Applied Machine Learning: Module 3 (Evaluation)

03-01: Evaluation for Classification

Preamble

In [2]:

```
%matplotlib notebook
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.datasets import load_digits

dataset = load_digits() # Loads the digits dataset
X, y = dataset.data, dataset.target

for class_name, class_count in zip(dataset.target_names, np.bincount(dataset.tar
get)):
    print(class_name,class_count) # count the number of instances of each digit.
```

```
0 178
1 182
2 177
3 183
4 181
5 182
6 181
7 179
8 174
9 180
```

In [3]:

```
# Creating a dataset with imbalanced binary classes:
# Negative class (0) is 'not digit 1'
# Positive class (1) is 'digit 1'
y_binary_imbalanced = y.copy()
y_binary_imbalanced[y_binary_imbalanced != 1] = 0

print('Original labels:\t', y[1:30])
print('New binary labels:\t', y_binary_imbalanced[1:30])
```

```
Original labels:         [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]
New binary labels:       [1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1
0 0 0 0 0 0 0 0]
```

In [4]:

```
np.bincount(y_binary_imbalanced)    # Negative class (0) is the most frequent cl
ass
```

Out[4]:

```
array([1615,  182])
```

In [5]:

```
X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced, rand
om_state=0)

# Accuracy of Support Vector Machine classifier
from sklearn.svm import SVC

svm = SVC(kernel='rbf', C=1).fit(X_train, y_train)
svm.score(X_test, y_test)
```

Out[5]:

```
0.9088888888888886
```

Dummy Classifiers

DummyClassifier is a classifier that makes predictions using simple rules, which can be useful as a baseline for comparison against actual classifiers, especially with imbalanced classes.

In [6]:

```
from sklearn.dummy import DummyClassifier

# Negative class (0) is most frequent
dummy_majority = DummyClassifier(strategy = 'most_frequent').fit(X_train, y_trai
n)
# Therefore the dummy 'most_frequent' classifier always predicts class 0
# Most frequent parameter is used to predict the most frequent class
y_dummy_predictions = dummy_majority.predict(X_test)

y_dummy_predictions
```

Out[6]:

```
array([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, 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, 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, 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, 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, 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, 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, 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, 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, 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,
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, 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, 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, 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, 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, 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, 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, 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])
```

In [7]:

```
dummy_majority.score(X_test, y_test)
```

Out[7]:

```
0.9044444444444445
```

Change the Type of Kernel

In [8]:

```
svm = SVC(kernel='linear', C=1).fit(X_train, y_train)
svm.score(X_test, y_test)
```

Out[8]:

```
0.9777777777777775
```

Confusion matrices

Binary (two-class) confusion matrix on Dummy Classifier with `strategy = 'most_frequent'`

In [9]:

```
from sklearn.metrics import confusion_matrix

# Negative class (0) is most frequent
dummy_majority = DummyClassifier(strategy = 'most_frequent').fit(X_train, y_trai
n)
y_majority_predicted = dummy_majority.predict(X_test)
# To get the confusion matrix, we simply pass the y-test set of predicted label
s,
# and the y-predicted labels into the confusion matrix
# and then print the output.

confusion = confusion_matrix(y_test, y_majority_predicted)

print('Most frequent class (dummy classifier)\n', confusion)
```

```
Most frequent class (dummy classifier)
 [[407   0]
 [ 43   0]]
```

The order of the cells of the little matrix output here is the same as the one in the slides

```
[[TN     FP]
  FN     TP]]
```

In particular, the successful predictions of the classifier are **on the diagonal**, where the true class matches the predicted class. Elements on the **subdiagonal** represents errors of different types.

Here we compute the confusion matrices for different choices of classifier in the problem so we can see how they shift slightly with different choice of model.

Binary (Two Class) confusion matrix on Dummy Classifier with `strategy = 'stratified'`

In [10]:

```
# produces random predictions w/ same class proportion as training set
dummy_classprop = DummyClassifier(strategy='stratified').fit(X_train, y_train)
y_classprop_predicted = dummy_classprop.predict(X_test)
confusion = confusion_matrix(y_test, y_classprop_predicted)

print('Random class-proportional prediction (dummy classifier)\n', confusion)
```

```
Random class-proportional prediction (dummy classifier)
 [[368  39]
 [ 39   4]]
```

Binary (Two Class) Confusion matrix on Support Linear Vector Machine with Linear Kernel

In [11]:

```
svm = SVC(kernel='linear', C=1).fit(X_train, y_train)
svm_predicted = svm.predict(X_test)
confusion = confusion_matrix(y_test, svm_predicted)

print('Support vector machine classifier (linear kernel, C=1)\n', confusion)
```

```
Support vector machine classifier (linear kernel, C=1)
 [[402   5]
 [  5  38]]
```

Binary (Two Class) Confusion matrix on Logistic Regression model

In [12]:

```
from sklearn.linear_model import LogisticRegression

lr = LogisticRegression().fit(X_train, y_train)
lr_predicted = lr.predict(X_test)
confusion = confusion_matrix(y_test, lr_predicted)

print('Logistic regression classifier (default settings)\n', confusion)
```

```
Logistic regression classifier (default settings)
 [[401   6]
 [  6  37]]
```

Binary (Two Class) Confusion matrix on Decision Tree Classifier of max_depth 2

In [13]:

```
from sklearn.tree import DecisionTreeClassifier

dt = DecisionTreeClassifier(max_depth=2).fit(X_train, y_train)
tree_predicted = dt.predict(X_test)
confusion = confusion_matrix(y_test, tree_predicted)

print('Decision tree classifier (max_depth = 2)\n', confusion)
```

```
Decision tree classifier (max_depth = 2)
 [[400   7]
 [ 17  26]]
```

Note that the decision tree makes **twice as more** false negative errors as false positive errors.

03-02: Evaluation metrics for binary classification

Evaluation Metrics for Binary Classification - Decision Tree Classifier

In [14]:

```
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_sc
ore
# Accuracy = TP + TN / (TP + TN + FP + FN)
# Precision = TP / (TP + FP)
# Recall = TP / (TP + FN)  Also known as sensitivity, or True Positive Rate
# F1 = 2 * Precision * Recall / (Precision + Recall)
print('Accuracy: {:.2f}'.format(accuracy_score(y_test, tree_predicted)))
print('Precision: {:.2f}'.format(precision_score(y_test, tree_predicted)))
print('Recall: {:.2f}'.format(recall_score(y_test, tree_predicted)))
print('F1: {:.2f}'.format(f1_score(y_test, tree_predicted)))
```

```
Accuracy: 0.95
Precision: 0.79
Recall: 0.60
F1: 0.68
```

Using `classification_report`

In [15]:

```
# Combined report with all above metrics
from sklearn.metrics import classification_report

print(classification_report(y_test, tree_predicted, target_names=['not 1', '1'
])) # Look at the SKL documentation
# to see what other output options are available to you.
```

```
             precision    recall  f1-score   support

      not 1       0.96      0.98      0.97       407
          1       0.79      0.60      0.68        43

avg / total       0.94      0.95      0.94       450
```

Classification Report on Dummy Classifier

In [16]:

```
print('Random class-proportional (dummy)\n',
      classification_report(y_test, y_classprop_predicted, target_names=['not 1'
, '1']))
```

```
Random class-proportional (dummy)
              precision    recall  f1-score   support

      not 1       0.90      0.90      0.90       407
          1       0.09      0.09      0.09        43

avg / total       0.83      0.83      0.83       450
```

Classification Report on SVM Classifier

In [17]:

```
print('SVM\n',
      classification_report(y_test, svm_predicted, target_names = ['not 1', '1'
]))
```

```
SVM
              precision    recall  f1-score   support

      not 1       0.99      0.99      0.99       407
          1       0.88      0.88      0.88        43

avg / total       0.98      0.98      0.98       450
```

Classification Report on Logistic Regression Classifier

In [18]:

```
print('Logistic regression\n',
      classification_report(y_test, lr_predicted, target_names = ['not 1', '1'
]))
```

```
Logistic regression
              precision    recall  f1-score   support

      not 1       0.99      0.99      0.99       407
          1       0.86      0.86      0.86        43

avg / total       0.97      0.97      0.97       450
```

Classification Report on Decision Tree Classifier

In [19]:

```
print('Decision tree\n',
      classification_report(y_test, tree_predicted, target_names = ['not 1', '1'
]))
```

```
Decision tree
              precision    recall  f1-score   support

      not 1       0.96      0.98      0.97       407
          1       0.79      0.60      0.68        43

avg / total       0.94      0.95      0.94       450
```

03-03: Classifier Decision functions

Using `decision_function()` method

In [20]:

```
X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced, rand
om_state=0)
#lr was actually a logistic regression classifier from the previous lecture.
# lr = LogisticRegression().fit(X_train, y_train)
y_scores_lr = lr.fit(X_train, y_train).decision_function(X_test)
y_score_list = list(zip(y_test[0:20], y_scores_lr[0:20]))

# show the decision_function scores for first 20 instances
y_score_list
```

Out[20]:

```
[(0, -23.172292973469546),
 (0, -13.542576515500063),
 (0, -21.717588760007867),
 (0, -18.903065133316439),
 (0, -19.733169947138638),
 (0, -9.7463217496747667),
 (1, 5.2327155658831135),
 (0, -19.308012306288916),
 (0, -25.099330209728528),
 (0, -21.824312362996),
 (0, -24.14378275072049),
 (0, -19.578811099762508),
 (0, -22.568371393280199),
 (0, -10.822590225240777),
 (0, -11.907918741521932),
 (0, -10.977026853802803),
 (1, 11.206811164226373),
 (0, -27.64415761980748),
 (0, -12.857692102545409),
 (0, -25.848149140240199)]
```

Using the `predict_proba()` method

In [21]:

```
X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced, rand
om_state=0)
y_proba_lr = lr.fit(X_train, y_train).predict_proba(X_test)
y_proba_list = list(zip(y_test[0:20], y_proba_lr[0:20,1]))

# show the probability of positive class for first 20 instances
y_proba_list
```

Out[21]:

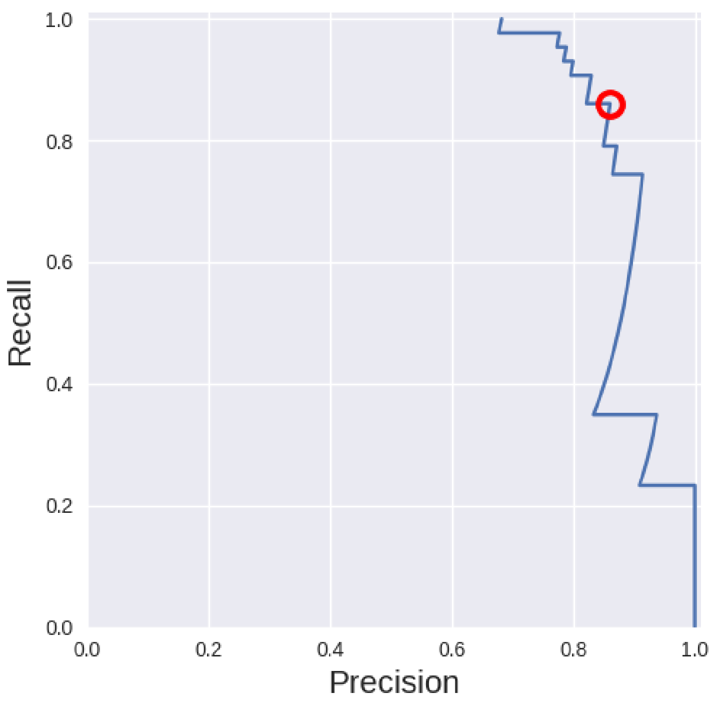
```
[(0, 8.6377579220606777e-11),
 (0, 1.3138118599563783e-06),
 (0, 3.6997386039099529e-10),
 (0, 6.1730972504865465e-09),
 (0, 2.6914925394345074e-09),
 (0, 5.8506057771143608e-05),
 (1, 0.99468934644404694),
 (0, 4.1175302368500096e-09),
 (0, 1.2574750894253029e-11),
 (0, 3.3252290754668869e-10),
 (0, 3.2695529799373086e-11),
 (0, 3.1407283576084884e-09),
 (0, 1.5800864117150149e-10),
 (0, 1.9943442430612578e-05),
 (0, 6.7368003023860014e-06),
 (0, 1.7089540581641637e-05),
 (1, 0.9999864188091131),
 (0, 9.8694940340195476e-13),
 (0, 2.6059983600823893e-06),
 (0, 5.9469113009063784e-12)]
```

03-04: Precision-recall and ROC Curves

Precision Recall Curves

In [22]:

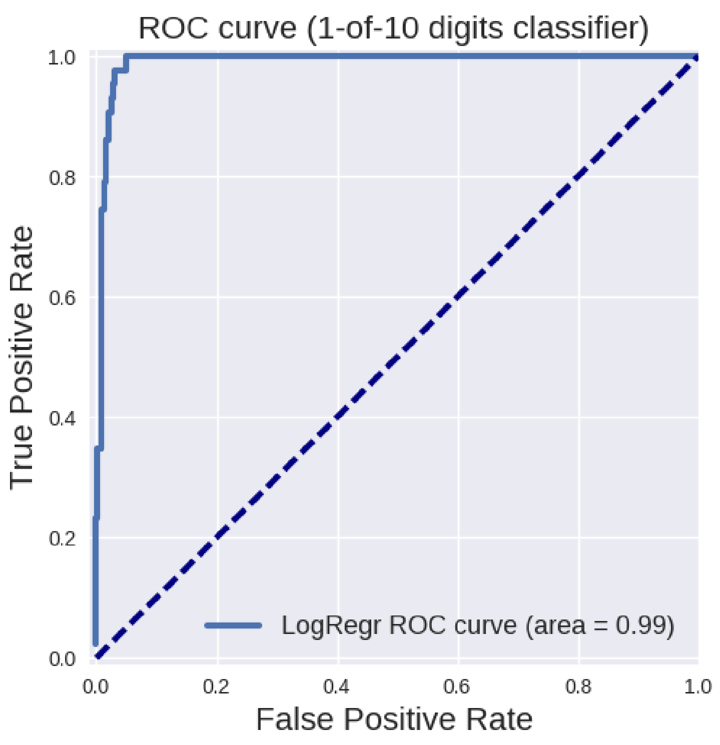
```
from sklearn.metrics import precision_recall_curve

precision, recall, thresholds = precision_recall_curve(y_test, y_scores_lr) ## c
all its constructor
# this returns an array of tuples in the above stated order, where all indices a
re shared across the 3 parameters.
closest_zero = np.argmin(np.abs(thresholds)) # this gives the index of the point
with a threshold closest to 0
closest_zero_p = precision[closest_zero] # Find the precision of the closest_zer
o threshold element
closest_zero_r = recall[closest_zero] #Find the recall of the closest_zero thres
hold element.

# Plot a graph of recall against precision
plt.figure()
plt.xlim([0.0, 1.01])
plt.ylim([0.0, 1.01])
plt.plot(precision, recall, label='Precision-Recall Curve')
plt.plot(closest_zero_p, closest_zero_r, 'o', markersize = 12, fillstyle = 'non
e', c='r', mew=3)
plt.xlabel('Precision', fontsize=16)
plt.ylabel('Recall', fontsize=16)
plt.axes().set_aspect('equal')
plt.show()
```



ROC curves, Area-Under-Curve (AUC)

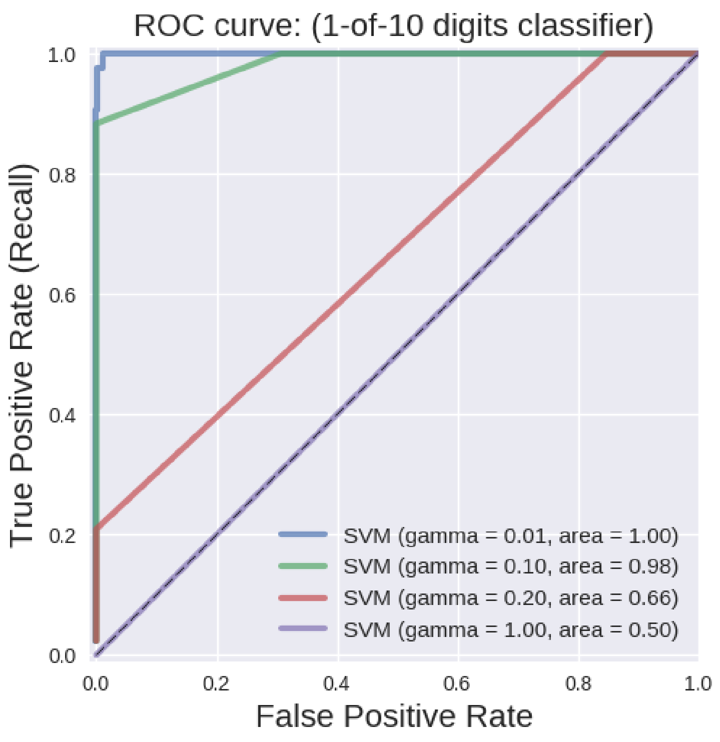
In [23]:

```
from sklearn.metrics import roc_curve, auc

X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced, rand
om_state=0)
# Lr represents the logistic regression classifier - fit the LRC with data and r
un the decision function on it
y_score_lr = lr.fit(X_train, y_train).decision_function(X_test)
#False positive rate, true positive rate and one extra parameter which we don't
 need - so we just pass it off as _
fpr_lr, tpr_lr, _ = roc_curve(y_test, y_score_lr)
#Area under the ROC curve.
roc_auc_lr = auc(fpr_lr, tpr_lr)

# Plot the ROC curve
plt.figure()
plt.xlim([-0.01, 1.00])
plt.ylim([-0.01, 1.01])
plt.plot(fpr_lr, tpr_lr, lw=3, label='LogRegr ROC curve (area = {:0.2f})'.format
(roc_auc_lr))
plt.xlabel('False Positive Rate', fontsize=16)
plt.ylabel('True Positive Rate', fontsize=16)
plt.title('ROC curve (1-of-10 digits classifier)', fontsize=16)
plt.legend(loc='lower right', fontsize=13)
plt.plot([0, 1], [0, 1], color='navy', lw=3, linestyle='--') # random classifie
r.
plt.axes().set_aspect('equal')
plt.show()
```



In [24]:

```
from matplotlib import cm #colour map

X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced, rand
om_state=0)
# Plot a figure of the TPR with respect to the FPR for varying gamma
plt.figure()
plt.xlim([-0.01, 1.00])
plt.ylim([-0.01, 1.01])
# Range of values of gamma
for g in [0.01, 0.1, 0.20, 1]:
    # Create a SVM classifier with RBF kernel and fit the training data to the m
odel
    svm = SVC(gamma=g).fit(X_train, y_train)
    # Find the decision_function
    y_score_svm = svm.decision_function(X_test)
    # Find the false positive rate and true positive rate for this SVM
    fpr_svm, tpr_svm, _ = roc_curve(y_test, y_score_svm)
    # Find the area under the curve as an evaluation metric
    roc_auc_svm = auc(fpr_svm, tpr_svm)
    # Calculate its accuracy on the test data
    accuracy_svm = svm.score(X_test, y_test)
    print("gamma = {:.2f}  accuracy = {:.2f}   AUC = {:.2f}".format(g, accuracy_
svm,
                                                                      roc_auc_svm
))
    # Plot the ROC curve for this value of gamma
    plt.plot(fpr_svm, tpr_svm, lw=3, alpha=0.7,
             label='SVM (gamma = {:0.2f}, area = {:0.2f})'.format(g, roc_auc_svm
))
    # Repeat for other values of gamma

# Label the rest of your axes
plt.xlabel('False Positive Rate', fontsize=16)
plt.ylabel('True Positive Rate (Recall)', fontsize=16)
plt.plot([0, 1], [0, 1], color='k', lw=0.5, linestyle='--')
plt.legend(loc="lower right", fontsize=11)
plt.title('ROC curve: (1-of-10 digits classifier)', fontsize=16)
plt.axes().set_aspect('equal')

plt.show()
```



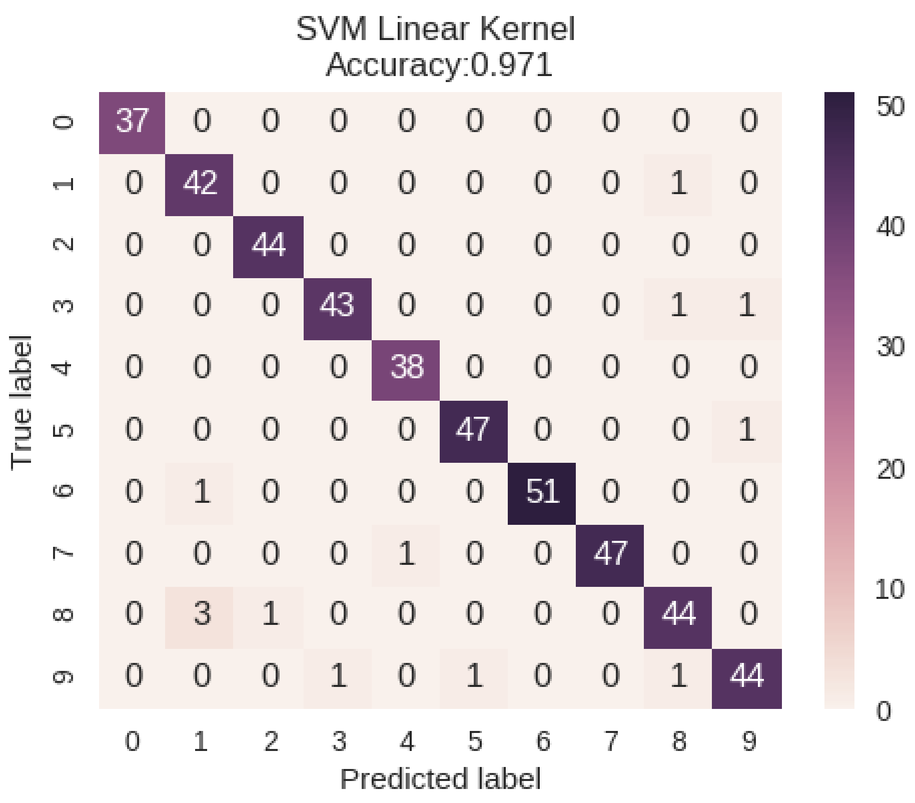
```
gamma = 0.01  accuracy = 0.91   AUC = 1.00
gamma = 0.10  accuracy = 0.90   AUC = 0.98
gamma = 0.20  accuracy = 0.90   AUC = 0.66
gamma = 1.00  accuracy = 0.90   AUC = 0.50
```

03-05: Evaluation measures for multi-class classification

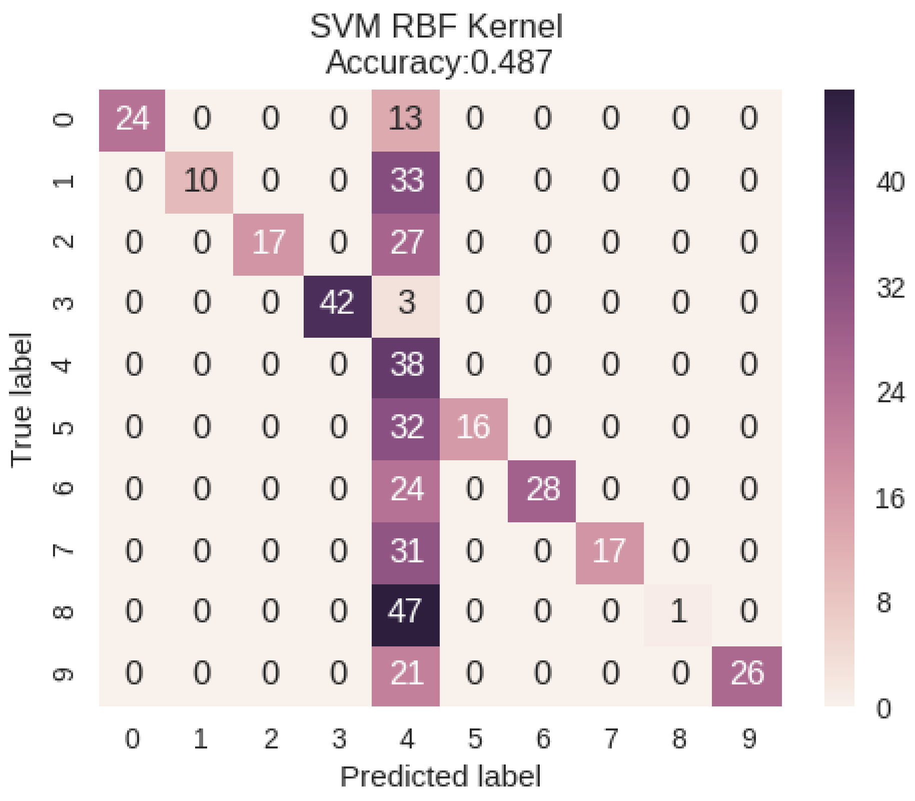
Multi-class confusion matrix

In [25]:

```
dataset = load_digits()
X, y = dataset.data, dataset.target
X_train_mc, X_test_mc, y_train_mc, y_test_mc = train_test_split(X, y, random_sta
te=0)

# Create an SVC with linear kernel
svm = SVC(kernel = 'linear').fit(X_train_mc, y_train_mc)
# Get a list of predictions
svm_predicted_mc = svm.predict(X_test_mc)
# Create a multiclass confusion matrix of name confusion_mc
confusion_mc = confusion_matrix(y_test_mc, svm_predicted_mc)
# Create a dataframe to store the values where each row is the true value and ea
ch column is the predicted value
df_cm = pd.DataFrame(confusion_mc,
                     index = [i for i in range(0,10)], columns = [i for i in ran
ge(0,10)])

# Plot the confusion matrix
plt.figure(figsize=(5.5,4))
# HEY HELLO SEABORN
sns.heatmap(df_cm, annot=True)
# Other MPL support
plt.title('SVM Linear Kernel \nAccuracy:{0:.3f}'.format(accuracy_score(y_test_mc
,
                                                                         svm_predi
cted_mc)))
plt.ylabel('True label')
plt.xlabel('Predicted label')

# Here is the 2nd classifier for comparison that uses an SVC rbf kernel - this c
lassifier is meant to perform
# much worse than the prior.
svm = SVC(kernel = 'rbf').fit(X_train_mc, y_train_mc)
svm_predicted_mc = svm.predict(X_test_mc)
confusion_mc = confusion_matrix(y_test_mc, svm_predicted_mc)
df_cm = pd.DataFrame(confusion_mc, index = [i for i in range(0,10)],
                  columns = [i for i in range(0,10)])

plt.figure(figsize = (5.5,4))
sns.heatmap(df_cm, annot=True)
plt.title('SVM RBF Kernel \nAccuracy:{0:.3f}'.format(accuracy_score(y_test_mc,
                                                                    svm_predicte
d_mc)))
plt.ylabel('True label')
plt.xlabel('Predicted label');
```



	0	1	2	3	4	5	6	7	8	9
0	37	0	0	0	0	0	0	0	0	0
1	0	42	0	0	0	0	0	0	1	0
2	0	0	44	0	0	0	0	0	0	0
3	0	0	0	43	0	0	0	0	1	1
4	0	0	0	0	38	0	0	0	0	0
5	0	0	0	0	0	47	0	0	0	1
6	0	1	0	0	0	0	51	0	0	0
7	0	0	0	0	1	0	0	47	0	0
8	0	3	1	0	0	0	0	0	44	0
9	0	0	0	1	0	1	0	0	1	44



As an aside, it sometimes is useful to display a confusion matrix as a **heat map** in order to highlight the relative frequencies of different kinds of errors.

For comparison, I've included the RBF kernel SVM which did substantially worse on the dataset.

Although you can see from the accuracy score, the RBF kernel has an accuracy of 0.487 compared to the linear kernel, but this accuracy metric alone doesn't give much insight into why this is the case.

For some reason, the SVM RBF kernel **keeps predicting the digit 4.** For instance, out of 44 instances of the digit 2 the classifier only correctly classified 17 of them, and the rest of them was predicted as the digit 4. This would mean an error in the **feature preprocessing** which has caused too many numbers to map to the digit 4. It is **the confusion matrix** that gives you insight into these issues.

Multi-class classification report

In [26]:

```
print(classification_report(y_test_mc, svm_predicted_mc))
```

```
             precision    recall  f1-score   support

          0       1.00      0.65      0.79        37
          1       1.00      0.23      0.38        43
          2       1.00      0.39      0.56        44
          3       1.00      0.93      0.97        45
          4       0.14      1.00      0.25        38
          5       1.00      0.33      0.50        48
          6       1.00      0.54      0.70        52
          7       1.00      0.35      0.52        48
          8       1.00      0.02      0.04        48
          9       1.00      0.55      0.71        47

avg / total       0.93      0.49      0.54       450
```

Micro- vs. macro-averaged metrics using the `average` = parameter

In [29]:

```
print('Micro-averaged precision = {:.2f} (treat instances equally)'
      .format(precision_score(y_test_mc, svm_predicted_mc, average = 'micro')))
print('Macro-averaged precision = {:.2f} (treat classes equally)'
      .format(precision_score(y_test_mc, svm_predicted_mc, average = 'macro')))
```

```
Micro-averaged precision = 0.49 (treat instances equally)
Macro-averaged precision = 0.91 (treat classes equally)
```

In [28]:

```
print('Micro-averaged f1 = {:.2f} (treat instances equally)'
      .format(f1_score(y_test_mc, svm_predicted_mc, average = 'micro')))
print('Macro-averaged f1 = {:.2f} (treat classes equally)'
      .format(f1_score(y_test_mc, svm_predicted_mc, average = 'macro')))
```

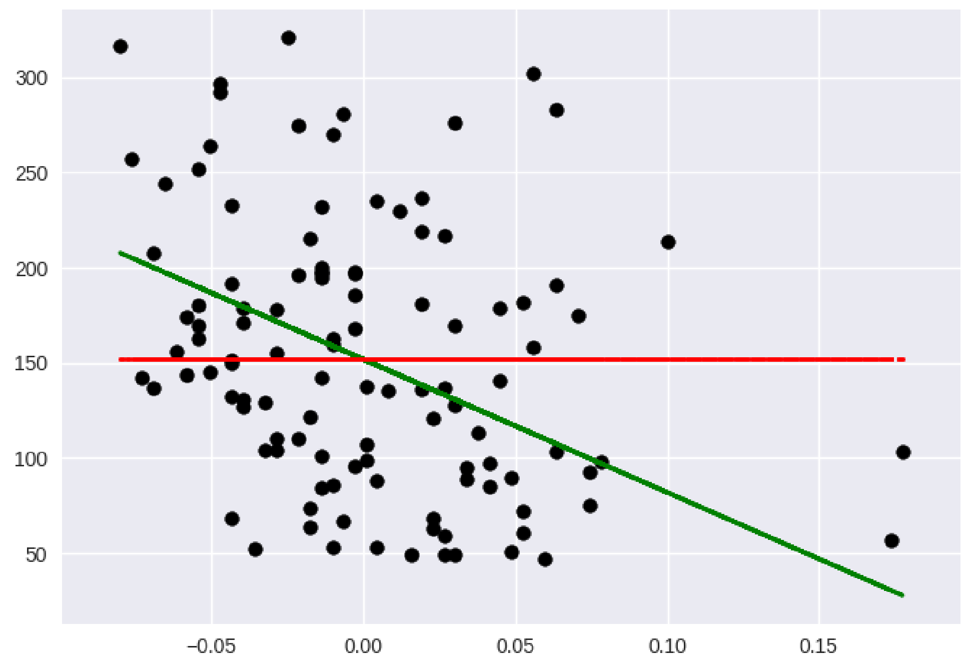
```
Micro-averaged f1 = 0.49 (treat instances equally)
Macro-averaged f1 = 0.54 (treat classes equally)
```

03-06: Regression evaluation metrics

In [30]:

```
%matplotlib notebook
import matplotlib.pyplot as plt
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn import datasets
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.dummy import DummyRegressor

diabetes = datasets.load_diabetes()

X = diabetes.data[:, None, 6]
y = diabetes.target

X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
# Least Squares Regression
lm = LinearRegression().fit(X_train, y_train)
# Dummy Regressor
lm_dummy_mean = DummyRegressor(strategy = 'mean').fit(X_train, y_train)
# Get both predicted values for both models.
y_predict = lm.predict(X_test)
y_predict_dummy_mean = lm_dummy_mean.predict(X_test)

# Output the coefficients to the linear model using the coef_ attribute
print('Linear model, coefficients: ', lm.coef_)

# Calculate the mean_Squared error for the dummy and for the linear model
print("Mean squared error (dummy): {:.2f}".format(mean_squared_error(y_test,
                                                                     y_predict_d
ummy_mean)))
print("Mean squared error (linear model): {:.2f}".format(mean_squared_error(y_te
st, y_predict)))

# Calculate the r2 score for the dummy and linear model
print("r2_score (dummy): {:.2f}".format(r2_score(y_test, y_predict_dummy_mean)))
print("r2_score (linear model): {:.2f}".format(r2_score(y_test, y_predict)))

# Plot outputs
plt.scatter(X_test, y_test,  color='black')
plt.plot(X_test, y_predict, color='green', linewidth=2)
plt.plot(X_test, y_predict_dummy_mean, color='red', linestyle = 'dashed',
         linewidth=2, label = 'dummy')

plt.show()
```

```
Linear model, coefficients:  [-698.80206267]
Mean squared error (dummy): 4965.13
Mean squared error (linear model): 4646.74
r2_score (dummy): -0.00
r2_score (linear model): 0.06
```



We can see that, as expected, the dummy regressor achieves an R^2 score of 0, since it always makes a constant prediction without looking at the output. In this instance, the linear model provides only **slightly better fit** than the dummy regressor according to both the **mean squared error** and the R^2 **score.**

03-07: Model selection using evaluation metrics

Cross-validation example

In [31]:

```
from sklearn.model_selection import cross_val_score
from sklearn.svm import SVC

dataset = load_digits()
# again, making this a binary problem with 'digit 1' as positive class
# and 'not 1' as negative class
X, y = dataset.data, dataset.target == 1 # appreciate how neat this syntax look
s!
# Create an SVC linear kernel with default value of C
clf = SVC(kernel='linear', C=1)

# accuracy is the default scoring metric
print('Cross-validation (accuracy)', cross_val_score(clf, X, y, cv=5))
# use AUC as scoring metric
print('Cross-validation (AUC)', cross_val_score(clf, X, y, cv=5, scoring = 'roc_
auc'))
# use recall as scoring metric
print('Cross-validation (recall)', cross_val_score(clf, X, y, cv=5, scoring = 'r
ecall'))
```

```
Cross-validation (accuracy) [ 0.91944444  0.98611111  0.97214485  0.
97493036  0.96935933]
Cross-validation (AUC) [ 0.9641871   0.9976571   0.99372205  0.99699
002  0.98675611]
Cross-validation (recall) [ 0.81081081  0.89189189  0.83333333  0.83
333333  0.83333333]
```

Grid search example

In [32]:

```
from sklearn.svm import SVC
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import roc_auc_score

dataset = load_digits()
X, y = dataset.data, dataset.target == 1
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

# Create a classifier with an rbf kernel
clf = SVC(kernel='rbf')
# Parameter values of the variable gamma
grid_values = {'gamma': [0.001, 0.01, 0.05, 0.1, 1, 10, 100]}

# --------------- default metric to optimize over grid parameters: accuracy-----
---------
# Call the GridSearchCV constructor and assign it the grid_clf_acc variable
grid_clf_acc = GridSearchCV(clf, param_grid = grid_values)
# Fit the model to the data
grid_clf_acc.fit(X_train, y_train)
# Run the decision_function on it
y_decision_fn_scores_acc = grid_clf_acc.decision_function(X_test)

# Use the best_params_ method from the GridSearchCV object to obtain the best pa
rameter for gamma
print('Grid best parameter (max. accuracy): ', grid_clf_acc.best_params_)
# And the score for this best gamma
print('Grid best score (accuracy): ', grid_clf_acc.best_score_)

# ----------------- Do the same thing for the alternative metric to optimize ove
r grid parameters: AUC ----------
grid_clf_auc = GridSearchCV(clf, param_grid = grid_values, scoring = 'roc_auc')
grid_clf_auc.fit(X_train, y_train)
y_decision_fn_scores_auc = grid_clf_auc.decision_function(X_test)

print('Test set AUC: ', roc_auc_score(y_test, y_decision_fn_scores_auc))
print('Grid best parameter (max. AUC): ', grid_clf_auc.best_params_)
print('Grid best score (AUC): ', grid_clf_auc.best_score_)
```

```
Grid best parameter (max. accuracy):  {'gamma': 0.001}
Grid best score (accuracy):  0.996288047513
Test set AUC:  0.999828581224
Grid best parameter (max. AUC):  {'gamma': 0.001}
Grid best score (AUC):  0.99987412783
```

In this case, they are the same. But you'll see for some cases that this value of γ is different.

Evaluation metrics supported for model selection

In [33]:

```
from sklearn.metrics.scorer import SCORERS

print(sorted(list(SCORERS.keys())))
```

```
['accuracy', 'adjusted_rand_score', 'average_precision', 'f1', 'f1_m
acro', 'f1_micro', 'f1_samples', 'f1_weighted', 'log_loss', 'mean_ab
solute_error', 'mean_squared_error', 'median_absolute_error', 'neg_l
og_loss', 'neg_mean_absolute_error', 'neg_mean_squared_error', 'neg_
median_absolute_error', 'precision', 'precision_macro', 'precision_m
icro', 'precision_samples', 'precision_weighted', 'r2', 'recall', 'r
ecall_macro', 'recall_micro', 'recall_samples', 'recall_weighted',
'roc_auc']
```

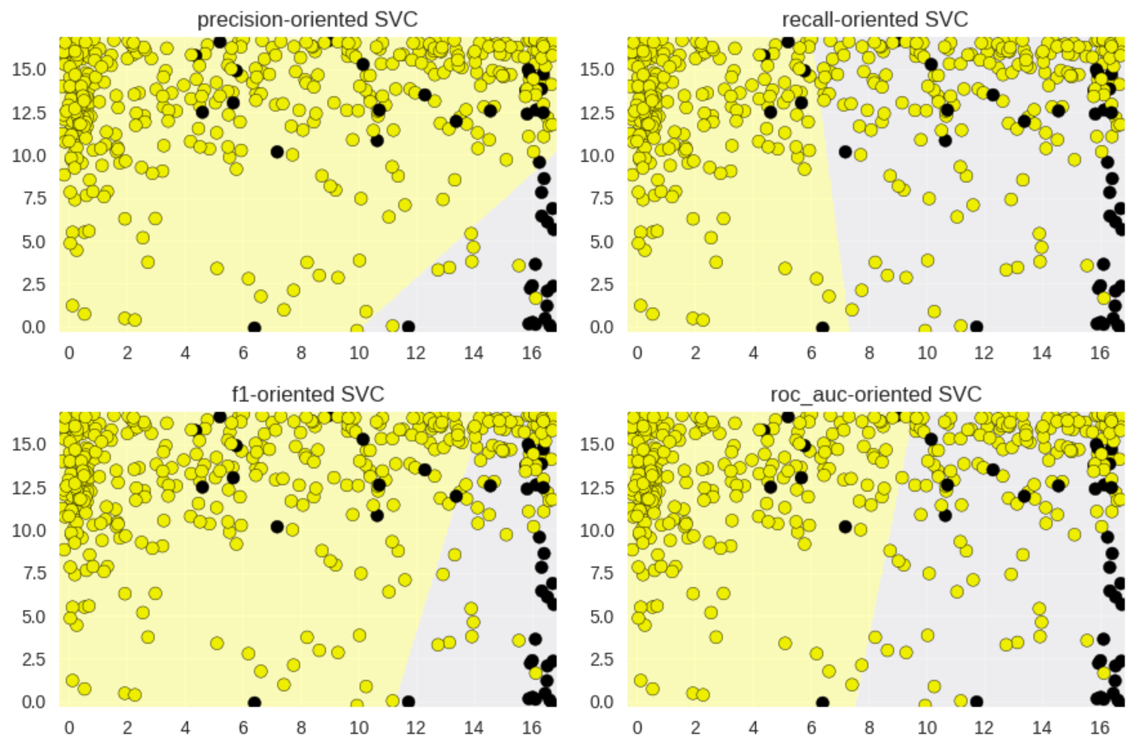
You can see stuff like **precision_micro** that represents micro-averaged-precision and also the **r2** metric for R^2 regression loss.

Two-feature classification example using the digits dataset

Optimizing a classifier using different evaluation metrics

In [34]:

```
from sklearn.datasets import load_digits
from sklearn.model_selection import train_test_split
from adspy_shared_utilities import plot_class_regions_for_classifier_subplot
from sklearn.svm import SVC
from sklearn.model_selection import GridSearchCV


dataset = load_digits()
X, y = dataset.data, dataset.target == 1
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

# Create a two-feature input vector matching the example plot above
# We jitter the points (add a small amount of random noise) in case there are ar
eas
# in feature space where many instances have the same features.
jitter_delta = 0.25
X_twovar_train = X_train[:,[20,59]]+ np.random.rand(X_train.shape[0], 2) - jitte
r_delta
X_twovar_test  = X_test[:,[20,59]] + np.random.rand(X_test.shape[0], 2) - jitter
_delta
# Create an SVC linear kernel and fit the training data to it
clf = SVC(kernel = 'linear').fit(X_twovar_train, y_train)

# Wait what is this??
grid_values = {'class_weight':['balanced', {1:2},{1:3},{1:4},{1:5},{1:10},{1:20
},{1:50}]}

# Plot the figure of 4 graphs - a precision oriented SVC, recall oriented SVC, f
1 oriented SVC and a roc_auc SVC
plt.figure(figsize=(9,6))
for i, eval_metric in enumerate(('precision','recall', 'f1','roc_auc')):
    # Call the constructor with the classifier used, grid values we want to opti
mise and the scoring metric we want
    # to optimise by.
    grid_clf_custom = GridSearchCV(clf, param_grid=grid_values, scoring=eval_met
ric)
    # Fit the parameters to this model
    grid_clf_custom.fit(X_twovar_train, y_train)
    # Find the best parameter.
    print('Grid best parameter (max. {0}): {1}'
          .format(eval_metric, grid_clf_custom.best_params_))
    print('Grid best score ({0}): {1}'
          .format(eval_metric, grid_clf_custom.best_score_))
    # some MPL support to plot the SVC
    plt.subplots_adjust(wspace=0.3, hspace=0.3)
    plot_class_regions_for_classifier_subplot(grid_clf_custom, X_twovar_test, y_
test, None,
                                             None, None,  plt.subplot(2, 2, i+1
))

    plt.title(eval_metric+'-oriented SVC')
plt.tight_layout()
plt.show()
```



```
Grid best parameter (max. precision): {'class_weight': {1: 2}}
Grid best score (precision): 0.5403571723170832
Grid best parameter (max. recall): {'class_weight': {1: 50}}
Grid best score (recall): 0.9284310837047003
Grid best parameter (max. f1): {'class_weight': {1: 4}}
Grid best score (f1): 0.500943108983028
Grid best parameter (max. roc_auc): {'class_weight': {1: 20}}
Grid best score (roc_auc): 0.8874264392933449
```

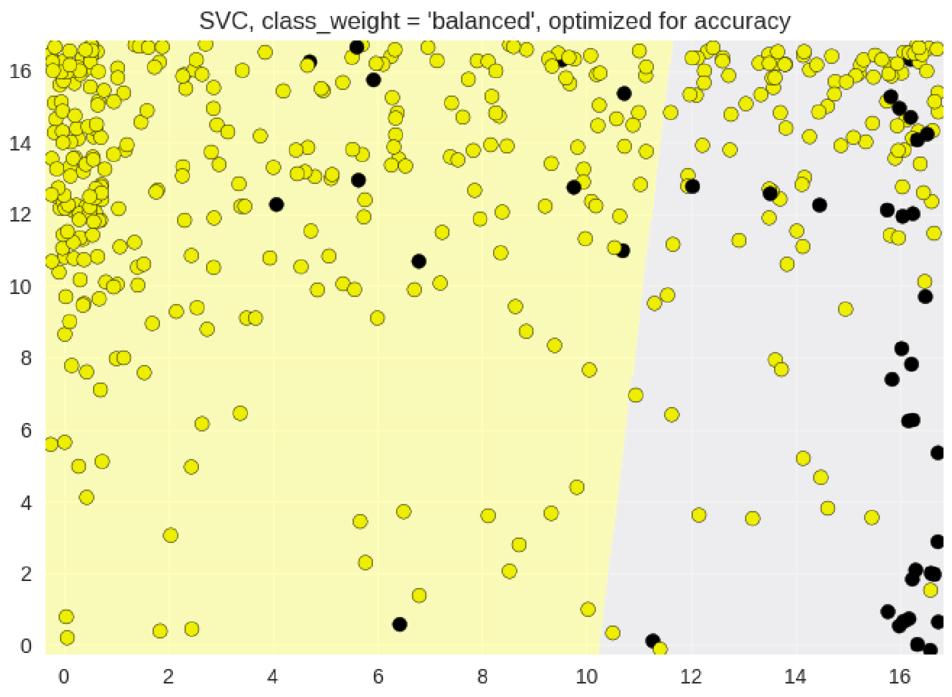
Note that the **F1-oriented** SVC is kind of in the middle of the precision and recall SVCs. This makes sense, because F1 is the **harmonic mean of precision and recall**.

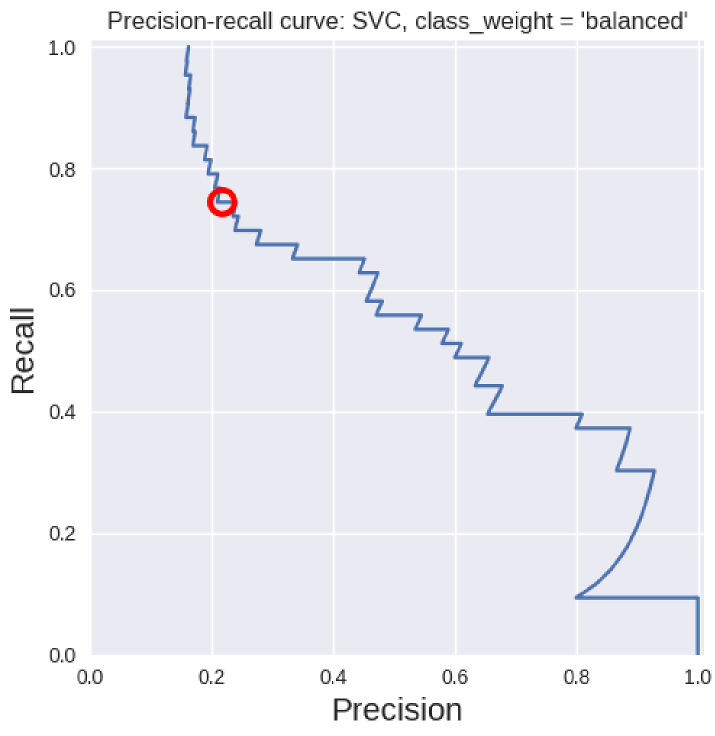
The AUC oriented classifier with an optimal class weight of 5 has a similar decision boundary to the F1-oriented classifier, but shifted slightly in favour of higher recall.

Precision-recall curve for the default SVC classifier (with balanced class weights)

In [35]:

```
from sklearn.model_selection import train_test_split
from sklearn.metrics import precision_recall_curve
from adspy_shared_utilities import plot_class_regions_for_classifier
from sklearn.svm import SVC

dataset = load_digits()
X, y = dataset.data, dataset.target == 1
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

# create a two-feature input vector matching the example plot above
jitter_delta = 0.25
X_twovar_train = X_train[:,[20,59]]+ np.random.rand(X_train.shape[0], 2) - jitte
r_delta
X_twovar_test  = X_test[:,[20,59]] + np.random.rand(X_test.shape[0], 2) - jitter
_delta

clf = SVC(kernel='linear', class_weight='balanced').fit(X_twovar_train, y_train)

y_scores = clf.decision_function(X_twovar_test)

precision, recall, thresholds = precision_recall_curve(y_test, y_scores)
closest_zero = np.argmin(np.abs(thresholds))
closest_zero_p = precision[closest_zero]
closest_zero_r = recall[closest_zero]

plot_class_regions_for_classifier(clf, X_twovar_test, y_test)
plt.title("SVC, class_weight = 'balanced', optimized for accuracy")
plt.show()

plt.figure()
plt.xlim([0.0, 1.01])
plt.ylim([0.0, 1.01])
plt.title ("Precision-recall curve: SVC, class_weight = 'balanced'")
plt.plot(precision, recall, label = 'Precision-Recall Curve')
plt.plot(closest_zero_p, closest_zero_r, 'o', markersize=12, fillstyle='none', c
='r', mew=3)
plt.xlabel('Precision', fontsize=16)
plt.ylabel('Recall', fontsize=16)
plt.axes().set_aspect('equal')
plt.show()
print('At zero threshold, precision: {:.2f}, recall: {:.2f}'
      .format(closest_zero_p, closest_zero_r))
```





```
At zero threshold, precision: 0.22, recall: 0.74
```

Take a moment to imagine how the extreme lower right part of the curve represents a decision boundary that is highly precision oriented. As the decision threshold is shifted to become less and less conservative, tracing the curve up and into the left, the classifier becomes more and more like the **recall-oriented** SVC example. Again the red circle represents the precision-recall trade-off achieved at the **zero score mark**, which is the actual decision boundary chosen for the trained classifier.

```
In [ ]:
```