude:

Assuming that class 1 (malignant) is the positive class in this example, our model correctly classified 71 of the examples that belong to class 0 (true negatives) and 40 examples that belong to class 1 (true positives), respectively. However, our model also incorrectly misclassified 1 example from class 0 as class 1 (false positive), and it predicted that 2 examples are benign although it is a malignant tumor (false negatives).

7.2 Optimizing the precision and recall of a classification model

```
[ ]: from sklearn.metrics import precision_score, recall_score, f1_score

     print('Precision: %.3f' % precision_score(y_true=y_test, y_pred=y_pred))
     print('Recall: %.3f' % recall_score(y_true=y_test, y_pred=y_pred))
     print('F1: %.3f' % f1_score(y_true=y_test, y_pred=y_pred))
```

```
Precision: 0.976
Recall: 0.952
F1: 0.964
```

```
[ ]: from sklearn.metrics import make_scorer

     scorer = make_scorer(f1_score, pos_label=0)

     c_gamma_range = [0.01, 0.1, 1.0, 10.0]

     param_grid = [{'svc__C': c_gamma_range,
                    'svc__kernel': ['linear']},
                   {'svc__C': c_gamma_range,
                    'svc__gamma': c_gamma_range,
                    'svc__kernel': ['rbf']}]

     gs = GridSearchCV(estimator=pipe_svc,
                       param_grid=param_grid,
                       scoring=scorer,
                       cv=10,
```

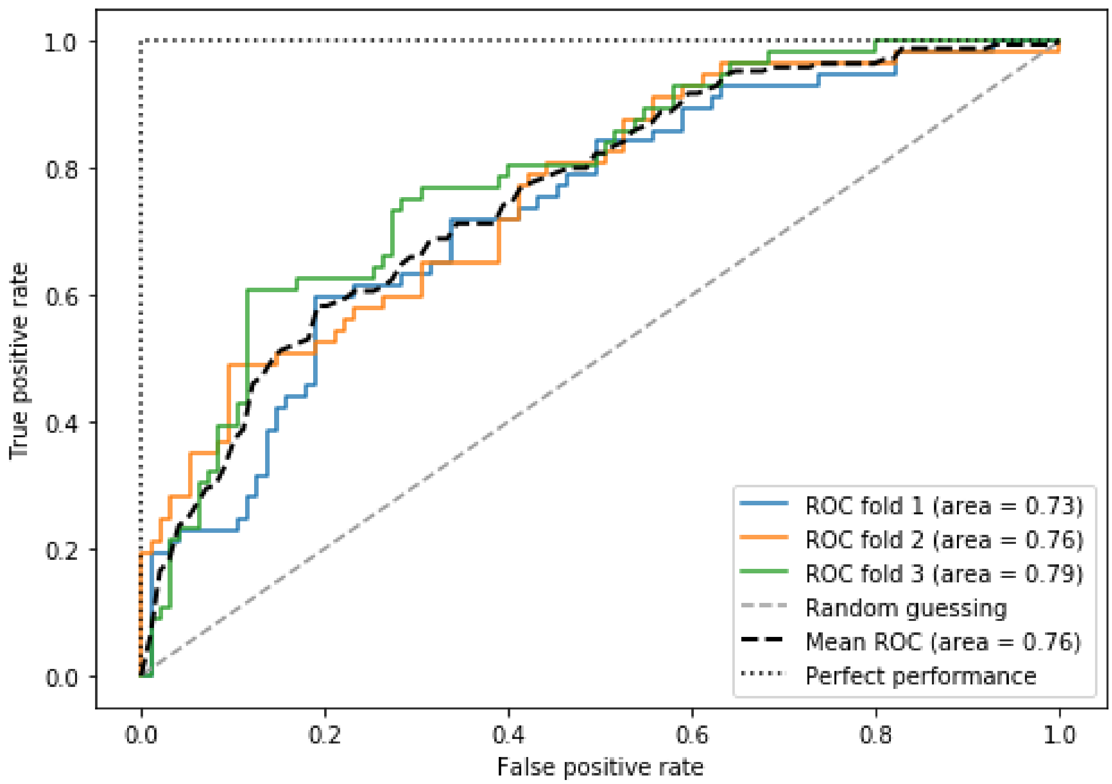
```
                  n_jobs=-1)
gs = gs.fit(X_train, y_train)
print(gs.best_score_)
print(gs.best_params_)
```

```
0.9861994953378878
{'svc__C': 10.0, 'svc__gamma': 0.01, 'svc__kernel': 'rbf'}
```

7.3 Plotting a receiver operating characteristic

[ ]:
```
from sklearn.metrics import roc_curve, auc
from distutils.version import LooseVersion as Version
from scipy import __version__ as scipy_version


if scipy_version >= Version('1.4.1'):
    from numpy import interp
else:
    from scipy import interp


pipe_lr = make_pipeline(StandardScaler(),
                        PCA(n_components=2),
                        LogisticRegression(penalty='l2',
                                           random_state=1,
                                           solver='lbfgs',
                                           C=100.0))

X_train2 = X_train[:, [4, 14]]


cv = list(StratifiedKFold(n_splits=3).split(X_train, y_train))

fig = plt.figure(figsize=(7, 5))

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

for i, (train, test) in enumerate(cv):
    probas = pipe_lr.fit(X_train2[train],
                         y_train[train]).predict_proba(X_train2[test])

    fpr, tpr, thresholds = roc_curve(y_train[test],
                                     probas[:, 1],
                                     pos_label=1)
    mean_tpr += interp(mean_fpr, fpr, tpr)
```

```
    mean_tpr[0] = 0.0
    roc_auc = auc(fpr, tpr)
    plt.plot(fpr,
             tpr,
             label='ROC fold %d (area = %0.2f)'
                   % (i+1, roc_auc))

plt.plot([0, 1],
         [0, 1],
         linestyle='--',
         color=(0.6, 0.6, 0.6),
         label='Random guessing')

mean_tpr /= len(cv)
mean_tpr[-1] = 1.0
mean_auc = auc(mean_fpr, mean_tpr)
plt.plot(mean_fpr, mean_tpr, 'k--',
         label='Mean ROC (area = %0.2f)' % mean_auc, lw=2)
plt.plot([0, 0, 1],
         [0, 1, 1],
         linestyle=':',
         color='black',
         label='Perfect performance')

plt.xlim([-0.05, 1.05])
plt.ylim([-0.05, 1.05])
plt.xlabel('False positive rate')
plt.ylabel('True positive rate')
plt.legend(loc="lower right")

plt.tight_layout()
# plt.savefig('images/06_10.png', dpi=300)
plt.show()
```



7.4 The scoring metrics for multiclass classification

[ ]:
```
pre_scorer = make_scorer(score_func=precision_score,
                         pos_label=1,
                         greater_is_better=True,
                         average='micro')
```

7.5 Dealing with class imbalance

[ ]:
```
X_imb = np.vstack((X[y == 0], X[y == 1][:40]))
y_imb = np.hstack((y[y == 0], y[y == 1][:40]))
```

[ ]:
```
y_pred = np.zeros(y_imb.shape[0])
np.mean(y_pred == y_imb) * 100
```

[ ]: 89.92443324937027

[ ]:
```
from sklearn.utils import resample

print('Number of class 1 examples before:', X_imb[y_imb == 1].shape[0])

X_upsampled, y_upsampled = resample(X_imb[y_imb == 1],
```

```
                                     y_imb[y_imb == 1],
                                     replace=True,
                                     n_samples=X_imb[y_imb == 0].shape[0],
                                     random_state=123)

print('Number of class 1 examples after:', X_upsampled.shape[0])
```

```
Number of class 1 examples before: 40
Number of class 1 examples after: 357
```

[ ]:
```
X_bal = np.vstack((X[y == 0], X_upsampled))
y_bal = np.hstack((y[y == 0], y_upsampled))
```

[ ]:
```
y_pred = np.zeros(y_bal.shape[0])
np.mean(y_pred == y_bal) * 100
```

[ ]: 50.0

8 Summary

…

Readers may ignore the next cell.

[ ]:
```
! python ../.convert_notebook_to_script.py --input ch06.ipynb --output ch06.py
```

```
[NbConvertApp] Converting notebook ch06.ipynb to script
[NbConvertApp] Writing 17510 bytes to ch06.py
```