# ROC Curve with Digits Dataset

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In [1]:
```
from IPython.display import IFrame

url = "https://paulvanderlaken.com/2019/08/16/roc-auc-precision-and-rec
IFrame(url, width=700, height=350)
```

Out[1]:

# Data

I will keep it simple and use the Digits dataset from scikit-learn.

In [5]:
```
from operator import itemgetter

import numpy as np
import pandas as pd
from sklearn.datasets import load_digits
from sklearn import datasets
from sklearn.metrics import roc_curve, auc
from sklearn.preprocessing import label_binarize
from sklearn.multiclass import OneVsRestClassifier

from matplotlib import pyplot as plt

%matplotlib inline

DEBUG=False

random_state = 0
```

In [7]:
```
digits = load_digits()
digits
```

Out[7]:
```
{'data': array([[ 0.,  0.,  5., ...,  0.,  0.,  0.],
        [ 0.,  0.,  0., ..., 10.,  0.,  0.],
        [ 0.,  0.,  0., ..., 16.,  9.,  0.],
        ...,
        [ 0.,  0.,  1., ...,  6.,  0.,  0.],
        [ 0.,  0.,  2., ..., 12.,  0.,  0.],
        [ 0.,  0., 10., ..., 12.,  1.,  0.]]),
 'target': array([0, 1, 2, ..., 8, 9, 8]),
 'frame': None,
 'feature_names': ['pixel_0_0',
  'pixel_0_1',
  'pixel_0_2',
  'pixel_0_3',
  'pixel_0_4',
  'pixel_0_5',
  'pixel_0_6',
  'pixel_0_7',
  'pixel_1_0',
  'pixel_1_1',
```

In [8]:
```
X = digits.data
Y = labels = digits.target

feature_names = digits.feature_names
Y_names = digits.target_names

n_labels = len(Y_names)

n_samples, n_features = X.shape

print("n_labels=%d \t n_samples=%d \t n_features=%d" % (n_labels, n_sam
```

```
n_labels=10      n_samples=1797          n_features=64
```

We will binarize the labels so that we can analyze each case separately:

In [9]:
```
Y = label_binarize(Y, classes=range(n_labels))
n_classes = Y.shape[1]
Y
```

Out[9]:
```
array([[1, 0, 0, ..., 0, 0, 0],
       [0, 1, 0, ..., 0, 0, 0],
       [0, 0, 1, ..., 0, 0, 0],
       ...,
       [0, 0, 0, ..., 0, 1, 0],
       [0, 0, 0, ..., 0, 0, 1],
       [0, 0, 0, ..., 0, 1, 0]])
```

# Generating the Model Probabilities

Our goal is just to work on the ROC curve, so we won't split the data into train and test sets. Let's use OneVsRestClassifier to make predictions on the dataset:

In [10]:
```
from sklearn.linear_model import LogisticRegression

classifier = OneVsRestClassifier(LogisticRegression(solver='lbfgs',
                                                   random_state=random_state))

classifier.fit(X, Y)
```

```
/Users/gulsum/opt/anaconda3/lib/python3.9/site-packages/sklearn/linear_mo
del/_logistic.py:444: ConvergenceWarning: lbfgs failed to converge (statu
s=1):
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown i
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    https://scikit-learn.org/stable/modules/preprocessing.html (https://s
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Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-re
gression (https://scikit-learn.org/stable/modules/linear_model.html#logis
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  n_iter_i = _check_optimize_result(
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Increase the number of iterations (max_iter) or scale the data as shown i
n:
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cikit-learn.org/stable/modules/preprocessing.html)
```

```
Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression (https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression)
  n_iter_i = _check_optimize_result(
/Users/gulsum/opt/anaconda3/lib/python3.9/site-packages/sklearn/linear_model/_logistic.py:444: ConvergenceWarning: lbfgs failed to converge (status=1):
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in:
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Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression (https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression)
  n_iter_i = _check_optimize_result(
/Users/gulsum/opt/anaconda3/lib/python3.9/site-packages/sklearn/linear_model/_logistic.py:444: ConvergenceWarning: lbfgs failed to converge (status=1):
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Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression (https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression)
  n_iter_i = _check_optimize_result(
```

Out[10]:

```
OneVsRestClassifier(estimator=LogisticRegression(random_state=0))
```

**In a Jupyter environment, please rerun this cell to show the HTML representation or trust the notebook.**
**On GitHub, the HTML representation is unable to render, please try loading this page with nbviewer.org.**

In [11]:

```
Y_pred = classifier.predict(X)
Y_pred
```

Out[11]:

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

But for the ROC curve we will use the probabilities classifier computed for each class:

In [13]:
```
Y_pred_prob = classifier.predict_proba(X)
Y_pred_prob
```

Out[13]:
```
array([[9.99999821e-01, 6.56683912e-15, 6.15172252e-09, ...,
        4.11842902e-06, 1.23278672e-05, 4.64888967e-05],
       [2.56426395e-18, 9.99812412e-01, 8.35546984e-10, ...,
        2.25726579e-13, 2.79910942e-04, 4.28740892e-10],
       [2.52085554e-11, 1.89954796e-03, 9.99943784e-01, ...,
        9.17817086e-16, 8.03875431e-02, 9.50605177e-13],
       ...,
       [3.44164617e-12, 4.49357761e-05, 2.58705096e-08, ...,
        1.36737987e-15, 9.96618504e-01, 7.79311255e-11],
       [2.75119772e-03, 2.65589373e-07, 5.10839922e-11, ...,
        2.27906489e-12, 1.43340013e-02, 9.99985790e-01],
       [1.95552713e-10, 5.78202594e-08, 8.26407634e-09, ...,
        1.91193011e-18, 9.54117694e-01, 3.52039231e-06]])
```

So, the model used the maximum of each row to predict the final class.

# Using the Metrics Module

We will use the metrics package to compute the ROC curve and AUC for each class:

In [61]:
```
fpr = dict()
tpr = dict()
roc_auc = dict()
thresholds = dict()
for n_class in range(n_classes):
    fpr[n_class], tpr[n_class], thresholds[n_class] = roc_curve(Y[:, n_
    roc_auc[n_class] = auc(fpr[n_class], tpr[n_class])
```

Let's plot the ROC curve for each class. Here are the colors we will use:

In [62]:
```
colors = ["blue", "red", "green"]
for name, color in zip(Y_names, colors):
    print("{0} <-> {1}".format(name, color))
```

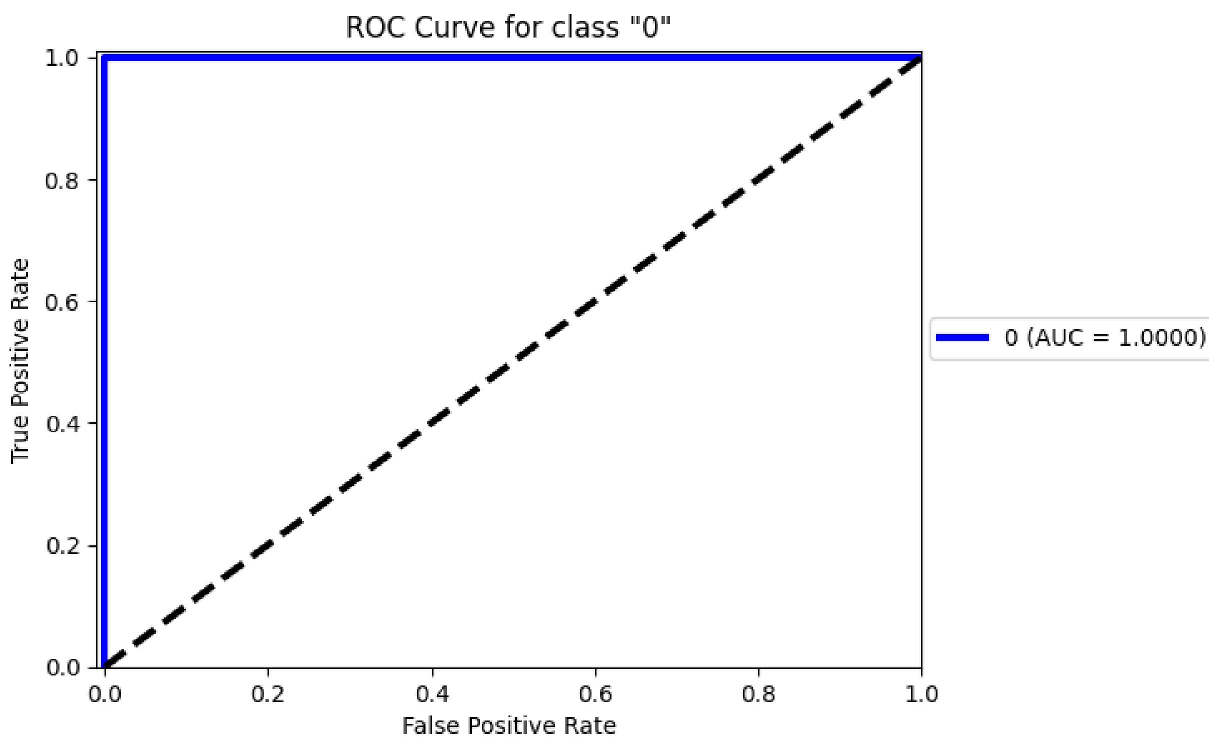
```
0 <-> blue
1 <-> red
2 <-> green
```

We will use the same code repeatedly, so let's write a function for it:

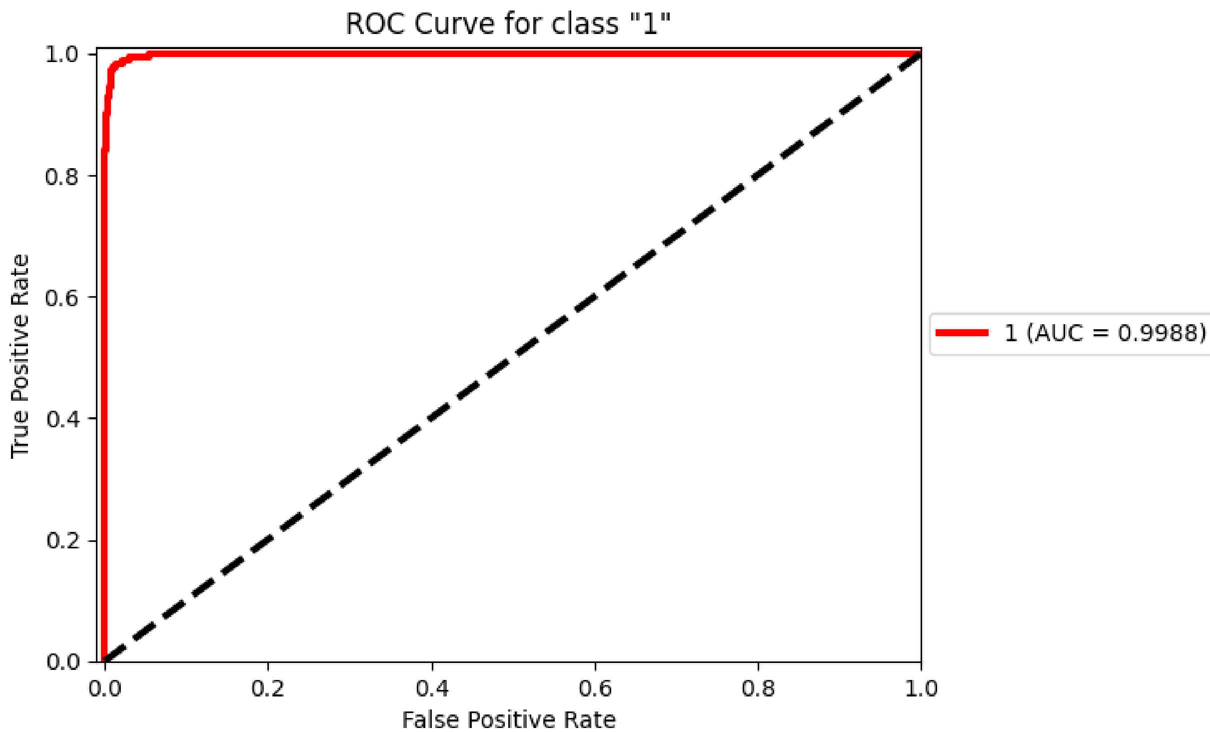
In [63]:
```
def plot_ROC_curve(n_class, fpr, tpr, roc_auc):

    buffer = 0.01 # to be able to clearly visualize the graph close to
    lw = 3  # line width

    plt.figure()
    plt.plot(fpr[n_class], tpr[n_class], color=colors[n_class],
             lw=lw, label="{} (AUC = {:0.4f})".format(Y_names[n_class],

    plt.plot([0, 1], [0, 1], color='black', lw=lw, linestyle='--')
    plt.xlim([-buffer, 1.0])
    plt.ylim([0.0, 1.0+buffer])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('ROC Curve for class \"{}\"'.format(Y_names[n_class]))
    plt.legend(loc=(1.01, 0.5))
    plt.show()
```

Here is the plot of the ROC curve for the each class:

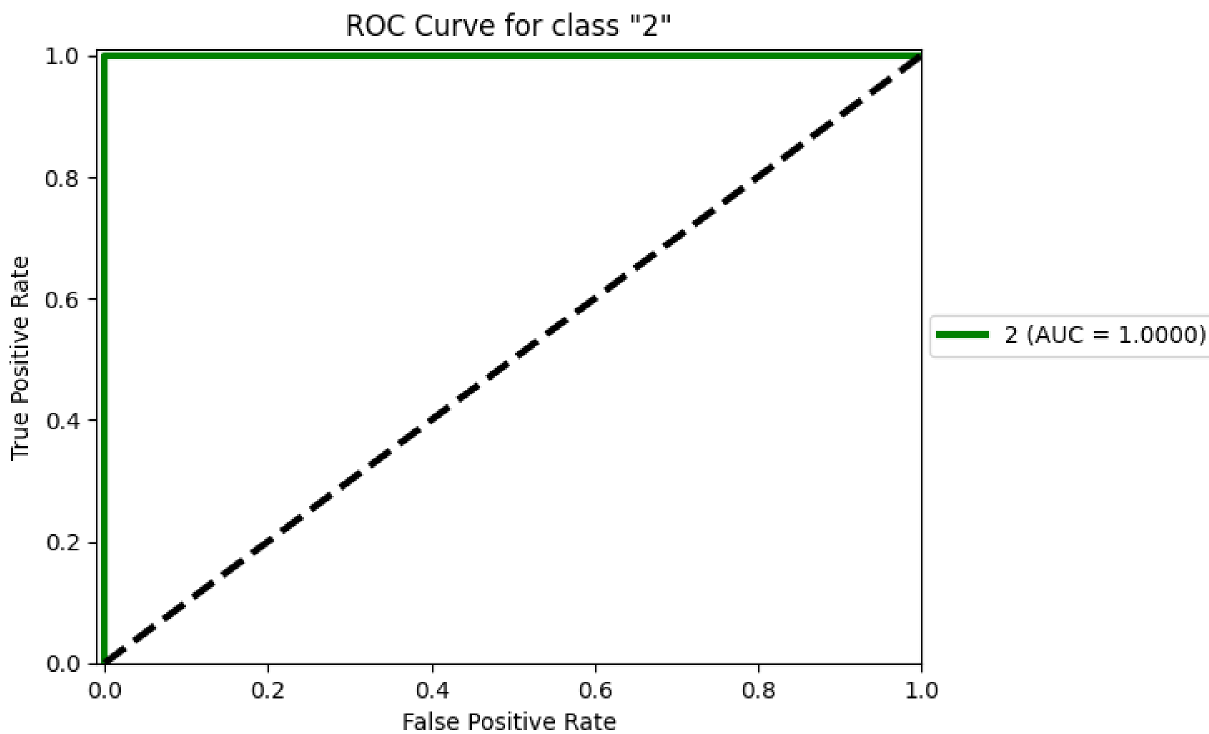
In [64]:
```
plot_ROC_curve(0, fpr, tpr, roc_auc)
```



In [65]:
```
plot_ROC_curve(1, fpr, tpr, roc_auc)
```



In [66]:
```
plot_ROC_curve(2, fpr, tpr, roc_auc)
```




# Computing from the Ground up

Now, let's compute the ROC curve points ourselves. For a given threshold, we will compute the TPR and FPR of the results. Let's start with an example threshold of 0.5:

In [71]:
```
threshold = 0.5

n_class = 2

N, P, TP, FP = 0, 0, 0, 0

for j in range(len(Y_pred_prob)):
    if Y[j][n_class] == 1:
        P += 1
    if Y[j][n_class] == 0:
        N += 1
    if Y_pred_prob[j][n_class] >= threshold:
        if Y[j][n_class] == 1:
            TP += 1
        if Y[j][n_class] == 0:
            FP += 1

my_fpr = FP/float(N)
my_tpr = TP/float(P)

print(N, P, TP, FP, my_fpr, my_tpr)
```

```
1620 177 177 0 0.0 1.0
```

This is just one of the points on the plot. We need to repeat this for a set of thresholds. We will use 100 values in the range [0, 1], i.e. 0.00, 0.01, 0.02, ..., 1.00:

In [ ]:
```
n_class = 1

NUM_THRESHOLDS = 10000

my_fpr = {}
my_tpr = {}

my_fpr[n_class] = []
my_tpr[n_class] = []

for i in range(0, NUM_THRESHOLDS+1):
    threshold = i/float(NUM_THRESHOLDS)
    N, P, TP, FP = 0, 0, 0, 0

    for j in range(len(Y_pred_prob)):
        if Y[j][n_class] == 1:
            P += 1
        if Y[j][n_class] == 0:
            N += 1
        if Y_pred_prob[j][n_class] >= threshold:
            if Y[j][n_class] == 1:
                TP += 1
            if Y[j][n_class] == 0:
                FP += 1

    my_fpr[n_class].append(FP/float(N))
    my_tpr[n_class].append(TP/float(P))

print(my_fpr[n_class], my_tpr[n_class])
```

Let's compute the AUC using the rectanges formed by the y coordinates with all widths equal to 1/NUM_THRESHOLDS :

In [73]:
```
1/float(NUM_THRESHOLDS)
```

Out[73]:
```
0.0001
```

To compute the AUC, first we have to sort the points with respect to the first and second coordinates, so that they form the staircase shape of the ROC Curve:

In [75]:

```
all_points = list(zip(my_fpr[n_class], my_tpr[n_class]))
all_points.sort(key=itemgetter(0, 1))
all_points
```

Out[75]:

```
[(0.0, 0.0),
 (0.0, 0.15934065934065933),
 (0.0, 0.1978021978021978),
 (0.0, 0.22527472527472528),
 (0.0, 0.26373626373626374),
 (0.0, 0.29120879120879123),
 (0.0, 0.3131868131868132),
 (0.0, 0.33516483516483514),
 (0.0, 0.34615384615384615),
 (0.0, 0.3626373626373626),
 (0.0, 0.3626373626373626),
 (0.0, 0.3626373626373626),
 (0.0, 0.3791208791208791),
 (0.0, 0.38461538461538464),
 (0.0, 0.3956043956043956),
 (0.0, 0.41208791208791207),
 (0.0, 0.4175824175824176),
 (0.0, 0.4230769230769231),
 (0.0, 0.42857142857142855),
```

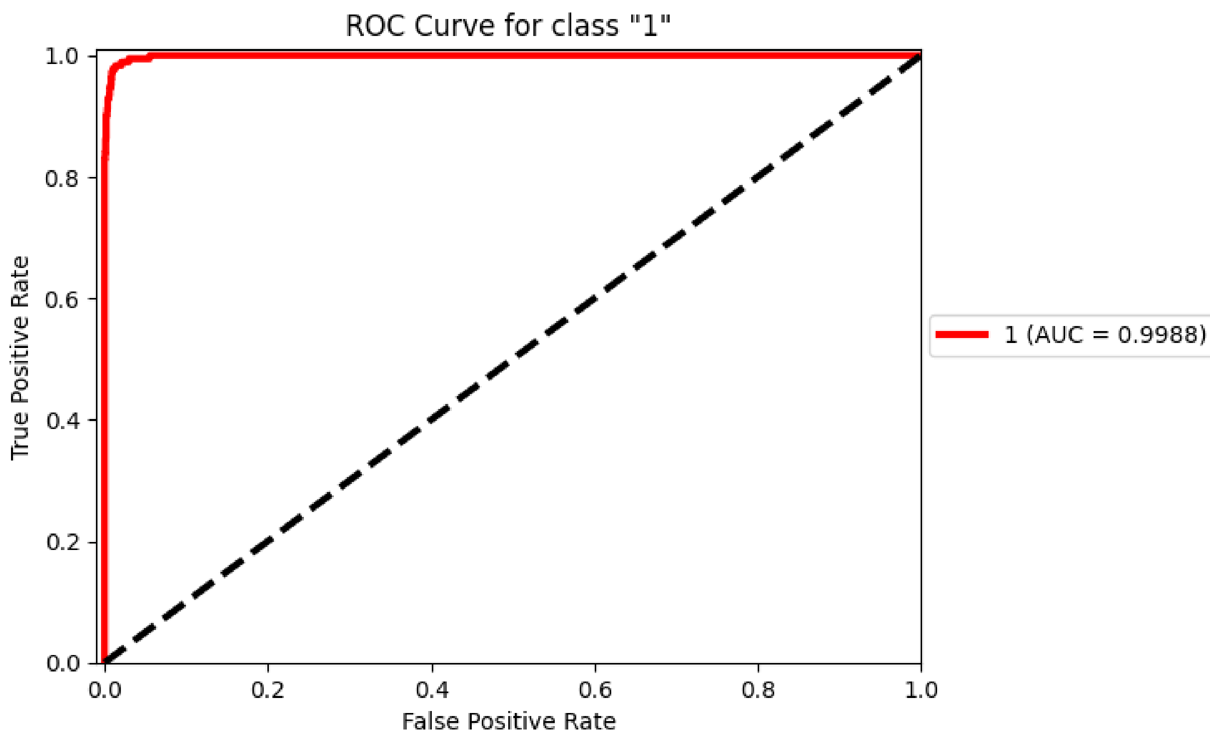
In [76]:

```
my_roc_auc = {}
my_roc_auc[n_class] = 0

for i in range(1,len(all_points)):
    height = all_points[i][0] - all_points[i-1][0]
    base_average = (all_points[i][1] + all_points[i-1][1]) / float(2)
    my_roc_auc[n_class] += height * base_average

print(my_roc_auc[n_class])
```

```
0.998766713162998
```

Let's plot this using our earlier example:

In [77]:
```
plot_ROC_curve(1, my_fpr, my_tpr, my_roc_auc)
```




Let's combine all the above and repeat it for all classes:

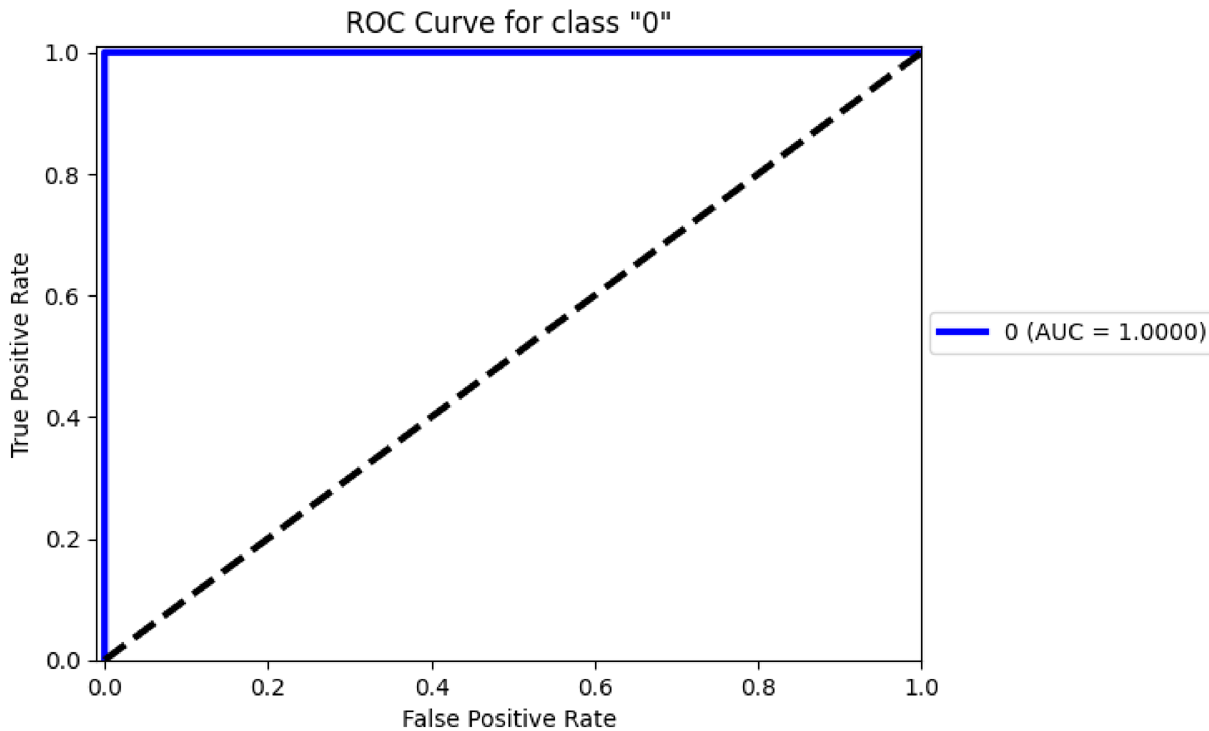
In [78]:
```
my_fpr = {}
my_tpr = {}
my_roc_auc = {}

for n_class in range(n_classes):

    my_fpr[n_class] = []
    my_tpr[n_class] = []

    for i in range(0, NUM_THRESHOLDS+1):
        threshold = i/float(NUM_THRESHOLDS)
        N, P, TP, FP = 0, 0, 0, 0

        for j in range(len(Y_pred_prob)):
            if Y[j][n_class] == 1:
                P += 1
            if Y[j][n_class] == 0:
                N += 1
            if Y_pred_prob[j][n_class] >= threshold:
                if Y[j][n_class] == 1:
                    TP += 1
                if Y[j][n_class] == 0:
                    FP += 1

        my_fpr[n_class].append(FP/float(N))
        my_tpr[n_class].append(TP/float(P))

    all_points = list(zip(my_fpr[n_class], my_tpr[n_class]))
    all_points.sort(key=itemgetter(0,1))

    my_roc_auc[n_class] = 0

    for i in range(1,len(all_points)):
        height = all_points[i][0] - all_points[i-1][0]
        base_average = (all_points[i][1] + all_points[i-1][1]) / float(
        my_roc_auc[n_class] += height * base_average

    print(my_fpr[n_class], my_tpr[n_class], my_roc_auc[n_class])
```

```
[1.0, 0.06176652254478073, 0.04941321803582458, 0.042001235330450894, 0.0
35206917850525016, 0.029647930821494475, 0.027794935145151328, 0.026559604
694255712, 0.025324274243360, 0.024088943792464484, 0.02285361334156887,
0.021000617665225447, 0.020382952439777764, 0.019765287214329835, 0.019147
621988882025, 0.019147621988882025, 0.017294626312538603, 0.0166769610870
90797, 0.016059295861642990, 0.016059295861642990, 0.016059295861642990, 0.0
15441630636195183, 0.015441630636195183, 0.014823965410747375, 0.01482396
5410747375, 0.014823965410747375, 0.014823965410747375, 0.014823965410747
375, 0.014206300185299567, 0.014206300185299567, 0.014206300185299567, 0.
013588634959851761, 0.012970969734403953, 0.012353304508956145, 0.0111179
74058060531, 0.009882643607164917, 0.009882643607164917, 0.00988264360716
4917, 0.009882643607164917, 0.009882643607164917, 0.009264978381717111, 0.
008647313156269302, 0.008647313156269302, 0.008647313156269302, 0.0074119
827053736875, 0.0074119827053736875, 0.0074119827053736875, 0.00741198270
53736875, 0.0074119827053736875, 0.0074119827053736875, 0.007411982705373
6875, 0.0074119827053736875, 0.006794317479925880 5, 0.006794317479925880
5, 0.006794317479925880 5, 0.006794317479925880 5, 0.006794317479925880 5,
0.006794317479925880 5, 0.006794317479925880 5, 0.006794317479925880 5, 0.00
```

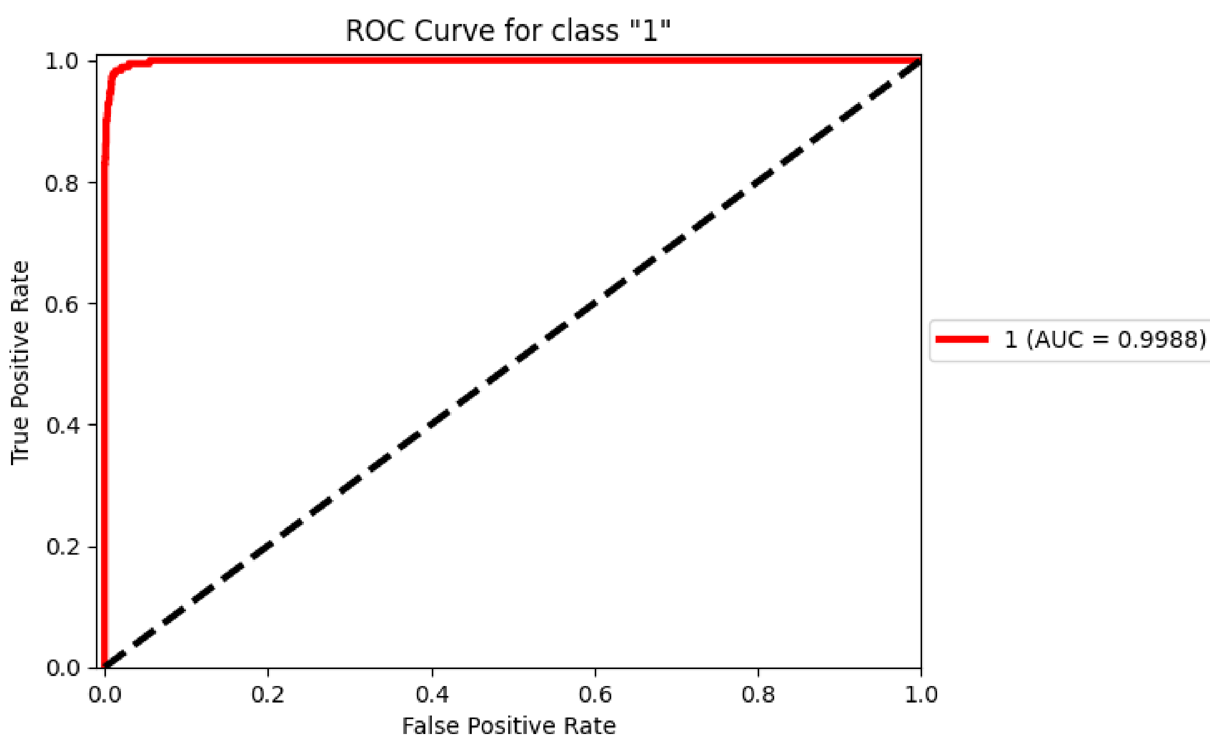
```
67943174799258805, 0.0067943174799258805, 0.0067943174799258805, 0.006794
```

Let's plot these new values now:

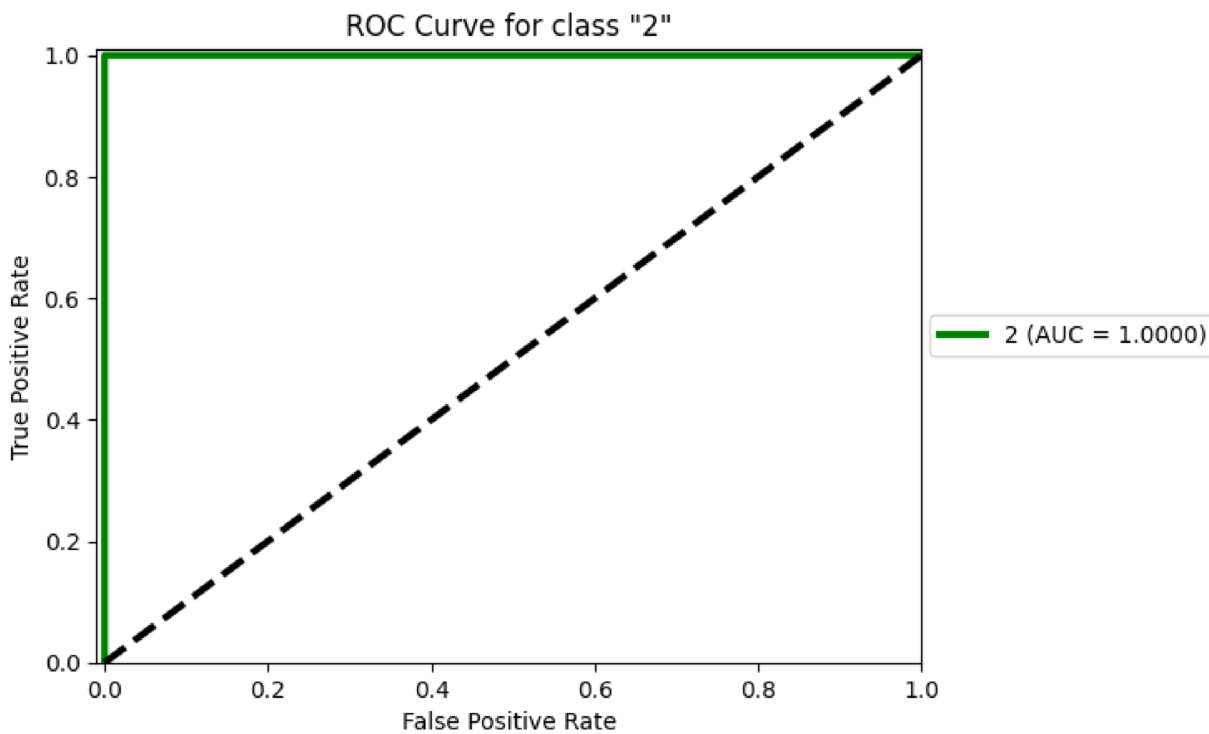
In [79]:
```
plot_ROC_curve(0, my_fpr, my_tpr, my_roc_auc)
```




In [80]:
```
plot_ROC_curve(1, my_fpr, my_tpr, my_roc_auc)
```



In [81]:
```
plot_ROC_curve(2, my_fpr, my_tpr, my_roc_auc)
```




The results are identical to the ones computed by the metrics module. There might have been small differences here due to different set of thresholds used and roundoff errors, e.g. is you choose to work with 1000 points, you may see some differences.

We can check our results by using the "auc" function of the metrics module on our data:

In [83]:
```
for n_class in range(n_classes):
    my_auc = auc(my_fpr[n_class], my_tpr[n_class])
    print("Class {}  auc={:0.4f}".format(Y_names[n_class], my_auc))
```

```
Class 0  auc=1.0000
Class 1  auc=0.9988
Class 2  auc=1.0000
Class 3  auc=0.9999
Class 4  auc=1.0000
Class 5  auc=1.0000
Class 6  auc=1.0000
Class 7  auc=1.0000
Class 8  auc=0.9902
Class 9  auc=0.9962
```

These are exactly the same results as our AUC computation, so our FPR and TPR computations are correct.

In [ ]:
```

```