Homework 3

Rodrigo Valle

27 November 2018

VC Dimension

We define a set of concepts

$$H = \{\operatorname{sgn}(ax^2 + bx + c) \mid a, b, c \in \mathbb{R}\}$$

where

$$\operatorname{sgn}(x) = \begin{cases} 1 \text{ if } x \geq 0 \\ 0 \text{ otherwise} \end{cases}$$

What is the VC dimension of H? Prove your claim.

The VC dimension of H is 3.

Proof

We first show that we can shatter a set of size 3 using functions from our hypothesis space. A set of size 3 in the context of our classification space is just three points along an axis, call it the x-axis. For every possible labeling of these points, we show graphically in Figure 1 that there is a function from our hypothesis space that can correctly classify these points. This function is a parabola, when the parabola is above the x-axis it is classifying points on the x-axis as positive; when the parabola is below the x-axis those points on the x-axis are classified as negative, i.e. we classify according to the sign of parabola's output.

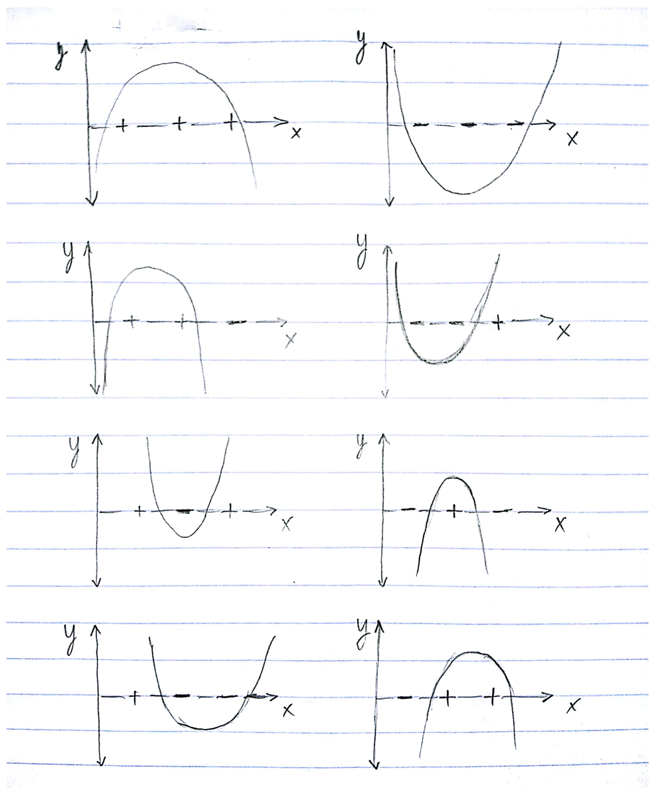


Figure 1: Shattering over all labelings of a set whose size is 3

Now that we have shown that a set of size 3 points is shatterable by our class of hypothesis functions by exhaustively showing every case, we can continue to show that a set of 4 points is not shatterable by considering the counterexample of four labeled points along the x-axis:

$$+ \quad - \quad + \quad -$$

A parabola can partition the continous x-axis into as many as three parts, one line segment with label y and two rays on either side with label $\overline{y}$. If we model this as a change of state along the x-axis we can say that the parabola can flip its current classification "state" twice along the entire x-axis. From the counter example, we observe that in order to correctly classify this case we would have to flip state three times, which is more than any parabolic hypothesis function can represent as a parabola can intersect the x-axis only twice. So, a set of any 4 points is not shatterable, but a set of 3 points is shatterable by our class of hypotheses functions. Since the VC dimension is defined as the cardinality of the largest set of points that our model can shatter, the VC dimension of H is three.

Kernels

Given vectors $\mathbf{x}$ and $\mathbf{z}$ in $\mathbb{R}^2$, define the kernel $K_\beta(\mathbf{x}, \mathbf{z}) = (1 + \beta\mathbf{x} \cdot \mathbf{z})^3$ for any value $\beta > 0$. Find the corresponding feature map $\phi(\cdot)$. What are the similarities/differences from the kernel $K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^3$, and what role does β play?

$$\begin{aligned}
K(\mathbf{x}, \mathbf{z}) =& \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \\
=& (1 + \beta\mathbf{x} \cdot \mathbf{z})^3 \\
=& 1 + 3(\beta\mathbf{x} \cdot \mathbf{z}) + 3(\beta\mathbf{x} \cdot \mathbf{z})^2 + (\beta\mathbf{x} \cdot \mathbf{z})^3 \\
=& 1 + 3\beta(x_0 z_0 + x_1 z_1) + 3\beta^2(x_0 z_0 + x_1 z_1)^2 + \beta^3(x_0 z_0 + x_1 z_1)^3 \\
=& 1 + \\
& 3\beta x_0 z_0 + \\
& 3\beta x_1 z_1 + \\
& 3\beta^2 x_0^2 z_0^2 + \\
& 6\beta^2 x_0 x_1 z_0 z_1 + \\
& 3\beta^2 x_1^2 z_1^2 + \\
& \beta^3 x_0^3 z_0^3 \\
& 3\beta^3 x_0^2 x_1 z_0^2 z_1 \\
& 3\beta^3 x_0 x_1^2 z_0 z_1^2 \\
& \beta^3 x_1^3 z_1^3
\end{aligned}$$

$$\phi(\mathbf{v}) = \begin{pmatrix} 1 \\ \sqrt{3\beta} v_0 \\ \sqrt{3\beta} v_1 \\ \sqrt{3}\beta v_0^2 \\ \sqrt{6}\beta v_0 v_1 \\ \sqrt{3}\beta v_1^2 \\ \sqrt{\beta^3} v_0^3 \\ \sqrt{3\beta^3} v_0^2 v_1 \\ \sqrt{3\beta^3} v_0 v_1^2 \\ \sqrt{\beta^3} v_1^3 \end{pmatrix}$$

It seems that β scales each polynomial dimension by an amount related to the number of features from the original vector in $\mathbb{R}^2$ that make up the polynomial dimension. For example, linear dimensions like $\sqrt{3\beta} v_0$ are scaled by an amount proportional to $\sqrt{\beta}$. Quadratic dimensions are scaled by an amount proportional to β, and cubic dimensions are scaled by an amount proportional to $\sqrt{\beta^3}$. From this observation, it would seem that β really scales the distance that is reported by the kernel function from computing the dot product in this higher dimensional space mapped to by ϕ — that is, beta scales the similarity between vectors reported by the kernel function.

SVM

Suppose we are looking for a maximum-margin linear classifer *through the origin*, i.e. $b = 0$ (also hard margin, i.e., no slack variables). In other words, we minimize $\frac{1}{2}||\mathbf{w}||^2$ subject to $y_n \mathbf{w}^T \mathbf{x}_n \geq 1$ where $n = 1 \dots N$.

a) Suppose we have two training examples, $\mathbf{x}_1 = (1,1)^T$ and $\mathbf{x}_2 = (1,0)^T$ with labels $y_1 = 1$ and $y_2 = -1$. What is $\mathbf{w}^*$ in this case?

$$\mathbf{w}^* = \begin{pmatrix} -1 \\ 2 \end{pmatrix}$$

This choice of $\mathbf{w}^*$ minimizes $\frac{1}{2}||\mathbf{w}||^2$ because $y_n \mathbf{w}^{*T} x_n = \gamma = 1$ over all n examples. That is:

$$y_1 \mathbf{w}^* x_1 = 1 \cdot \begin{pmatrix} -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 1 \cdot (-1 \cdot 1 + 2 \cdot 1) = 1$$
$$y_2 \mathbf{w}^* x_2 = -1 \cdot \begin{pmatrix} -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -1 \cdot (-1 \cdot 1 + 2 \cdot 0) = 1$$

Choosing a smaller $\mathbf{w}^*$ would cause these predictions to become less than 1, which violates our optimization constraint. Additionally, since SVM is a convex optimization problem, the minimal $\mathbf{w}^*$ that we have discovered must be a global minimum in the optimization problem, which means we have the best possible $\mathbf{w}^*$.

b) Suppose we now allow the offset parameter b to be non-zero. How would the classifier and the margin change in the previous question? What are the $(\mathbf{w}^*, \mathbf{b}^*)$? compare your solutions with and without the offset.

$$(\mathbf{w}^*, \mathbf{b}^*) = \left(\begin{pmatrix} 0 \\ 2 \end{pmatrix}, -1 \right)$$

We see that for this choice of $(\mathbf{w}^*, \mathbf{b}^*)$, $\mathbf{w}^*$ is minimal because $y_n \mathbf{w}^{*T} x_n = \gamma = 1$ over all n examples. If we were to choose a smaller $\mathbf{w}^*$ our margins would be less than 1, which violates our constraint. Additionally, since SVM is a convex optimization problem, the minimal $\mathbf{w}^*$ that we have discovered must be a global minimum in the optimization problem, which means we have the best possible $\mathbf{w}^*$.

$$y_1(\mathbf{w}^* x_1 + b) = 1 \cdot \begin{pmatrix} 0 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 1 \cdot ((0 \cdot 1 + 2 \cdot 1) - 1) = 1$$
$$y_2(\mathbf{w}^* x_2 + b) = -1 \cdot \begin{pmatrix} 0 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -1 \cdot ((0 \cdot 1 + 2 \cdot 0) - 1) = 1$$

With the bias, our minimized separating hyperplane normal of the hard-margin linear SVM has a magnitude of 2. Without the bias, the separating hyperplane normal has a magnitude of $\sqrt{5}$, which is greater than 2.

The SVM that is allowed to choose a bias offset has more possible hyperplanes to choose from, and is thus more expressive, than the SVM that must choose a hyperplane through the origin. So, it makes sense that SVM with more freedom to choose selects a more optimal weight vector ($\frac{1}{2}||\mathbf{w}^*||^2$ is smaller for the more expressive SVM).

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from IPython.display import HTML, Math
np.random.seed(1234)
```

4.1 Feature Extraction

In [2]:
```
from sklearn.model_selection import train_test_split
from src.twitter import extract_words, read_vector_file
```

(a) Implement `extract_dictionary(...)` that uses `extract_words(...)` to read all unique words contained in a file into a dictionary. Process the tweets in the order they appear in the file to create this dictionary of d unique words/punctuations.

In [3]:
```
def extract_dictionary(infile):
    """
    Given a filename, reads the text file and builds a dictionary of
    unique words/punctuations.

    Parameters
    ----------
        infile -- string, filename
    Returns
    ----------
        word_list -- dictionary, (key, value) pairs are
                     (word, index)
    """
    with open(infile, 'r') as fid:
        unique_words = set(extract_words(fid.read()))
        return {word: i for i, word in enumerate(unique_words)}
```

(b) Next, implement `extract_feature_vectors(...)` that produces the bag-of-words representation of a file based on the extracted dictionary. That is, for each tweet i, construct a feature vector of length d, where the j^{th} entry in the feature vectors is 1 if the j^{th} word in the dictionary is present in tweet i, or 0 otherwise. For n tweets, save the feature vectors in a feature matrix, where the rows correspond to tweets (examples) and the columns correspond to words (features). Maintain the order of the tweets as they appear in the file.

In [4]:
```
def extract_feature_vectors(infile, word_list):
    """
    Produces a bag-of-words representation of a text file specified
    by the filename infile based on the dictionary word_list.

    Parameters
    ----------
        infile -- string, filename
        world_list -- dictionary, (key, value) pairs are
                      (word, index)

    Returns
    ----------
        feature_matrix -- numpy array of shape (n,d)
                          boolean (0,1) array indicating words
                          presence in a string

    """
    num_lines = sum(1 for line in open(infile, 'r'))
    num_words = len(word_list)
    feature_matrix = np.zeros((num_lines, num_words))

    with open(infile, 'r') as fid:
        for j, tweet in enumerate(fid):
            for word in extract_words(tweet):
                i = word_list[word]
                feature_matrix[j][i] = 1

    return feature_matrix
```

In [5]:
```
data_file = 'data/tweets.txt'
dictionary = extract_dictionary(data_file)
X = extract_feature_vectors(data_file, dictionary)
y = read_vector_file('data/labels.txt')
```

In [6]:
```
pd.options.display.max_rows = 12
pd.options.display.max_columns = 12
pd.DataFrame(X)
```

Out[6]:

	0	1	2	3	4	5	...	1805	1806	1807	1808	1809	1810
0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	1.0	0.0	0.0
...	...	...	...	...	...	...	...	...	...	...	...	...	...
624	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
625	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
626	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
627	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
628	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0
629	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0

630 rows × 1811 columns

In [7]:
```
with open(data_file, 'r') as f:
    display(next(f))
feature_vec = sorted(zip(X[0], dictionary.keys()), reverse=True)
display(feature_vec[:20], len(feature_vec))
```

```
'2012, Micheal:This Is it && A Christmas Carol Are Cool Movies\n'

[(1.0, 'this'),
 (1.0, 'movies'),
 (1.0, 'micheal'),
 (1.0, 'it'),
 (1.0, 'is'),
 (1.0, 'cool'),
 (1.0, 'christmas'),
 (1.0, 'carol'),
 (1.0, 'are'),
 (1.0, 'a'),
 (1.0, ':'),
 (1.0, '2012'),
 (1.0, ','),
 (1.0, '&'),
 (0.0, '|'),
 (0.0, 'zigster'),
 (0.0, 'z'),
 (0.0, 'yumm'),
 (0.0, 'your'),
 (0.0, 'you')]

1811
```

(c) Split the feature matrix and corresponding labels into your training and test sets. **The first 560 tweets will be used for training and the last 70 tweets will be used for testing.**

In [8]:
```
# note: the data is being shuffled implicitly by train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=
560)
```

```
/usr/lib/python3.7/site-packages/sklearn/model_selection/_split.py:20
69: FutureWarning: From version 0.21, test_size will always complemen
t train_size unless both are specified.
  FutureWarning)
```

(d) Indicate that you have finished the feature extraction and generated the train/test splits in your write-up. ✓

4.2 Hyper-parameter Selection for a Linear-Kernel SVM

In [9]:
```
from sklearn.svm import SVC
from sklearn.model_selection import StratifiedKFold
from sklearn import metrics
```

(a) The result of a hyperparameter selection often depends upon the choice of performance measure. Here, we will consider the following performance measures: **accuracy**, **F1-score**, and **AUROC**.

Implement `performance(...)` . All measures are implemented in `sklearn.metrics` .

In [10]:
```
def performance(y_true, y_pred, metric="accuracy"):
    """
    Calculates the performance metric based on the agreement between
    the true labels and the predicted labels.

    Parameters
    --------------------
        y_true -- numpy array of shape (n,), known labels
        y_pred -- numpy array of shape (n,), (continuous-valued)
                  predictions
        metric -- string, option used to select the performance
                  measure
                  options: 'accuracy', 'f1-score', 'auroc'

    Returns
    --------------------
        score  -- float, performance score
    """
    # map continuous-valued predictions to binary labels
    y_label = np.sign(y_pred)
    y_label[y_label==0] = 1

    scorer = {
        'accuracy': metrics.accuracy_score,
        'f1_score': metrics.f1_score,
        'auroc': metrics.roc_auc_score,
    }[metric]

    return scorer(y_true, y_label)
```

(b) Next, implement `cv_performance(...)` to return the mean k-fold CV performance for the performance metric passed into the function. Here, you will make use of `SVC.fit(X,y)` and the `SVC.decision_function(X)` , as well as your `performance(...)` function.

You may have noticed that the proportion of the two classes (positive and negative) are not equal in the training data. When dividing the data into folds for CV, you should try to keep the class proportions roughly the same across folds. In your write-up briefly describe why it might be beneficial to maintain class proportions across folds. Then, use `sklearn.cross_validation.StratifiedKFold(...)` to split the data for 5-fold CV, making sure to stratify using only the training labels.

We would want to try to keep class proportions the same across folds to avoid oversampling any one class accidentally. If this were to happen, we might choose a set of examples of all the same class for example. In this scenario, even a trivial classifier that always predicts the majority class can get 100% training accuracy (but will probably have horrible test accuracy because its not a very expressive model). Essentially, it's impossible to learn the class separation when there's an overwhelming majority of a single class, so we use stratified sampling to avoid this situation and keep similar class distributions between the whole data set and any sampled training sets.

In [11]:
```
def cv_performance(clf, X, y, kf, metric="accuracy"):
    """
    Splits the data, X and y, into k-folds and runs k-fold
    cross-validation. Trains classifier on k-1 folds and tests on the
    remaining fold. Calculates the k-fold cross-validation
    performance metric for classifier by averaging the performance
    across folds.

    Parameters
    --------------------
        clf    -- classifier (instance of SVC)
        X      -- numpy array of shape (n,d), feature vectors
                    n = number of examples
                    d = number of features
        y      -- numpy array of shape (n,), binary labels {1,-1}
        kf     -- cross_validation.KFold or
                  cross_validation.StratifiedKFold
        metric -- string, option used to select performance measure

    Returns
    --------------------
        score   -- float, average cross-validation performance across
                   k folds
    """
    scores = []

    for train_index, test_index in kf.split(X, y):
        X_train_fold, X_test_fold = X[train_index], X[test_index]
        y_train_fold, y_test_fold = y[train_index], y[test_index]

        svm = clf.fit(X_train_fold, y_train_fold)
        y_pred = svm.decision_function(X_test_fold)
        scores.append(performance(y_test_fold, y_pred, metric=metric
))

    return sum(scores)/len(scores)
```

In [12]:
```
cv_performance(SVC(gamma='auto'), X_train, y_train, StratifiedKFold(n
_splits=5), metric='accuracy')
```

Out[12]:
```
0.6535764114303937
```

(c) Now, implement `select_param_linear(...)` to choose a setting for C for a linear SVM based on the training data and the specified metric. Your function should call `cv_performance(...)` , passing in instances of `SVC(kernel='linear', C=c)` with different values for `C` , e.g. $C = 10^{-3}, 10^{-2}, 10^{-1}, 1, 10, 10^2$

In [13]:
```
def select_param_linear_helper(c_range, X, y, kf, metric='accuracy'):
    return {
        c:
        cv_performance(
            SVC(kernel='linear', C=c, gamma='auto'),
            X, y, kf, metric=metric
        )
        for c in c_range
    }
```

In [14]:
```
def select_param_linear(X, y, kf, metric="accuracy"):
    """
    Sweeps different settings for the hyperparameter of a linear-
    kernel SVM, calculating the k-fold CV performance for each
    setting, then selecting the hyperparameter that 'maximize'
    the average k-fold CV performance.

    Parameters
    --------------------
        X      -- numpy array of shape (n,d), feature vectors
                     n = number of examples
                     d = number of features
        y      -- numpy array of shape (n,), binary labels {1,-1}
        kf     -- cross_validation.KFold or
                  cross_validation.StratifiedKFold
        metric -- string, option used to select performance measure

    Returns
    --------------------
        C -- float, optimal parameter value for linear-kernel SVM
    """

    print('Linear SVM Hyperparameter Selection based on ' + str(metri
c) + ':')
    c_range = 10.0 ** np.arange(-3, 3)
    results = select_param_linear_helper(c_range, X, y, kf, c_range,
metric=metric)
    return c_range[np.argmax(results)]
```

(d) Finally, using the training data from Section 4.1 and the functions implemented here, find the best setting for C for each performance measure mentioned above. Report your findings in tabular format (up to the fourth decimal place).

In [15]:
```
c_range = 10.0 ** np.arange(-3, 3)
kf = StratifiedKFold(n_splits=5)
scores = {
    metric: select_param_linear_helper(
        c_range,
        X_train,
        y_train,
        kf,
        metric=metric,
    )
    for metric in ['accuracy', 'f1_score', 'auroc']
}
```

In [16]:
```
df = pd.DataFrame(data=scores)
df = df.rename_axis('C', axis='columns')
df.append(df.idxmax().rename('best C')).round(4)
```

Out[16]:

C	accuracy	f1_score	auroc
0.001	0.6536	0.7905	0.5000
0.01	0.7822	0.8497	0.7109
0.1	0.8072	0.8584	0.7688
1.0	0.8250	0.8675	0.8019
10.0	0.8196	0.8636	0.7953
100.0	0.8196	0.8636	0.7953
best C	1.0000	1.0000	1.0000

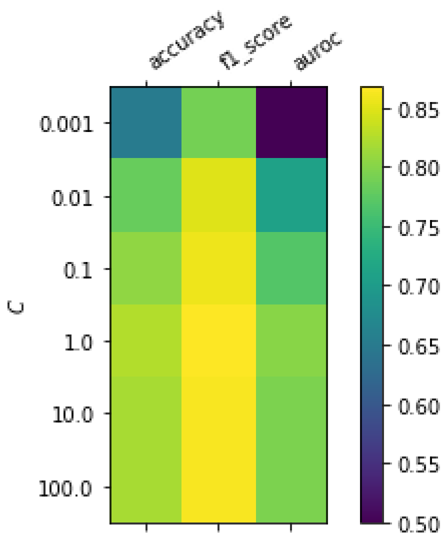
Your `select_param_linear(...)` function returns the 'best' C given a range of values. How does the 5-fold CV performance vary with C and the performance metric?

In general, it seems that AUROC is the most pessimistic metric of the three, F1 is optimistic, and accuracy is middle-of-the-road.

For lower values of C, i.e. $C < 1$, the accuracy of the SVM across all performance metrics grows worse as C decreases. For $C > 1$, we note that the performance seems to level off across all performance metrics as the SVM becomes less willing to provide slack and penalizes misclassified examples more harshly. Performance peaks at $C = 1$ for all metrics because $C = 1$ is the choice for this dataset where enough slack is afforded to account for any outlier examples while still maintaining a hard enough margin to accurately separate all other data.

In [17]:
```
fig, ax = plt.subplots(ncols=1)

ax.set_ylabel('$C$')
ax.set_xticklabels(['', 'accuracy', 'f1_score', 'auroc'], rotation=35
, ha='left')
ax.set_yticklabels([''] + list(map(str, c_range)))
im = ax.matshow(df)
fig.colorbar(im, ax=ax);
```



4.3 Test Set Performance

(a) Based on the results you obtained in Section 4.2, choose a hyperparameter setting for the linear-kernel SVM. Then, using the training data extracted in Section 4.1 and `SVC.fit(...)` , train a linear-kernel SVM with your chosen settings.

In [18]:
```
clf = SVC(kernel='linear', gamma='auto', C=1.0)
clf.fit(X_train, y_train)
```

Out[18]:
```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape='ovr', degree=3, gamma='auto', kernel='line
ar',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

(b) Implement `performance_test(...)` which returns the value of a performance measure, given the test data and a trained classifier.

In [19]:
```
def performance_test(clf, X, y, metric="accuracy"):
    """
    Estimates the performance of the classifier using the 95% CI.

    Parameters
    --------------------
        clf    -- classifier (instance of SVC) [already fit to data]
        X      -- numpy array of shape (n,d), feature vectors of test
                  set
                    n = number of examples
                    d = number of features
        y      -- numpy array of shape (n,), binary labels {1,-1} of
                  test set
        metric -- string, option used to select performance measure

    Returns
    --------------------
        score  -- float, classifier performance
    """

    y_pred = clf.decision_function(X)
    return performance(y, y_pred, metric=metric)
```

(c) For each performance metric, use `performance_test(...)` and the trained linear-kernel SVM classifier to measure performance on the test data. Report the results. Be sure to include the name of the performance metric employed and the performance on the test data.

In [20]:
```
performance_scores = {
    metric: performance_test(clf, X_test, y_test, metric=metric)
    for metric in ['accuracy', 'f1_score', 'auroc']
}
```

In [21]:
```
pd.DataFrame(performance_scores, index=['performance:'])
```

Out[21]:

	accuracy	f1_score	auroc
performance:	0.857143	0.9	0.849359

NOTE: training data has been shuffled

In [ ]: