Module 3

April 12, 2021

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*You are currently looking at **version 1.0** of this notebook. To download notebooks and datafiles, as well as get help on Jupyter notebooks in the Coursera platform, visit the Jupyter Notebook FAQ course resource.*

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1 Applied Machine Learning: Module 3 (Evaluation)

1.1 Evaluation for Classification

1.1.1 Preamble

```
In [ ]: %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()
        X, y = dataset.data, dataset.target

        for class_name, class_count in zip(dataset.target_names, np.bincount(datase
            print(class_name,class_count)
```

```
In [ ]: # 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])
```

```
In [ ]: np.bincount(y_binary_imbalanced)    # Negative class (0) is the most freque
```

```
In [ ]: X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced,

        # 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)
```

1.1.2 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 [ ]: from sklearn.dummy import DummyClassifier

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

        y_dummy_predictions
```

```
In [ ]: dummy_majority.score(X_test, y_test)
```

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

1.1.3 Confusion matrices

Binary (two-class) confusion matrix

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

        # Negative class (0) is most frequent
        dummy_majority = DummyClassifier(strategy = 'most_frequent').fit(X_train, y
        y_majority_predicted = dummy_majority.predict(X_test)
        confusion = confusion_matrix(y_test, y_majority_predicted)

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

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

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

```
In [ ]: 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
```

In [ ]:
```
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)
```

In [ ]:
```
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)
```

1.1.4 Evaluation metrics for binary classification

In [ ]:
```
from sklearn.metrics import accuracy_score, precision_score, recall_score,
# 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)))
```

In [ ]:
```
# Combined report with all above metrics
from sklearn.metrics import classification_report

print(classification_report(y_test, tree_predicted, target_names=['not 1',
```

In [ ]:
```
print('Random class-proportional (dummy)\n',
      classification_report(y_test, y_classprop_predicted, target_names=['r
print('SVM\n',
      classification_report(y_test, svm_predicted, target_names = ['not 1',
print('Logistic regression\n',
      classification_report(y_test, lr_predicted, target_names = ['not 1',
print('Decision tree\n',
      classification_report(y_test, tree_predicted, target_names = ['not 1'
```

1.1.5 Decision functions

In [ ]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced,
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
```

```
In [ ]: X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced,
        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
```

1.1.6 Precision-recall curves

```
In [ ]: from sklearn.metrics import precision_recall_curve

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

        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 =
        plt.xlabel('Precision', fontsize=16)
        plt.ylabel('Recall', fontsize=16)
        plt.axes().set_aspect('equal')
        plt.show()
```

1.1.7 ROC curves, Area-Under-Curve (AUC)

```
In [ ]: from sklearn.metrics import roc_curve, auc

        X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced,

        y_score_lr = lr.fit(X_train, y_train).decision_function(X_test)
        fpr_lr, tpr_lr, _ = roc_curve(y_test, y_score_lr)
        roc_auc_lr = auc(fpr_lr, tpr_lr)

        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})'.f
        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='--')
plt.axes().set_aspect('equal')
plt.show()
```

In [ ]:
```
from matplotlib import cm

X_train, X_test, y_train, y_test = train_test_split(X, y_binary_imbalanced,

plt.figure()
plt.xlim([-0.01, 1.00])
plt.ylim([-0.01, 1.01])
for g in [0.01, 0.1, 0.20, 1]:
    svm = SVC(gamma=g).fit(X_train, y_train)
    y_score_svm = svm.decision_function(X_test)
    fpr_svm, tpr_svm, _ = roc_curve(y_test, y_score_svm)
    roc_auc_svm = auc(fpr_svm, tpr_svm)
    accuracy_svm = svm.score(X_test, y_test)
    print("gamma = {:.2f}  accuracy = {:.2f}   AUC = {:.2f}".format(g, accu
                                                                     roc_auc
    plt.plot(fpr_svm, tpr_svm, lw=3, alpha=0.7,
             label='SVM (gamma = {:0.2f}, area = {:0.2f})'.format(g, roc_au

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()
```

1.1.8 Evaluation measures for multi-class classification

Multi-class confusion matrix

In [ ]:
```
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, rando


svm = SVC(kernel = 'linear').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 i

plt.figure(figsize=(5.5,4))
sns.heatmap(df_cm, annot=True)
```

```
plt.title('SVM Linear Kernel \nAccuracy:{0:.3f}'.format(accuracy_score(y_te
                                                                        svm_
plt.ylabel('True label')
plt.xlabel('Predicted label')


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_
                                                                      svm_pre
plt.ylabel('True label')
plt.xlabel('Predicted label');
```

Multi-class classification report

```
In [ ]: print(classification_report(y_test_mc, svm_predicted_mc))
```

Micro- vs. macro-averaged metrics

```
In [ ]: 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

In [ ]: 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')))
```

1.1.9 Regression evaluation metrics

```
In [ ]: %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)

lm = LinearRegression().fit(X_train, y_train)
lm_dummy_mean = DummyRegressor(strategy = 'mean').fit(X_train, y_train)

y_predict = lm.predict(X_test)
y_predict_dummy_mean = lm_dummy_mean.predict(X_test)

print('Linear model, coefficients: ', lm.coef_)
print("Mean squared error (dummy): {:.2f}".format(mean_squared_error(y_test
                                                                      y_prec
print("Mean squared error (linear model): {:.2f}".format(mean_squared_error
print("r2_score (dummy): {:.2f}".format(r2_score(y_test, y_predict_dummy_me
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()
```

1.1.10 Model selection using evaluation metrics

Cross-validation example

```
In [ ]: 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
        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 =
        # use recall as scoring metric
        print('Cross-validation (recall)', cross_val_score(clf, X, y, cv=5, scoring
```

Grid search example

```
In [ ]: 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)

        clf = SVC(kernel='rbf')
        grid_values = {'gamma': [0.001, 0.01, 0.05, 0.1, 1, 10, 100]}

        # default metric to optimize over grid parameters: accuracy
        grid_clf_acc = GridSearchCV(clf, param_grid = grid_values)
        grid_clf_acc.fit(X_train, y_train)
        y_decision_fn_scores_acc = grid_clf_acc.decision_function(X_test)

        print('Grid best parameter (max. accuracy): ', grid_clf_acc.best_params_)
        print('Grid best score (accuracy): ', grid_clf_acc.best_score_)

        # alternative metric to optimize over grid parameters: AUC
        grid_clf_auc = GridSearchCV(clf, param_grid = grid_values, scoring = 'roc_a
        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_)
```

Evaluation metrics supported for model selection

```
In [ ]: from sklearn.metrics.scorer import SCORERS

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

1.1.11 Two-feature classification example using the digits dataset

Optimizing a classifier using different evaluation metrics

```
In [ ]: from sklearn.datasets import load_digits
        from sklearn.model_selection import train_test_split
        from adspy_shared_utilities import plot_class_regions_for_classifier_subplo
        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 a
# 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) -
X_twovar_test  = X_test[:,[20,59]] + np.random.rand(X_test.shape[0], 2) - j

clf = SVC(kernel = 'linear').fit(X_twovar_train, y_train)
grid_values = {'class_weight':['balanced', {1:2},{1:3},{1:4},{1:5},{1:10},{
plt.figure(figsize=(9,6))
for i, eval_metric in enumerate(('precision','recall', 'f1','roc_auc')):
    grid_clf_custom = GridSearchCV(clf, param_grid=grid_values, scoring=eva
    grid_clf_custom.fit(X_twovar_train, y_train)
    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_))
    plt.subplots_adjust(wspace=0.3, hspace=0.3)
    plot_class_regions_for_classifier_subplot(grid_clf_custom, X_twovar_tes
                                              None, None,  plt.subplot(2, 2,

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

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

In [ ]:
```
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) -
X_twovar_test  = X_test[:,[20,59]] + np.random.rand(X_test.shape[0], 2) - j

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

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='non
    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))
```

```
In [ ]:
```