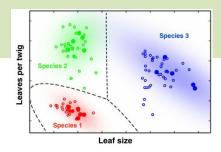


Unit 04: **The Classification Pipeline**



Outline

- Look at the big picture
- 2. Get, explore and prepare data
- Select and train model
 - 1) Binary Classification
 - i. Accuracy
 - ii. Confusion Matrix
 - iii. Precision, Recall and F1 score
 - iv. Precision vs Recall (PR) Curve
 - v. Receiver Operating Curve (ROC)
 - vi. Area Under Curve (AUC)
 - 2) Multi-class classification
- Fine-tune model

Python Libraries & Tools

- To learn the classification pipeline, we will be using the following Python libraries and tools:
 - Numpy, Pandas, Matplotlib, Scikit-Learn
 - Jupyter Notebook
- Dataset needed for the hand-on exercise:
 - MNIST dataset

Will practice the classification pipeline in Lab 6

Dataset used in this lecture

MNIST Digit





- A set of 70,000 small images of digits written by high school students and employees of US Census Bureau
- First 60,000 samples for training, remaining 10,000 for testing
- All images are 28x28 pixels in size, gray scale with values of 0 ~ 255
- Comes with Scikit-Learn
- Task: given an image, classify what digit is in the image

Look at the Big Picture

What do we want to do?



- Binary Classification: Detect images with digit 5 in the dataset. Classify images with digit 5 as true and the others as false.
- Multi-class Classification: Detect images with digit 0 to 9 in the dataset.

Get data

Fetch dataset and look at data structure



MNIST dataset is provided by Scikit-Learn

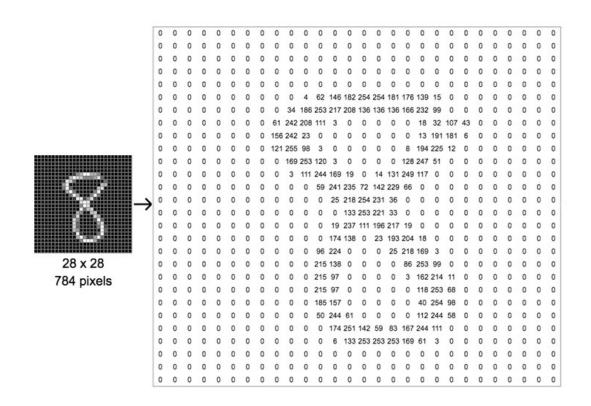
```
from sklearn.datasets import fetch_openml
X, y = fetch_openml('mnist_784', version=1, return_X_y=True)

print('Shape of X:', X.shape)
print('Shape of y:', y.shape)

Shape of X: (70000, 784)
Shape of y: (70000,)
```

- Total 70,000 samples
- Each sample has **784 attributes** (pixels) which are acquired by flattening the image $(784 = 28 \times 28)$.
- Each pixel has a value between 0 (black) and 255 (white)
- X stores the images in rows as float
- y stores the labels of corresponding images as pandas 'CategoricalDtype'

Image Representation



Explore data



Looking at the distribution of digits, it is quite even

```
print('label frequency')
print(pd.Series(y).value_counts())
label frequency
     7877
1
    7293
3
    7141
2
   6990
9
   6958
0
    6903
    6876
    6825
4
    6824
     6313
dtype: int64
```

Prepare data



- First, define the input matrix X and output variable y
- Then, split the dataset into training and testing set

```
X_train, X_test, y_train, y_test = X[:60000], X[60000:], y[:60000], y[60000:]
print('Shape of X_train:', X_train.shape, ' y_train:', y_train.shape)
print('Shape of X_test:', X_test.shape, ' y_test:', y_test.shape)

Shape of X_train: (60000, 784) y_train: (60000,)
Shape of X_test: (10000, 784) y_test: (10000,)
```

```
print('Labels of first 10 training samples:', y_train[:10]) # show the first 10 samples
Labels of first 10 training samples: ['5' '0' '4' '1' '9' '2' '1' '3' '1' '4']
```

Outline

- 1. Look at the big picture
- 2. Get, explore and prepare data
- Select and train model
 - 1) Binary Classification
 - i. Accuracy
 - ii. Confusion Matrix
 - iii. Precision, Recall and F1 score
 - iv. Precision vs Recall (PR) Curve
 - v. Receiver Operating Curve (ROC)
 - vi. Area Under Curve (AUC)
 - 2) Multi-class classification
- Fine-tune model

Binary Classification

Binary classifier: distinguish between two classes,
 5 (true) and not-5 (false) images



 First, let's create the targeted variable y_train_5 and y_test_5 which is *True* only for samples with digit 5 and False otherwise

```
y_train_5 = (y_train == '5')
y_test_5 = (y_test == '5')
```

y_train_5
False
False
False
True
False

Select and Train a Model

Training a binary classifier: SGDClassifier



Train the SGDClassifier classifier:

```
from sklearn.linear_model import SGDClassifier
sgd_clf = SGDClassifier (random_state = 42, max_iter = 5, tol = None)
sgd_clf.fit(X_train, y_train_5)
```

After we have trained it, we can now use it to classify 5 / not-5 images

```
y_pred = sgd_clf.predict(X_train)
y_pred
```

```
array([False, False, False, ..., False, False, False], dtype=bool)
```

SGDCLassifier is a **linear classifier** that uses stochastic gradient descent (SGD) which which has the advantage of being capable of handling very large datasets efficiently.

Classification Accuracy

One way to measure the performance of a classifier is accuracy measure:

$$Accuracy = \frac{\text{\#Correctly predicted samples}}{\text{\#samples}}$$

Evaluating accuracy of predicted labels



```
from sklearn.metrics import accuracy_score
train_acc = accuracy_score(y_train_5, y_pred)
print("Training accuracy: {:.4f}".format(train_acc))
Training accuracy: 0.9648
```

accuracy_score helper function computes the accuracy score given the
actual and predicted labels

Evaluation using Cross-Validation

A good way to evaluate a model is to use the K-fold cross-validation:

3-fold cross-validation



```
from sklearn.model_selection import cross_val_score
k_scores = cross_val_score(sgd_clf, X_train, y_train_5, cv=3, scoring='accuracy')
k_scores
array([0.9502 , 0.96565, 0.96495])
```

Performance on all folds are above 0.95. This looks very amazing. But is it really so?

cross_validate allows specifying multiple metrics for evaluation

Issues with Accuracy

 Accuracy measure may not give a true idea about the performance of the system especially for skewed dataset

Problem with accuracy for skewed dataset



```
from sklearn.metrics import accuracy_score

y_train_pred = sgd_clf.predict(X_train)
print('Accuracy using prediction values:', accuracy_score(y_train_5, y_train_pred))

y_train_allfalse = np.zeros(len(y_train_5), dtype=bool)
print('Accuracy if set to all false:', accuracy_score(y_train_5, y_train_allfalse))
```

Accuracy using prediction values: 0.9648 Accuracy if set to all false: 0.90965

- Although we predict all images with digit 5 wrongly, we still get a high accuracy value of over 90%
- This is because only 10% of the images are 5

Confusion matrix

A better way to present our results is the confusion matrix

False True False True Negative (TN) False Positive(FP) Actual Class False Negative (FN) True Positive(TP)

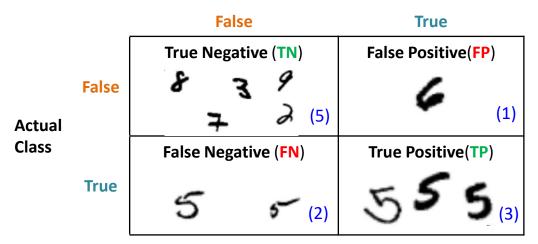
y_pred
False
False
True
True
False

TP (true positives): number of positive samples that are correctly predicted as positive FN (false negatives): number of positive samples that are falsely predicted as negative TN (true negatives): number of negative samples that are correctly predicted as negative FP (false positives): number of negative samples that are falsely predicted as positive

Confusion matrix

A better way to present our results is the confusion matrix

Predicted Class (a 5 image)



We can derive accuracy from the confusion matrix

Accuracy =
$$(TN + TP) / (TN + TP + FP + FN)$$
 Accuracy = $8 / 11$

Confusion Matrix



Compute the cross-validated prediction of all samples in training set

```
from sklearn.model_selection import cross_val_predict

y_train_pred = cross_val_predict (sgd_clf, X_train, y_train_5, cv=3)
y_train_pred
```

array([False, False, False, False, False], dtype=bool)

Compute the confusion matrix

```
from sklearn.metrics import confusion_matrix
cm = confusion_matrix (y_train_5, y_train_pred)
print(cm)
```

Prediction

False True

[53272 1307]
[1077 4344]

Actual

Question: What is the confusion matrix for the best possible performance?

cross_val_predict generates the cross-validated estimates for each sample
confusion_matrix computes the confusion matrix given the actual and predicted values

Precision and Recall

Precision or positive predictive value (PPV) measures the accuracy of the positive prediction:

If the system predicts something to be true, how reliable is its prediction?

 Recall or sensitivity or true positive rate (TPR) measures the ratio of positive samples that are correctly detected

How many positive samples in the dataset are correctly detected?

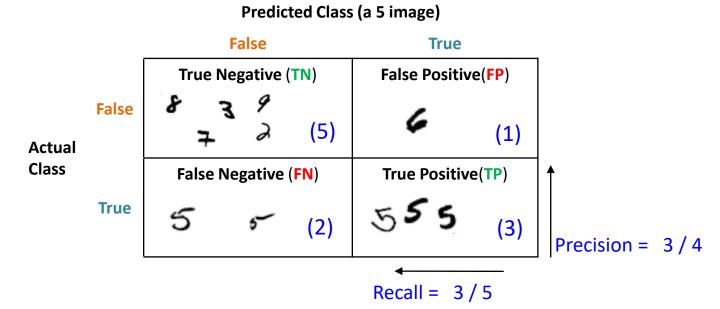
Recall =
$$TP / (FN + TP)$$

Pre

False Positive(FP)

True Positive(TP

Confusion matrix



The Precision/Recall trade-off: increase precision usually will lower the recall rate and vice versa

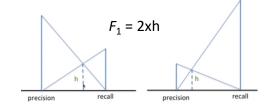
F₁ Score

- Combines the precision and recall into a single score
- The harmonic mean of precision and recall:

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = \frac{\text{TP}}{TP + \frac{FN + FP}{2}}$$

Examples:

Precision	Recall	Mean	F1-score
0.9	0.3	0.6	0.45
0.7	0.5	0.6	0.58



- F₁ is high only when both recall and precision are high (harmonic mean gives much more weight to the low values)
- F₁ favors classifiers that have similar precision and recall
- Used when both precision and recall are equally important

Precision, Recall and F1 Score



```
from sklearn.metrics import precision_score, recall_score, f1_score
print('precision = ', precision_score(y_train_5, y_train_pred))
print('recall = ', recall_score (y_train_5, y_train_pred))
print('f1 score = ', f1_score(y_train_5, y_train_pred))
```

```
precision = 0.768713502035
recall = 0.801328168235
f1 score = 0.784682080925
```

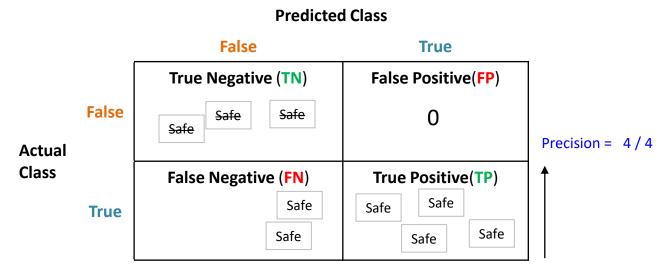
 The 5-detector does not look as good now (correct only 77% of the time and only detect 80% of the 5s).

precision_score computes the precision given the actual and predicted values
recall_score computes the recall given the actual and predicted values
f1_score computes the f1 score given the actual and predicted values

Review question

For a classifier that detect safe video contents for the kids, which performance measure is more important: precision or recall?

Want high precision (all selected videos are actually safe), able to tolerate low recall (some good videos are filtered out)



Review question

For a classifier that detect shoplifters, which performance measure is more important: precision or recall?

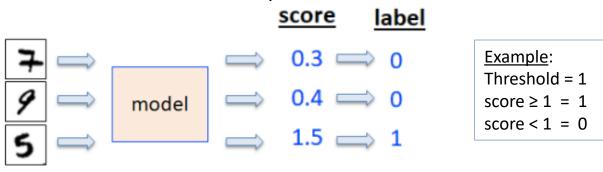
Want high recall (detect potential shoplifters). Low precision (detect non-shoplifters) can be screened manually. Want to catch all shoplifters.

Predicted Class

		False	True
Actual Class		True Negative (TN)	False Positive(FP)
	False		
		False Negative (FN)	True Positive(TP)
	True	0	

Precision/Recall Tradeoff

- Desirable to have high precision and high recall
- In reality, increasing precision reduces recall, and vice versa.
- Most classifiers compute a score (how likely a sample belongs to the positive class) based on a decision function, and then threshold on the score to output the label.

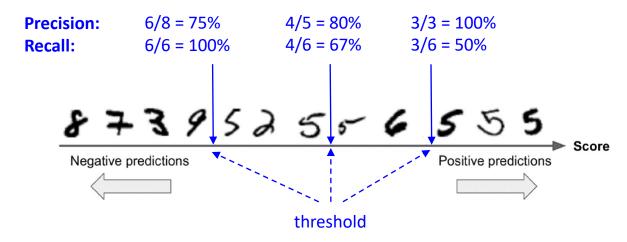


 Thus, we can set some threshold on the score to control the tradeoff between precision and recall.

Note that in SGDClassifier, the threshold value is fixed at 0

Precision/Recall Tradeoff

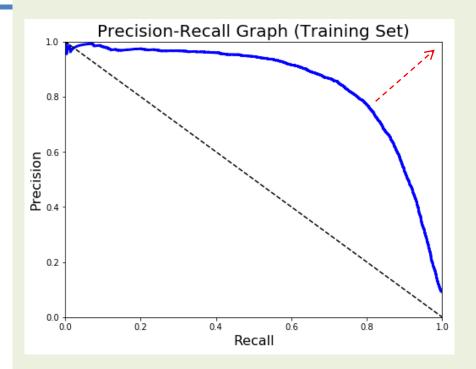
- The score threshold value controls precision and recall
- As we lower the threshold, recall increases but precision decreases (less precise but get more positive samples), and vice versa



- How to decide which threshold to use?
 - Plot the precision-recall graph and choose manually

Precision-Recall Curve





- P-R Curve shows the relationship of precision and recall when changing threshold values
- A good classifier should have a curve that is close to the top-right corner.

Precision and Recall scores for different threshold values



 We can retrieve the average cross-validated scores for all samples through the function cross_val_predict() with the parameter method="decision_fuction"

 Next, compute the precision and recall scores at threshold values using precision_recall_curve()

```
from sklearn.metrics import precision_recall_curve
precisions, recalls, thresholds = precision_recall_curve (y_train_5, y_scores_cv)
```

precision_recall_curve computes the precision and recall for different probability
thresholds. Note that this implementation is restricted to binary classification task

Plot Precision-Recall graph



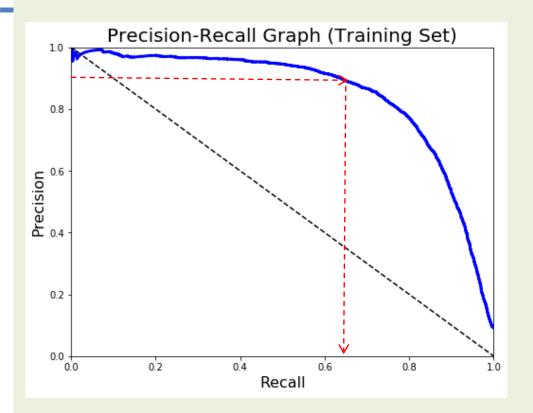
 Using the precision and recall values at different thresholds, we can now plot our precision-recall graph.

```
def plot_precision_vs_recall(precisions, recalls):
   plt.plot(recalls, precisions, "b-", linewidth=3)
   plt.plot(np.linspace(0, 1, 20), np.linspace(1, 0, 20), 'k--')
   plt.xlabel("Recall", fontsize=16)
   plt.ylabel("Precision", fontsize=16)
   plt.axis([0, 1, 0, 1])

plt.figure(figsize=(8, 6))
   plot_precision_vs_recall(precisions, recalls)
   plt.title ('Precision-Recall Graph (Training Set)', fontsize = 20)
   plt.show()
```

Precision-Recall Curve





When, Precision = 0.9, Recall = 0.64

Getting the desired threshold value



Suppose we desire a higher precision (0.9) and can tolerate a lower recall (between 0.6 and 0.7). The following code shows how to retrieve the desired threshold value when the precision is at least 0.9.

```
idx = np.argmax(precisions >= 0.9)  # the position of the first precision value that is >= 0.9
selected_threshold = thresholds[idx]

print('selected threshold = {:.2f}'.format(selected_threshold))
print('precision at selected threshold = {:.2f}'.format(precisions[idx]))
print('recall at selected threshold = {:.2f}'.format(recalls[idx]))

selected threshold = 103561.39
precision at selected threshold = 0.90
recall at selected threshold = 0.64
```

When threshold =103561, we can achieve 0.9 precision and 0.64 recall rate (compare to default threshold=0, precision=0.768, recall=0.801)

Prediction with manually selected threshold value

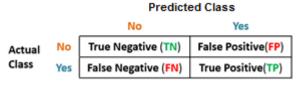


- Recall that in SGDClassifier, the threshold value is fixed at 0
- We can manually use the selected threshold value to perform prediction.

```
# evaluate on the first 200 training samples
samples = X train[:200]
samples label = y train 5[:200]
# use our model to compute the scores on selected samples
scores = sgd clf.decision function(samples)
# perform prediction
predictions = (scores > selected threshold)
# compute precision and recall
print ('precision =', precision score (samples label, predictions))
print ('recall =', recall score (samples label, predictions))
  precision = 0.9090909090909091
```

Receiver Operating Characteristics (ROC)

- Another common tool to evaluate binary classifier is the Receiver Operating Characteristic (ROC) curve
- ROC curve plots the True Positive Rate (TPR or recall) vs False Positive Rate (FPR)
 - TPR = ratio of the positive instances that are correctly predicted positive
 - = TP/(TP + FN)
 - FPR = ratio of negative instances that are incorrectly classified as positive
 - = FP/(TN + FP)



Plot ROC curve

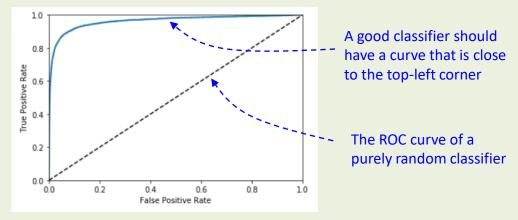
```
from sklearn.metrics import roc_curve
fpr, tpr, thresholds = roc_curve(y_train_5, y_scores_cv)
```

```
def plot_roc_curve (fpr, tpr, label = None):
    plt.plot(fpr, tpr, linewidth = 2, label = label)
    plt.plot([0,1], [0, 1], 'k--')
    plt.axis([0, 1, 0, 1])
    plt.xlabel ('False Positive Rate')
    plt.ylabel ('True Positive Rate')

plot_roc_curve(fpr, tpr)
```

Computes the FPR and TPR for different threshold values

Plots the ROC curve



roc_curve() computes the FPR and FPR for different threshold values

Area Under Curve (AUC)

- AUC converts the ROC curve into a quantitative value
- A perfect AUC has a value of 1
- A purely random classifier has a AUC value of 0.5

Compute the AUC

```
from sklearn.metrics import roc_auc_score
auc = roc_auc_score(y_train_5, y_scores_cv)
print('AUC = {:.4f}'.format(auc))
AUC = 0.9624
```

roc_auc_score() computes the AUC score given the predicted and actual value

Evaluate Model on Test Set

 The final model should be evaluated on unseen data (test set) before deployment.

```
from sklearn.linear_model import SGDClassifier
from sklearn.metrics import precision_score, recall_score, f1_score

sgd_clf = SGDClassifier(random_state = 42, max_iter = 5, tol = None)
sgd_clf.fit(X_train, y_train_5)
y_pred_test = sgd_clf.predict(X_test) # fit on test set

print('Test precision = {:.4f}'.format(precision_score(y_test_5, y_pred_test)))
print('Test recall = {:.4f}'.format(recall_score (y_test_5, y_pred_test)))
print('Test f1 score = {:.4f}'.format(f1_score(y_test_5, y_pred_test)))

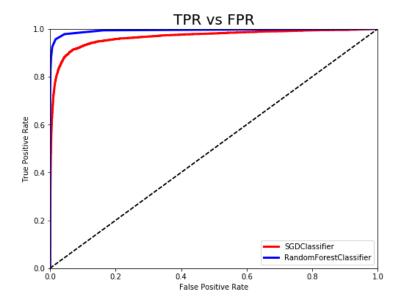
Test precision = 0.8188
Test recall = 0.8105
Test f1 score = 0.8146
```

The test performance results are close to the training results, indicating that the model is not overfitted.

Comparing classifiers using ROC curve

 We can use ROC curve and AUC measure to compare the performance of different classification models.

Example:



For this task, RandomForestClassifier should perform better than SGDClassifier

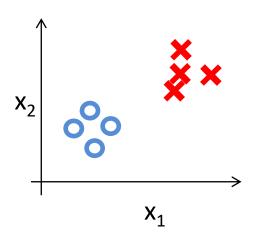
Outline

- 1. Look at the big picture
- 2. Get, explore and prepare data
- Select and train model
 - 1) Binary Classification
 - i. Accuracy
 - ii. Confusion Matrix
 - iii. Precision, Recall and F1 score
 - iv. Precision vs Recall (PR) Curve
 - v. Receiver Operating Curve (ROC)
 - vi. Area Under Curve (AUC)
 - 2) Multi-class classification
- Fine-tune model

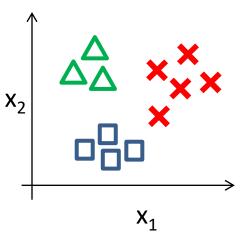
Multi-class Classification

What is a multi-class classification?

Binary classification:



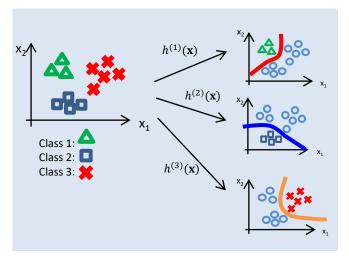
Multi-class classification:



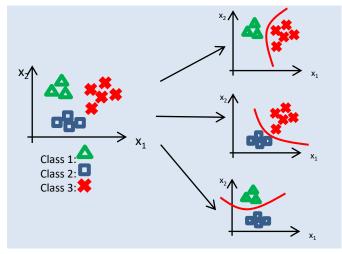
- Digit classification: 0, 1, 2, ..., 9
- Vehicle classification: car, bus, truck, ...

Multi-class Classification

- Some classifiers (e.g. Random Forest) can naturally handle multi-class classification.
- For binary classifiers (e.g. SGDClassifier, SVM), multi-class classification is supported through One-Versus-One (OVO) or One-Versus-All (OVA) schemes.







OVO (N(N-1)/2 classifiers)

Multi-class classification for SGDClassifier



- In Scikit-learn, by default all binary classifier uses OVA except for SVM which uses OVO
- SGDClassifier is a binary classifier. When it detects that targeted output has three or more classes, it will automatically runs OVA

```
from sklearn.linear_model import SGDClassifier

sgd_clf = SGDClassifier (random_state = 42, max_iter = 5, tol = None)
sgd_clf.fit(X_train, y_train)
print(sgd_clf.classes_) # show class labels

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

The syntax
remains
unchanged!
```

Measuring training accuracy

```
from sklearn.metrics import accuracy_score

y_pred = sgd_clf.predict(X_train)|
train_acc = accuracy_score(y_train, y_pred)
print("Training accuracy: {:.4f}".format(train_acc))

Training accuracy: 0.8639
```



Measuring training accuracy using Cross-Validation

```
from sklearn.model_selection import cross_val_score
cross_val_score(sgd_clf, X_train, y_train, cv=3, scoring="accuracy")
array([0.84063187, 0.84899245, 0.86652998])
```

- Achieve around 85% accuracy on all test folds
- If we scale the dataset, we can improve the performance to around 90%.
- If we use RandomForestClassifier, we can get around 94%

Performance Measure on Multiclass Classification

Multiclass Confusion Matrix

Model Predictions

	Α	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

Total number of samples = 80

Performance Metric for Class A

Model Predictions

	Α	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

True Positive (TP) = 9

False Positive (FP) = 6

True Negative (TN) = 64

Performance Metric for Class B

Model Predictions

	А	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

True Positive (TP) = 15

False Positive (FP) = 5

True Negative (TN) = 55

Performance Metric for Class C

Model Predictions

	Α	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

True Positive (TP) = 24

False Positive (FP) = 4

True Negative (TN) = 46

Performance Metric for Class D

Model Predictions

	Α	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

True Positive (TP) = 15

False Positive (FP) = 2

True Negative (TN) = 58

Accuracy

Model Predictions

	Α	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

Accuracy =
$$(9 + 15 + 24 + 15) / 80 = 0.7875$$

Precision (P) = TP / (TP+FP)

Model Predictions

	u	П
	Č	Ī
	?	
	ù	1
	Ų	
	(Ū
		ز
	٦	
-		
	(Q
		5
	4	_
	Ċ	5
	1	
		1
		1

	Α	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15
	_		_	

TP: 9 FP: 6

TP: 15 FP: 5

TP: 24 FP: 4

TP: 15 FP: 2

P(A) = 9/15 P(B) = 15/20 P(C) = 24/28 P(D) = 15/17

Average (macro) Precision = (P(A)+P(B)+P(C)+P(D)) / 4 = 0.7724

Model Predictions

	A	В	С	D
Α	9	1	0	0
В	1	15	3	1
С	5	0	24	1
D	0	4	1	15

FN: 1

R(A) = 9/10 R(B) = 15/20 R(C) = 24/30 R(D) = 15/20

Average (macro) Recall = (R(A)+R(B)+R(C)RP(D)) / 4 = 0.8

Outline

- Look at the big picture
- 2. Get, explore and prepare data
- Select and train model
 - 1) Binary Classification
 - i. Accuracy
 - ii. Confusion Matrix
 - iii. Precision, Recall and F1 score
 - iv. Precision vs Recall (PR) Curve
 - v. Receiver Operating Curve (ROC)
 - vi. Area Under Curve (AUC)
 - 2) Multi-class classification
- 4. Fine-tune model

Fine-tuning model

- Fine-tune model hyperparamters using grid search or random search
- Improve the model by analyzing the types of errors it makes. Strategy:
 - Plot the confusion matrix
 - Check the difficult cases.

Plot the confusion matrix



```
from sklearn.model selection import cross val predict
from sklearn.metrics import confusion matrix
y pred cv = cross val predict (sgd clf, X train, y train, cv=3)
cm = confusion matrix (y train, y pred cv)
print(cm)
0 [[5604
              81
                  25 8 44
                       20 22 8
      1 6292
              72
     59
                  218
                                82
                                             151
         73 5016
        16
            148 5315
                       19 199
                                23
                                    41 297
                                             331
     40
     24 26
            145
                   39 4746 - 22
                                63
                                            2261
    73 25
             74
                  375
                       62 3868 91
                                    22 | 771
                 13 84 105 5369
    50 19 128
            69 117 100 18
                                 2 5641 112 1221
    65 19
          96
             127 196 77 135
                                30
          45
     58
              59
                  199
                      233
                           59
                                    385
```

plt.matshow(cm, cmap=plt.cm.gray) # plot the confusion matrix

- True positive for digit 5 and 9 are a bit low: opportunity for improvement
- Many digits are misclassified as 8, especially 5 & 9

Possible Improvements:

- Get more training data for digits 5/8/9
- Preprocess the image, e.g. make sure digits are centered & not rotated.



Next:

Linear Regression and Gradient Descent