C1_W2_Assignment

September 7, 2024

1 Evaluation of Diagnostic Models

Welcome to the second assignment of course 1. In this assignment, we will be working with the results of the X-ray classification model we developed in the previous assignment. In order to make the data processing a bit more manageable, we will be working with a subset of our training, and validation datasets. We will also use our manually labeled test dataset of 420 X-rays.

As a reminder, our dataset contains X-rays from 14 different conditions diagnosable from an X-ray. We'll evaluate our performance on each of these classes using the classification metrics we learned in lecture.

By the end of this assignment you will learn about:

1. Accuracy
2. Prevalence
3. Specificity & Sensitivity
4. PPV and NPV
5. ROC curve and AUCROC (c-statistic)
6. Confidence Intervals

1.1 Table of Contents

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1. Packages

In this assignment, we'll make use of the following packages: - numpy is a popular library for scientific computing - matplotlib is a plotting library compatible with numpy - pandas is what we'll use to manipulate our data - sklearn will be used to measure the performance of our model

Run the next cell to import all the necessary packages as well as custom util functions.

```
In [26]: import numpy as np
         import matplotlib.pyplot as plt
         import pandas as pd

         import util
         from public_tests import *
         from test_utils import *
```

2. Overview

We'll go through our evaluation metrics in the following order.

- Metrics
  - TP, TN, FP, FN
  - Accuracy
  - Prevalence
  - Sensitivity and Specificity
  - PPV and NPV
  - AUC
- Confidence Intervals

Let's take a quick peek at our dataset. The data is stored in two CSV files called `train_preds.csv` and `valid_preds.csv`. We have precomputed the model outputs for our test cases. We'll work with these predictions and the true class labels throughout the assignment.

```
In [2]: train_results = pd.read_csv("data/train_preds.csv")
        valid_results = pd.read_csv("data/valid_preds.csv")

        # the labels in our dataset
        class_labels = ['Cardiomegaly',
         'Emphysema',
         'Effusion',
         'Hernia',
         'Infiltration',
         'Mass',
         'Nodule',
         'Atelectasis',
         'Pneumothorax',
```

```
 'Pleural_Thickening',
 'Pneumonia',
 'Fibrosis',
 'Edema',
 'Consolidation']

# the labels for prediction values in our dataset
pred_labels = [l + "_pred" for l in class_labels]
```

Extract the labels (y) and the predictions (pred).

```
In [3]: y = valid_results[class_labels].values
        pred = valid_results[pred_labels].values
```

Run the next cell to view them side by side.

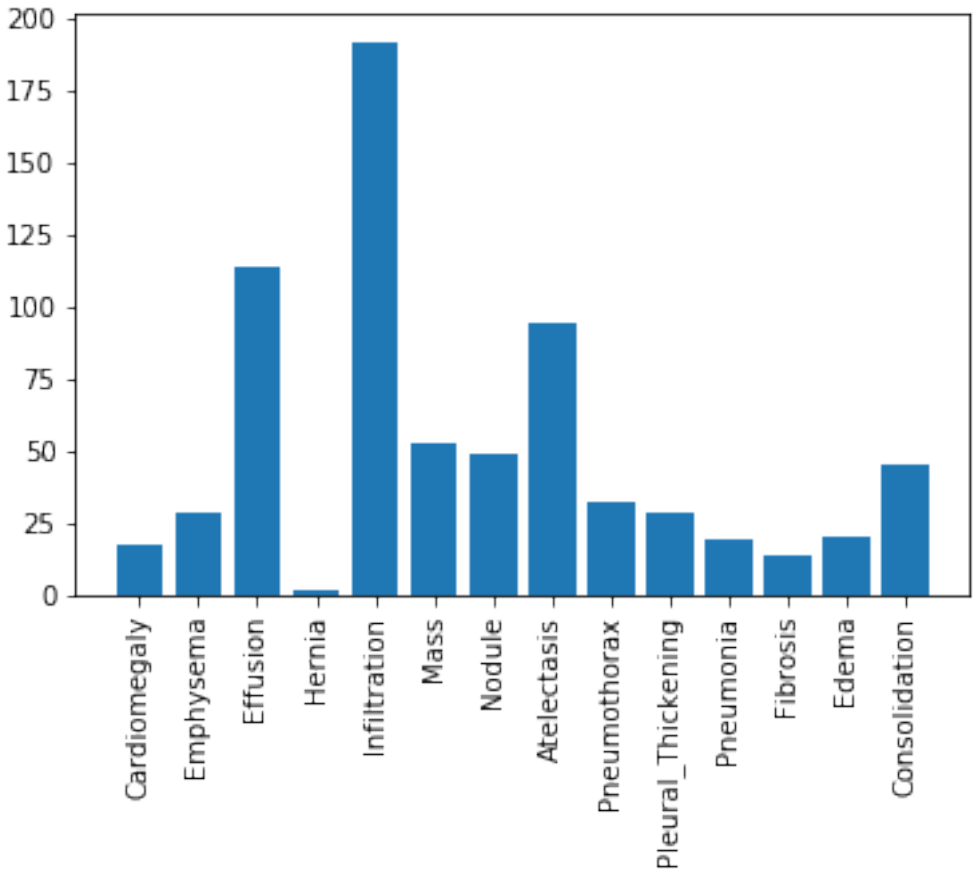
```
In [4]: # let's take a peek at our dataset
        valid_results[np.concatenate([class_labels, pred_labels])].head()
```

```
Out[4]:    Cardiomegaly  Emphysema  Effusion  Hernia  Infiltration  Mass  Nodule  \
        0             0          0         0       0             0     0       0
        1             0          0         0       0             1     0       1
        2             0          0         0       0             0     0       0
        3             0          0         0       0             0     0       0
        4             0          0         0       0             0     0       0

           Atelectasis  Pneumothorax  Pleural_Thickening  ...  Infiltration_pred  \
        0            0             0                   0  ...           0.256020
        1            0             0                   0  ...           0.382199
        2            0             0                   0  ...           0.427727
        3            0             0                   0  ...           0.158596
        4            0             0                   0  ...           0.536762

           Mass_pred  Nodule_pred  Atelectasis_pred  Pneumothorax_pred  \
        0   0.266928     0.312440          0.460342           0.079453
        1   0.176825     0.465807          0.489424           0.084595
        2   0.115513     0.249030          0.035105           0.238761
        3   0.259460     0.334870          0.266489           0.073371
        4   0.198797     0.273110          0.186771           0.242122

           Pleural_Thickening_pred  Pneumonia_pred  Fibrosis_pred  Edema_pred  \
        0                 0.271495        0.276861       0.398799    0.015867
        1                 0.377318        0.363582       0.638024    0.025948
        2                 0.167095        0.166389       0.262463    0.007758
        3                 0.229834        0.191281       0.344348    0.008559
        4                 0.309786        0.411771       0.244666    0.126930

           Consolidation_pred
        0            0.156320
```

```
1            0.144419
2            0.125790
3            0.119153
4            0.342409

[5 rows x 28 columns]
```

To further understand our dataset details, here's a histogram of the number of samples for each label in the validation dataset:

```
In [5]: plt.xticks(rotation=90)
        plt.bar(x = class_labels, height= y.sum(axis=0));
```



It seem like our dataset has an imbalanced population of samples. Specifically, our dataset has a small number of patients diagnosed with a `Hernia`.

3. Metrics

3.1 True Positives, False Positives, True Negatives and False Negatives

The most basic statistics to compute from the model predictions are the true positives, true negatives, false positives, and false negatives.

As the name suggests - True Positive (TP): The model classifies the example as positive, and the actual label also positive. - False Positive (FP): The model classifies the example as positive, **but**

the actual label is negative. - True Negative (TN): The model classifies the example as negative, and the actual label is also negative. - False Negative (FN): The model classifies the example as negative, **but** the label is actually positive.

We will count the number of TP, FP, TN and FN in the given data. All of our metrics can be built off of these four statistics.

Recall that the model outputs real numbers between 0 and 1. * To compute binary class predictions, we need to convert these to either 0 or 1. * We'll do this using a threshold value *th*. * Any model outputs above *th* are set to 1, and below *th* are set to 0.

All of our metrics (except for AUC at the end) will depend on the choice of this threshold.

Exercise 1 - true positives, false positives, true negatives and false negatives

Fill in the functions to compute the TP, FP, TN, and FN for a given threshold below.

The first one has been done for you.

```
In [7]: # UNQ_C1 (UNIQUE CELL IDENTIFIER, DO NOT EDIT)
        def true_positives(y, pred, th=0.5):
            """
            Count true positives.

            Args:
                y (np.array): ground truth, size (n_examples)
                pred (np.array): model output, size (n_examples)
                th (float): cutoff value for positive prediction from model
            Returns:
                TP (int): true positives
            """
            TP = 0

            # get thresholded predictions
            thresholded_preds = pred >= th

            # compute TP
            TP = np.sum((y == 1) & (thresholded_preds == 1))

            return TP

        def true_negatives(y, pred, th=0.5):
            """
            Count true negatives.

            Args:
                y (np.array): ground truth, size (n_examples)
                pred (np.array): model output, size (n_examples)
                th (float): cutoff value for positive prediction from model
            Returns:
                TN (int): true negatives
            """
            TN = 0
```

```
    # get thresholded predictions
    thresholded_preds = pred >= th

    ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

    # compute TN
    TN = np.sum((y == 0) & (thresholded_preds == 0))

    ### END CODE HERE ###

    return TN

def false_positives(y, pred, th=0.5):
    """
    Count false positives.

    Args:
        y (np.array): ground truth, size (n_examples)
        pred (np.array): model output, size (n_examples)
        th (float): cutoff value for positive prediction from model
    Returns:
        FP (int): false positives
    """
    FP = 0

    # get thresholded predictions
    thresholded_preds = pred >= th

    ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

    # compute FP
    FP = np.sum((y == 0) & (thresholded_preds == 1))

    ### END CODE HERE ###

    return FP

def false_negatives(y, pred, th=0.5):
    """
    Count false positives.

    Args:
        y (np.array): ground truth, size (n_examples)
        pred (np.array): model output, size (n_examples)
        th (float): cutoff value for positive prediction from model
    Returns:
        FN (int): false negatives
    """
```

```
            FN = 0

            # get thresholded predictions
            thresholded_preds = pred >= th

            ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

            # compute FN
            FN = np.sum((y == 1) & (thresholded_preds == 0))

            ### END CODE HERE ###

            return FN
```

```
In [8]: ### do not modify this cell
        get_tp_tn_fp_fn_test(true_positives, true_negatives, false_positives, false_negatives)
```

```
    y_test  preds_test category
0        1         0.8       TP
1        1         0.7       TP
2        0         0.4       TN
3        0         0.3       TN
4        0         0.2       TN
5        0         0.5       FP
6        0         0.6       FP
7        0         0.7       FP
8        0         0.8       FP
9        1         0.1       FN
10       1         0.2       FN
11       1         0.3       FN
12       1         0.4       FN
13       1         0.0       FN


Your functions calcualted:
    TP: 2
    TN: 3
    FP: 4
    FN: 5

 All tests passed. All tests passed. All tests passed. All tests passed.
```

Expected output

```
Your functions calcualted:
    TP: 2
    TN: 3
    FP: 4
    FN: 5
```

```
All tests passed.
All tests passed.
All tests passed.
All tests passed.
```

Run the next cell to see a summary of evaluative metrics for the model predictions for each class.

```
In [9]: util.get_performance_metrics(y, pred, class_labels)
```

Out[9]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	Specificity	PPV	NPV	AUC	F1	Threshold
Cardiomegaly	16	814	169	1	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	0.5
Emphysema	20	869	103	8	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	0.5
Effusion	99	690	196	15	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Hernia	1	743	255	1	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Infiltration	114	543	265	78	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Mass	40	789	158	13	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Nodule	28	731	220	21	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Atelectasis	64	657	249	30	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Pneumothorax	24	785	183	8	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Pleural_Thickening	24	713	259	4	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Pneumonia	14	661	320	5	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Fibrosis	10	725	261	4	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Edema	15	767	213	5	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	
Consolidation	36	658	297	9	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	Not Defined	

```
Effusion            Not Defined       0.5
Hernia              Not Defined       0.5
Infiltration        Not Defined       0.5
Mass                Not Defined       0.5
Nodule              Not Defined       0.5
Atelectasis         Not Defined       0.5
Pneumothorax        Not Defined       0.5
Pleural_Thickening  Not Defined       0.5
Pneumonia           Not Defined       0.5
Fibrosis            Not Defined       0.5
Edema               Not Defined       0.5
Consolidation       Not Defined       0.5
```

Right now it only has TP, TN, FP, FN. Throughout this assignment we'll fill in all the other metrics to learn more about our model performance.

3.2 - Accuracy

Let's use a threshold of .5 for the probability cutoff for our predictions for all classes and calculate our model's accuracy as we would normally do in a machine learning problem.

$$accuracy = \frac{\text{true positives} + \text{true negatives}}{\text{true positives} + \text{true negatives} + \text{false positives} + \text{false negatives}}$$

Exercise 2 - get_accuracy

Use this formula to compute accuracy below:

Hints

Remember to set the value for the threshold when calling the functions.

```
In [10]: # UNQ_C2 (UNIQUE CELL IDENTIFIER, DO NOT EDIT)
         def get_accuracy(y, pred, th=0.5):
             """
             Compute accuracy of predictions at threshold.

             Args:
                 y (np.array): ground truth, size (n_examples)
                 pred (np.array): model output, size (n_examples)
                 th (float): cutoff value for positive prediction from model
             Returns:
                 accuracy (float): accuracy of predictions at threshold
             """
             accuracy = 0.0

             ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

             # get TP, FP, TN, FN using our previously defined functions
             TP = true_positives(y, pred, th=0.5)
             FP = false_positives(y, pred, th=0.5)
             TN = true_negatives(y, pred, th=0.5)
             FN = false_negatives(y, pred, th=0.5)
```

```
            # Compute accuracy using TP, FP, TN, FN
            accuracy = (TP + TN) / (TP+FP+TN+FN)

            ### END CODE HERE ###

            return accuracy
```

```
In [11]: ### do not modify this cell
         get_accuracy_test(get_accuracy)
```

```
Test Case:

Test Labels:           [1 0 0 1 1]
Test Predictions:  [0.8 0.8 0.4 0.6 0.3]
Threshold:           0.5
Computed Accuracy: 0.6

 All tests passed.
```

Expected output:

```
Test Case:

Test Labels:       [1 0 0 1 1]
Test Predictions:  [0.8 0.8 0.4 0.6 0.3]
Threshold:       0.5
Computed Accuracy: 0.6

 All tests passed.
```

Run the next cell to see the accuracy of the model output for each class, as well as the number of true positives, true negatives, false positives, and false negatives.

```
In [12]: util.get_performance_metrics(y, pred, class_labels, acc=get_accuracy)
```

Out[12]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	\
Cardiomegaly	16	814	169	1	0.83	Not Defined	Not Defined	
Emphysema	20	869	103	8	0.889	Not Defined	Not Defined	
Effusion	99	690	196	15	0.789	Not Defined	Not Defined	
Hernia	1	743	255	1	0.744	Not Defined	Not Defined	
Infiltration	114	543	265	78	0.657	Not Defined	Not Defined	
Mass	40	789	158	13	0.829	Not Defined	Not Defined	
Nodule	28	731	220	21	0.759	Not Defined	Not Defined	
Atelectasis	64	657	249	30	0.721	Not Defined	Not Defined	
Pneumothorax	24	785	183	8	0.809	Not Defined	Not Defined	
Pleural_Thickening	24	713	259	4	0.737	Not Defined	Not Defined	
Pneumonia	14	661	320	5	0.675	Not Defined	Not Defined	
Fibrosis	10	725	261	4	0.735	Not Defined	Not Defined	

```
Edema                15  767  213   5    0.782  Not Defined  Not Defined
Consolidation        36  658  297   9    0.694  Not Defined  Not Defined

                    Specificity          PPV          NPV          AUC  \

Cardiomegaly        Not Defined  Not Defined  Not Defined  Not Defined
Emphysema           Not Defined  Not Defined  Not Defined  Not Defined
Effusion            Not Defined  Not Defined  Not Defined  Not Defined
Hernia              Not Defined  Not Defined  Not Defined  Not Defined
Infiltration        Not Defined  Not Defined  Not Defined  Not Defined
Mass                Not Defined  Not Defined  Not Defined  Not Defined
Nodule              Not Defined  Not Defined  Not Defined  Not Defined
Atelectasis         Not Defined  Not Defined  Not Defined  Not Defined
Pneumothorax        Not Defined  Not Defined  Not Defined  Not Defined
Pleural_Thickening  Not Defined  Not Defined  Not Defined  Not Defined
Pneumonia           Not Defined  Not Defined  Not Defined  Not Defined
Fibrosis            Not Defined  Not Defined  Not Defined  Not Defined
Edema               Not Defined  Not Defined  Not Defined  Not Defined
Consolidation       Not Defined  Not Defined  Not Defined  Not Defined

                                      F1 Threshold

Cardiomegaly        Not Defined       0.5
Emphysema           Not Defined       0.5
Effusion            Not Defined       0.5
Hernia              Not Defined       0.5
Infiltration        Not Defined       0.5
Mass                Not Defined       0.5
Nodule              Not Defined       0.5
Atelectasis         Not Defined       0.5
Pneumothorax        Not Defined       0.5
Pleural_Thickening  Not Defined       0.5
Pneumonia           Not Defined       0.5
Fibrosis            Not Defined       0.5
Edema               Not Defined       0.5
Consolidation       Not Defined       0.5
```

If we were to judge our model's performance based on the accuracy metric, we would say that our model is not very accurate for detecting the `Infiltration` cases (accuracy of 0.657) but pretty accurate for detecting `Emphysema` (accuracy of 0.889).

But is that really the case?...

Let's imagine a model that simply predicts that any patient does **Not** have `Emphysema`, regardless of patient's measurements. Let's calculate the accuracy for such a model.

```
In [13]: get_accuracy(valid_results["Emphysema"].values, np.zeros(len(valid_results)))
```

```
Out[13]: 0.972
```

As you can see above, such a model would be 97% accurate! Even better than our deep learning based model.

But is this really a good model? Wouldn't this model be wrong 100% of the time if the patient actually had this condition?

In the following sections, we will address this concern with more advanced model measures - **sensitivity and specificity** - that evaluate how well the model predicts positives for patients with the condition and negatives for cases that actually do not have the condition.

3.3 - Prevalence

Another important concept is **prevalence**. * In a medical context, prevalence is the proportion of people in the population who have the disease (or condition, etc). * In machine learning terms, this is the proportion of positive examples. The expression for prevalence is:

$$prevalence = \frac{1}{N}\sum_i y_i$$

where $y_i = 1$ when the example is 'positive' (has the disease).

Exercise 3 - get_prevalence

Let's measure prevalence for each disease:

Hints

You can use np.mean to calculate the formula.

Actually, the automatic grader is expecting numpy.mean, so please use it instead of using an equally valid but different way of calculating the prevalence. =)

```
In [14]: # UNQ_C3 (UNIQUE CELL IDENTIFIER, DO NOT EDIT)
         def get_prevalence(y):
             """
             Compute prevalence.

             Args:
                 y (np.array): ground truth, size (n_examples)
             Returns:
                 prevalence (float): prevalence of positive cases
             """
             prevalence = 0.0

             ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

             prevalence = np.sum(y == 1) /len(y)

             ### END CODE HERE ###

             return prevalence
```

```
In [15]: ### do npt modify this cell
         get_prevalence_test(get_prevalence)
```

```
Test Case:

Test Labels:              [1 0 0 1 1 0 0 0 0 1]
Computed Prevalence:  0.4

 All tests passed.
```

Expected output:

```
Test Case:

Test Labels:          [1 0 0 1 1 0 0 0 0 1]
Computed Prevalence:  0.4

 All tests passed.
```

```
In [16]: util.get_performance_metrics(y, pred, class_labels, acc=get_accuracy, prevalence=get_
```

Out[16]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	\
Cardiomegaly	16	814	169	1	0.83	0.017	Not Defined	
Emphysema	20	869	103	8	0.889	0.028	Not Defined	
Effusion	99	690	196	15	0.789	0.114	Not Defined	
Hernia	1	743	255	1	0.744	0.002	Not Defined	
Infiltration	114	543	265	78	0.657	0.192	Not Defined	
Mass	40	789	158	13	0.829	0.053	Not Defined	
Nodule	28	731	220	21	0.759	0.049	Not Defined	
Atelectasis	64	657	249	30	0.721	0.094	Not Defined	
Pneumothorax	24	785	183	8	0.809	0.032	Not Defined	
Pleural_Thickening	24	713	259	4	0.737	0.028	Not Defined	
Pneumonia	14	661	320	5	0.675	0.019	Not Defined	
Fibrosis	10	725	261	4	0.735	0.014	Not Defined	
Edema	15	767	213	5	0.782	0.02	Not Defined	
Consolidation	36	658	297	9	0.694	0.045	Not Defined	

	Specificity	PPV	NPV	AUC	\
Cardiomegaly	Not Defined	Not Defined	Not Defined	Not Defined	
Emphysema	Not Defined	Not Defined	Not Defined	Not Defined	
Effusion	Not Defined	Not Defined	Not Defined	Not Defined	
Hernia	Not Defined	Not Defined	Not Defined	Not Defined	
Infiltration	Not Defined	Not Defined	Not Defined	Not Defined	
Mass	Not Defined	Not Defined	Not Defined	Not Defined	
Nodule	Not Defined	Not Defined	Not Defined	Not Defined	
Atelectasis	Not Defined	Not Defined	Not Defined	Not Defined	
Pneumothorax	Not Defined	Not Defined	Not Defined	Not Defined	
Pleural_Thickening	Not Defined	Not Defined	Not Defined	Not Defined	
Pneumonia	Not Defined	Not Defined	Not Defined	Not Defined	
Fibrosis	Not Defined	Not Defined	Not Defined	Not Defined	
Edema	Not Defined	Not Defined	Not Defined	Not Defined	
Consolidation	Not Defined	Not Defined	Not Defined	Not Defined	

	F1	Threshold
Cardiomegaly	Not Defined	0.5
Emphysema	Not Defined	0.5

```
Effusion            Not Defined       0.5
Hernia              Not Defined       0.5
Infiltration        Not Defined       0.5
Mass                Not Defined       0.5
Nodule              Not Defined       0.5
Atelectasis         Not Defined       0.5
Pneumothorax        Not Defined       0.5
Pleural_Thickening  Not Defined       0.5
Pneumonia           Not Defined       0.5
Fibrosis            Not Defined       0.5
Edema               Not Defined       0.5
Consolidation       Not Defined       0.5
```

`Hernia` has a prevalence 0.002, which is the rarest among the studied conditions in our dataset.
3.4 Sensitivity and Specificity

Sensitivity and specificity are two of the most prominent numbers that are used to measure diagnostics tests. - Sensitivity is the probability that our test outputs positive given that the case is actually positive. - Specificity is the probability that the test outputs negative given that the case is actually negative.

We can phrase this easily in terms of true positives, true negatives, false positives, and false negatives:

$$sensitivity = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

$$specificity = \frac{\text{true negatives}}{\text{true negatives} + \text{false positives}}$$

Exercise 4 - get_sensitivity and get_specificity

Let's calculate sensitivity and specificity for our model:

```
In [23]: # UNQ_C4 (UNIQUE CELL IDENTIFIER, DO NOT EDIT)
         def get_sensitivity(y, pred, th=0.5):
             """
             Compute sensitivity of predictions at threshold.

             Args:
                 y (np.array): ground truth, size (n_examples)
                 pred (np.array): model output, size (n_examples)
                 th (float): cutoff value for positive prediction from model
             Returns:
                 sensitivity (float): probability that our test outputs positive given that th
             """
             sensitivity = 0.0

             ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

             # get TP and FN using our previously defined functions
             TP = true_positives(y, pred, th)
```

```
    FN = false_negatives(y, pred, th)

    # use TP and FN to compute sensitivity
    sensitivity = TP / (TP+FN) if (TP + FN) != 0 else 0

    ### END CODE HERE ###

    return sensitivity

def get_specificity(y, pred, th=0.5):
    """
    Compute specificity of predictions at threshold.

    Args:
        y (np.array): ground truth, size (n_examples)
        pred (np.array): model output, size (n_examples)
        th (float): cutoff value for positive prediction from model
    Returns:
        specificity (float): probability that the test outputs negative given that th
    """
    specificity = 0.0

    ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

    # get TN and FP using our previously defined functions
    TN = true_negatives(y, pred, th)
    FP = false_positives(y, pred, th)


    # use TN and FP to compute specificity
    specificity = TN / (TN+FP) if (TN + FP) != 0 else 0

    ### END CODE HERE ###

    return specificity
```

In [24]:
```
### do not modify this cell
get_sensitivity_specificity_test(get_sensitivity, get_specificity)
```

```
Test Case:

Test Labels:                [1 0 0 1 1]
Test Predictions:       [1 0 0 1 1]
Threshold:                  0.5
Computed Sensitivity:  0.6666666666666666
Computed Specificity:  0.5

 All tests passed. All tests passed.
```

Expected output:

```
Test Case:

Test Labels:           [1 0 0 1 1]
Test Predictions:      [1 0 0 1 1]
Threshold:           0.5
Computed Sensitivity:  0.6666666666666666
Computed Specificity:  0.5

 All tests passed.
 All tests passed.
```

```
In [25]: util.get_performance_metrics(y, pred, class_labels, acc=get_accuracy, prevalence=get_
                                sens=get_sensitivity, spec=get_specificity)
```

Out[25]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	\
Cardiomegaly	16	814	169	1	0.83	0.017	0.941	
Emphysema	20	869	103	8	0.889	0.028	0.714	
Effusion	99	690	196	15	0.789	0.114	0.868	
Hernia	1	743	255	1	0.744	0.002	0.5	
Infiltration	114	543	265	78	0.657	0.192	0.594	
Mass	40	789	158	13	0.829	0.053	0.755	
Nodule	28	731	220	21	0.759	0.049	0.571	
Atelectasis	64	657	249	30	0.721	0.094	0.681	
Pneumothorax	24	785	183	8	0.809	0.032	0.75	
Pleural_Thickening	24	713	259	4	0.737	0.028	0.857	
Pneumonia	14	661	320	5	0.675	0.019	0.737	
Fibrosis	10	725	261	4	0.735	0.014	0.714	
Edema	15	767	213	5	0.782	0.02	0.75	
Consolidation	36	658	297	9	0.694	0.045	0.8	

	Specificity	PPV	NPV	AUC	\
Cardiomegaly	0.828	Not Defined	Not Defined	Not Defined	
Emphysema	0.894	Not Defined	Not Defined	Not Defined	
Effusion	0.779	Not Defined	Not Defined	Not Defined	
Hernia	0.744	Not Defined	Not Defined	Not Defined	
Infiltration	0.672	Not Defined	Not Defined	Not Defined	
Mass	0.833	Not Defined	Not Defined	Not Defined	
Nodule	0.769	Not Defined	Not Defined	Not Defined	
Atelectasis	0.725	Not Defined	Not Defined	Not Defined	
Pneumothorax	0.811	Not Defined	Not Defined	Not Defined	
Pleural_Thickening	0.734	Not Defined	Not Defined	Not Defined	
Pneumonia	0.674	Not Defined	Not Defined	Not Defined	
Fibrosis	0.735	Not Defined	Not Defined	Not Defined	
Edema	0.783	Not Defined	Not Defined	Not Defined	
Consolidation	0.689	Not Defined	Not Defined	Not Defined	

```
                                F1 Threshold

Cardiomegaly        Not Defined       0.5
Emphysema           Not Defined       0.5
Effusion            Not Defined       0.5
Hernia              Not Defined       0.5
Infiltration        Not Defined       0.5
Mass                Not Defined       0.5
Nodule              Not Defined       0.5
Atelectasis         Not Defined       0.5
Pneumothorax        Not Defined       0.5
Pleural_Thickening  Not Defined       0.5
Pneumonia           Not Defined       0.5
Fibrosis            Not Defined       0.5
Edema               Not Defined       0.5
Consolidation       Not Defined       0.5
```

Note that specificity and sensitivity do not depend on the prevalence of the positive class in the dataset. * This is because the statistics are only computed within people of the same class * Sensitivity only considers output on people in the positive class * Similarly, specificity only considers output on people in the negative class.

3.5 PPV and NPV

Diagnostically, however, sensitivity and specificity are not helpful. Sensitivity, for example, tells us the probability our test outputs positive given that the person already has the condition. Here, we are conditioning on the thing we would like to find out (whether the patient has the condition)!

What would be more helpful is the probability that the person has the disease given that our test outputs positive. That brings us to positive predictive value (PPV) and negative predictive value (NPV).

- Positive predictive value (PPV) is the probability that subjects with a positive screening test truly have the disease.
- Negative predictive value (NPV) is the probability that subjects with a negative screening test truly don't have the disease.

Again, we can formulate these in terms of true positives, true negatives, false positives, and false negatives:

$$PPV = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

$$NPV = \frac{\text{true negatives}}{\text{true negatives} + \text{false negatives}}$$

Exercise 5 - get_ppv and get_npv

Let's calculate PPV & NPV for our model:

```
In [27]: # UNQ_C5 (UNIQUE CELL IDENTIFIER, DO NOT EDIT)
         def get_ppv(y, pred, th=0.5):
```

```
    """
    Compute PPV of predictions at threshold.

    Args:
        y (np.array): ground truth, size (n_examples)
        pred (np.array): model output, size (n_examples)
        th (float): cutoff value for positive prediction from model
    Returns:
        PPV (float): positive predictive value of predictions at threshold
    """
    PPV = 0.0

    ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

    # get TP and FP using our previously defined functions
    TP = true_positives(y, pred, th)

    FP =false_positives(y, pred, th)


    # use TP and FP to compute PPV
    PPV = TP / (TP + FP) if (TP + FP) != 0 else 0


    ### END CODE HERE ###

    return PPV

def get_npv(y, pred, th=0.5):
    """
    Compute NPV of predictions at threshold.

    Args:
        y (np.array): ground truth, size (n_examples)
        pred (np.array): model output, size (n_examples)
        th (float): cutoff value for positive prediction from model
    Returns:
        NPV (float): negative predictive value of predictions at threshold
    """
    NPV = 0.0

    ### START CODE HERE (REPLACE INSTANCES OF 'None' with your code) ###

    # get TN and FN using our previously defined functions
    TN = true_negatives(y, pred, th)

    FN = false_negatives(y, pred, th)
```

```
            # use TN and FN to compute NPV
            NPV = TN / (TN + FN) if (TN + FN) != 0 else 0


            ### END CODE HERE ###

            return NPV
```

```
In [28]: ### do not modify this cell
         get_ppv_npv_test(get_ppv, get_npv)
```

```
Test Case:

Test Labels:           [1 0 0 1 1]
Test Predictions:  [1 0 0 1 1]
Threshold:           0.5
Computed PPV:           0.6666666666666666
Computed NPV:           0.5

 All tests passed. All tests passed.
```

Expected output:

```
Test Case:

Test Labels:       [1 0 0 1 1]
Test Predictions:  [1 0 0 1 1]
Threshold:       0.5
Computed PPV:     0.6666666666666666
Computed NPV:     0.5

 All tests passed.
 All tests passed.
```

```
In [29]: util.get_performance_metrics(y, pred, class_labels, acc=get_accuracy, prevalence=get_
                                  sens=get_sensitivity, spec=get_specificity, ppv=get_ppv, npv=
```

Out[29]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	\
Cardiomegaly	16	814	169	1	0.83	0.017	0.941	
Emphysema	20	869	103	8	0.889	0.028	0.714	
Effusion	99	690	196	15	0.789	0.114	0.868	
Hernia	1	743	255	1	0.744	0.002	0.5	
Infiltration	114	543	265	78	0.657	0.192	0.594	
Mass	40	789	158	13	0.829	0.053	0.755	
Nodule	28	731	220	21	0.759	0.049	0.571	
Atelectasis	64	657	249	30	0.721	0.094	0.681	
Pneumothorax	24	785	183	8	0.809	0.032	0.75	
Pleural_Thickening	24	713	259	4	0.737	0.028	0.857	

```
Pneumonia            14  661  320   5    0.675      0.019       0.737
Fibrosis             10  725  261   4    0.735      0.014       0.714
Edema                15  767  213   5    0.782       0.02        0.75
Consolidation        36  658  297   9    0.694      0.045         0.8

                  Specificity    PPV    NPV          AUC           F1  \

Cardiomegaly            0.828  0.086  0.999  Not Defined  Not Defined
Emphysema               0.894  0.163  0.991  Not Defined  Not Defined
Effusion                0.779  0.336  0.979  Not Defined  Not Defined
Hernia                  0.744  0.004  0.999  Not Defined  Not Defined
Infiltration            0.672  0.301  0.874  Not Defined  Not Defined
Mass                    0.833  0.202  0.984  Not Defined  Not Defined
Nodule                  0.769  0.113  0.972  Not Defined  Not Defined
Atelectasis             0.725  0.204  0.956  Not Defined  Not Defined
Pneumothorax            0.811  0.116   0.99  Not Defined  Not Defined
Pleural_Thickening      0.734  0.085  0.994  Not Defined  Not Defined
Pneumonia               0.674  0.042  0.992  Not Defined  Not Defined
Fibrosis                0.735  0.037  0.995  Not Defined  Not Defined
Edema                   0.783  0.066  0.994  Not Defined  Not Defined
Consolidation           0.689  0.108  0.987  Not Defined  Not Defined

                  Threshold

Cardiomegaly            0.5
Emphysema               0.5
Effusion                0.5
Hernia                  0.5
Infiltration            0.5
Mass                    0.5
Nodule                  0.5
Atelectasis             0.5
Pneumothorax            0.5
Pleural_Thickening      0.5
Pneumonia               0.5
Fibrosis                0.5
Edema                   0.5
Consolidation           0.5
```

Notice that despite having very high sensitivity and accuracy, the PPV of the predictions could still be very low.

This is the case with `Edema`, for example. * The sensitivity for `Edema` is 0.75. * However, given that the model predicted positive, the probability that a person has Edema (its PPV) is only 0.066!

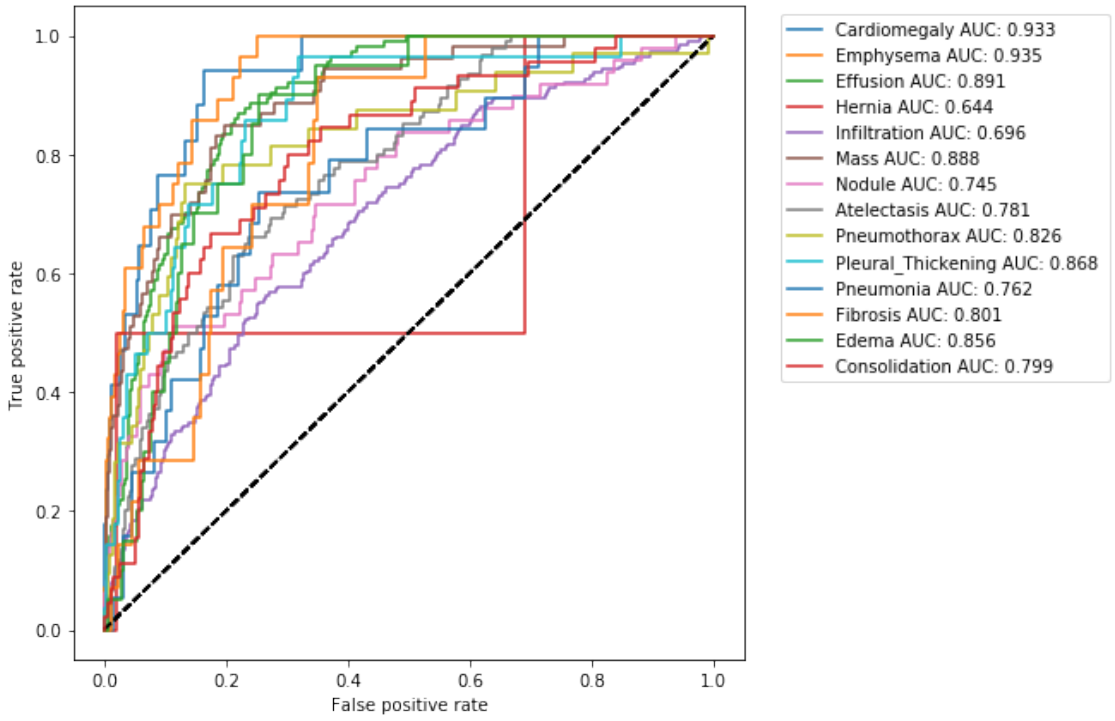
3.6 ROC Curve

So far we have been operating under the assumption that our model's prediction of `0.5` and above should be treated as positive and otherwise it should be treated as negative. This however was a rather arbitrary choice. One way to see this, is to look at a very informative visualization called the receiver operating characteristic (ROC) curve.

The ROC curve is created by plotting the true positive rate (TPR) against the false positive rate (FPR) at various threshold settings. The ideal point is at the top left, with a true positive rate of 1 and a false positive rate of 0. The various points on the curve are generated by gradually changing the threshold.

Let's look at this curve for our model:

```
In [30]: util.get_curve(y, pred, class_labels)
```



The area under the ROC curve is also called AUCROC or C-statistic and is a measure of goodness of fit. In medical literature this number also gives the probability that a randomly selected patient who experienced a condition had a higher risk score than a patient who had not experienced the event. This summarizes the model output across all thresholds, and provides a good sense of the discriminative power of a given model.

Let's use the `sklearn` metric function of `roc_auc_score` to add this score to our metrics table.

```
In [31]: from sklearn.metrics import roc_auc_score
         util.get_performance_metrics(y, pred, class_labels, acc=get_accuracy, prevalence=get_
                                      sens=get_sensitivity, spec=get_specificity, ppv=get_ppv, npv=
```

Out[31]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	\
Cardiomegaly	16	814	169	1	0.83	0.017	0.941	
Emphysema	20	869	103	8	0.889	0.028	0.714	
Effusion	99	690	196	15	0.789	0.114	0.868	
Hernia	1	743	255	1	0.744	0.002	0.5	

Infiltration	114	543	265	78	0.657	0.192	0.594
Mass	40	789	158	13	0.829	0.053	0.755
Nodule	28	731	220	21	0.759	0.049	0.571
Atelectasis	64	657	249	30	0.721	0.094	0.681
Pneumothorax	24	785	183	8	0.809	0.032	0.75
Pleural_Thickening	24	713	259	4	0.737	0.028	0.857
Pneumonia	14	661	320	5	0.675	0.019	0.737
Fibrosis	10	725	261	4	0.735	0.014	0.714
Edema	15	767	213	5	0.782	0.02	0.75
Consolidation	36	658	297	9	0.694	0.045	0.8

	Specificity	PPV	NPV	AUC	F1	Threshold
Cardiomegaly	0.828	0.086	0.999	0.933	Not Defined	0.5
Emphysema	0.894	0.163	0.991	0.935	Not Defined	0.5
Effusion	0.779	0.336	0.979	0.891	Not Defined	0.5
Hernia	0.744	0.004	0.999	0.644	Not Defined	0.5
Infiltration	0.672	0.301	0.874	0.696	Not Defined	0.5
Mass	0.833	0.202	0.984	0.888	Not Defined	0.5
Nodule	0.769	0.113	0.972	0.745	Not Defined	0.5
Atelectasis	0.725	0.204	0.956	0.781	Not Defined	0.5
Pneumothorax	0.811	0.116	0.99	0.826	Not Defined	0.5
Pleural_Thickening	0.734	0.085	0.994	0.868	Not Defined	0.5
Pneumonia	0.674	0.042	0.992	0.762	Not Defined	0.5
Fibrosis	0.735	0.037	0.995	0.801	Not Defined	0.5
Edema	0.783	0.066	0.994	0.856	Not Defined	0.5
Consolidation	0.689	0.108	0.987	0.799	Not Defined	0.5

4. Confidence Intervals

Of course our dataset is only a sample of the real world, and our calculated values for all above metrics is an estimate of the real world values. It would be good to quantify this uncertainty due to the sampling of our dataset. We'll do this through the use of confidence intervals. A 95% confidence interval for an estimate $\hat{s}$ of a parameter s is an interval $I = (a, b)$ such that 95% of the time when the experiment is run, the true value s is contained in I. More concretely, if we were to run the experiment many times, then the fraction of those experiments for which I contains the true parameter would tend towards 95%.

While some estimates come with methods for computing the confidence interval analytically, more complicated statistics, such as the AUC for example, are difficult. For these we can use a method called the *bootstrap*. The bootstrap estimates the uncertainty by resampling the dataset with replacement. For each resampling i, we will get a new estimate, $\hat{s}_i$. We can then estimate the distribution of $\hat{s}$ by using the distribution of $\hat{s}_i$ for our bootstrap samples.

In the code below, we create bootstrap samples and compute sample AUCs from those samples. Note that we use stratified random sampling (sampling from the positive and negative classes separately) to make sure that members of each class are represented.

```
In [32]: def bootstrap_auc(y, pred, classes, bootstraps = 100, fold_size = 1000):
             statistics = np.zeros((len(classes), bootstraps))
```

```
            for c in range(len(classes)):
                df = pd.DataFrame(columns=['y', 'pred'])
                df.loc[:, 'y'] = y[:, c]
                df.loc[:, 'pred'] = pred[:, c]
                # get positive examples for stratified sampling
                df_pos = df[df.y == 1]
                df_neg = df[df.y == 0]
                prevalence = len(df_pos) / len(df)
                for i in range(bootstraps):
                    # stratified sampling of positive and negative examples
                    pos_sample = df_pos.sample(n = int(fold_size * prevalence), replace=True)
                    neg_sample = df_neg.sample(n = int(fold_size * (1-prevalence)), replace=T

                    y_sample = np.concatenate([pos_sample.y.values, neg_sample.y.values])
                    pred_sample = np.concatenate([pos_sample.pred.values, neg_sample.pred.valu
                    score = roc_auc_score(y_sample, pred_sample)
                    statistics[c][i] = score
            return statistics

        statistics = bootstrap_auc(y, pred, class_labels)
```

Now we can compute confidence intervals from the sample statistics that we computed.

```
In [33]: util.print_confidence_intervals(class_labels, statistics)
```

```
Out[33]:                    Mean AUC (CI 5%-95%)
         Cardiomegaly           0.93 (0.89-0.97)
         Emphysema              0.93 (0.90-0.96)
         Effusion               0.89 (0.87-0.91)
         Hernia                 0.66 (0.31-0.98)
         Infiltration           0.70 (0.66-0.73)
         Mass                   0.89 (0.85-0.93)
         Nodule                 0.75 (0.69-0.81)
         Atelectasis            0.78 (0.75-0.82)
         Pneumothorax           0.82 (0.77-0.88)
         Pleural_Thickening     0.87 (0.80-0.91)
         Pneumonia              0.77 (0.68-0.85)
         Fibrosis               0.80 (0.73-0.86)
         Edema                  0.86 (0.81-0.90)
         Consolidation          0.80 (0.76-0.85)
```

As you can see, our confidence intervals are much wider for some classes than for others. Hernia, for example, has an interval around (0.30 - 0.98), indicating that we can't be certain it is better than chance (at 0.5).

5. Precision-Recall Curve

Precision-Recall are informative prediction metrics when significant class imbalance are present in the data.

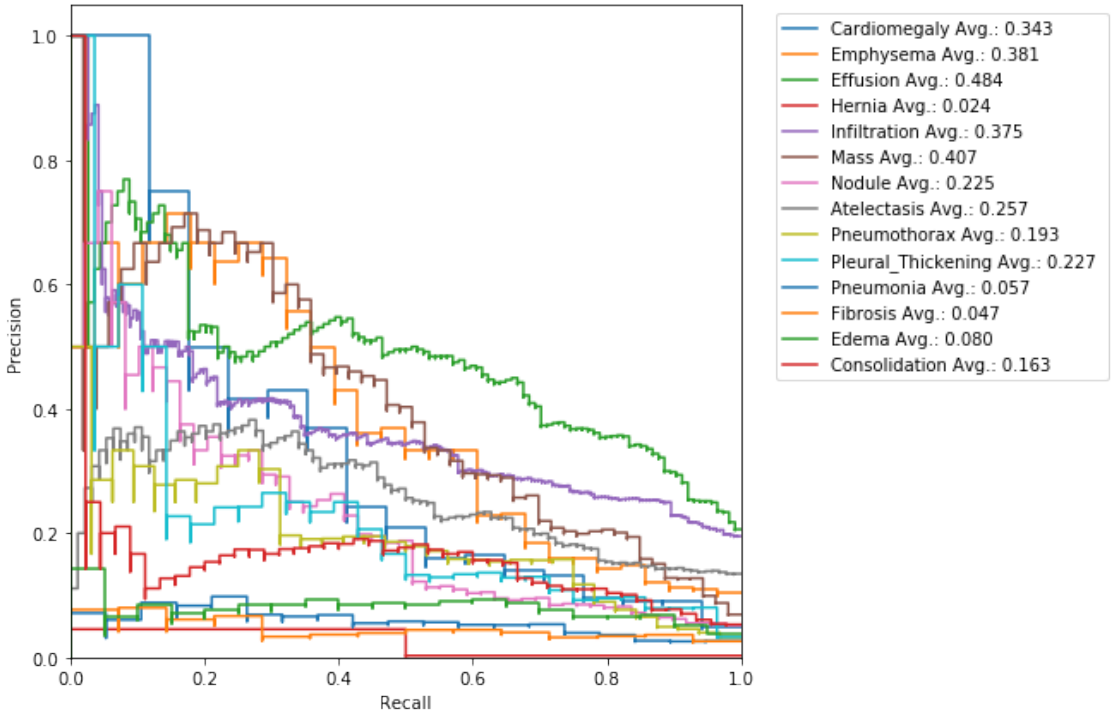
In information retrieval - Precision is a measure of result relevancy and that is equivalent to our previously defined PPV. - Recall is a measure of how many truly relevant results are returned and that is equivalent to our previously defined sensitivity measure.

The precision-recall curve (PRC) shows the trade-off between precision and recall for different thresholds. A high area under the curve represents both high recall and high precision, where high precision relates to a low false positive rate, and high recall relates to a low false negative rate.

High scores for both show that the classifier is returning accurate results (high precision), as well as returning a majority of all positive results (high recall).

Run the following cell to generate a PRC:

```
In [34]: util.get_curve(y, pred, class_labels, curve='prc')
```



6. F1 Score

F1 score is the harmonic mean of the precision and recall, where an F1 score reaches its best value at 1 (perfect precision and recall) and worst at 0.

Again, we can simply use `sklearn`'s utility metric function of `f1_score` to add this measure to our performance table.

```
In [35]: from sklearn.metrics import f1_score
         util.get_performance_metrics(y, pred, class_labels, acc=get_accuracy, prevalence=get_
                                      sens=get_sensitivity, spec=get_specificity, ppv=get_ppv, npv=
```

Out[35]:

	TP	TN	FP	FN	Accuracy	Prevalence	Sensitivity	\
Cardiomegaly	16	814	169	1	0.83	0.017	0.941	
Emphysema	20	869	103	8	0.889	0.028	0.714	
Effusion	99	690	196	15	0.789	0.114	0.868	

Hernia	1	743	255	1	0.744	0.002	0.5
Infiltration	114	543	265	78	0.657	0.192	0.594
Mass	40	789	158	13	0.829	0.053	0.755
Nodule	28	731	220	21	0.759	0.049	0.571
Atelectasis	64	657	249	30	0.721	0.094	0.681
Pneumothorax	24	785	183	8	0.809	0.032	0.75
Pleural_Thickening	24	713	259	4	0.737	0.028	0.857
Pneumonia	14	661	320	5	0.675	0.019	0.737
Fibrosis	10	725	261	4	0.735	0.014	0.714
Edema	15	767	213	5	0.782	0.02	0.75
Consolidation	36	658	297	9	0.694	0.045	0.8

	Specificity	PPV	NPV	AUC	F1	Threshold
Cardiomegaly	0.828	0.086	0.999	0.933	0.158	0.5
Emphysema	0.894	0.163	0.991	0.935	0.265	0.5
Effusion	0.779	0.336	0.979	0.891	0.484	0.5
Hernia	0.744	0.004	0.999	0.644	0.008	0.5
Infiltration	0.672	0.301	0.874	0.696	0.399	0.5
Mass	0.833	0.202	0.984	0.888	0.319	0.5
Nodule	0.769	0.113	0.972	0.745	0.189	0.5
Atelectasis	0.725	0.204	0.956	0.781	0.314	0.5
Pneumothorax	0.811	0.116	0.99	0.826	0.201	0.5
Pleural_Thickening	0.734	0.085	0.994	0.868	0.154	0.5
Pneumonia	0.674	0.042	0.992	0.762	0.079	0.5
Fibrosis	0.735	0.037	0.995	0.801	0.07	0.5
Edema	0.783	0.066	0.994	0.856	0.121	0.5
Consolidation	0.689	0.108	0.987	0.799	0.19	0.5

7. Calibration

When performing classification we often want not only to predict the class label, but also obtain a probability of each label. This probability would ideally give us some kind of confidence on the prediction. In order to observe how our model's generated probabilities are aligned with the real probabilities, we can plot what's called a *calibration curve*.

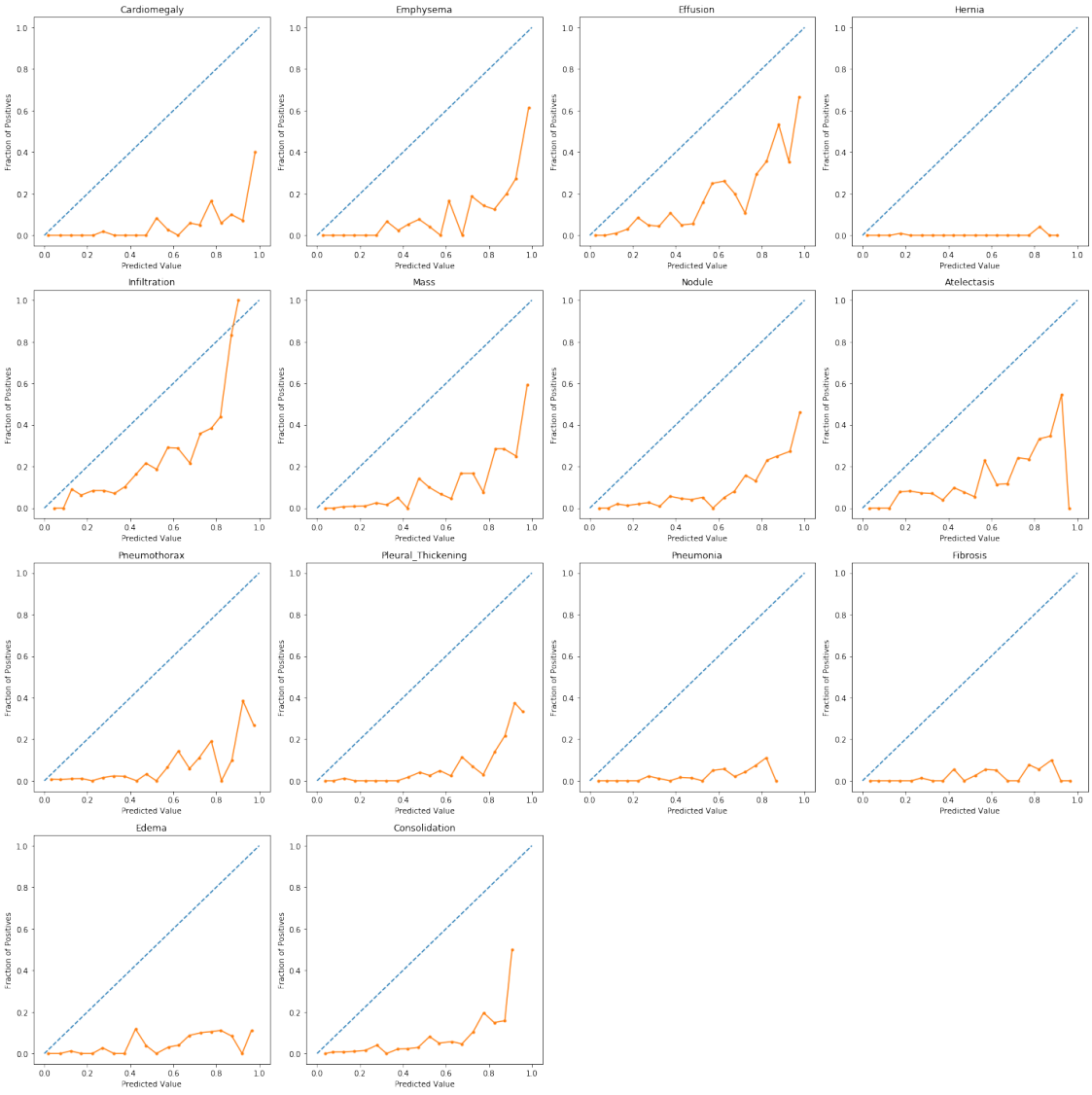
In order to generate a calibration plot, we first bucketize our predictions to a fixed number of separate bins (e.g. 5) between 0 and 1. We then calculate a point for each bin: the x-value for each point is the mean for the probability that our model has assigned to these points and the y-value for each point fraction of true positives in that bin. We then plot these points in a linear plot. A well-calibrated model has a calibration curve that almost aligns with the y=x line.

The `sklearn` library has a utility `calibration_curve` for generating a calibration plot. Let's use it and take a look at our model's calibration:

```
In [36]: from sklearn.calibration import calibration_curve
         def plot_calibration_curve(y, pred):
             plt.figure(figsize=(20, 20))
             for i in range(len(class_labels)):
                 plt.subplot(4, 4, i + 1)
                 fraction_of_positives, mean_predicted_value = calibration_curve(y[:,i], pred[
```

```
            plt.plot([0, 1], [0, 1], linestyle='--')
            plt.plot(mean_predicted_value, fraction_of_positives, marker='.')
            plt.xlabel("Predicted Value")
            plt.ylabel("Fraction of Positives")
            plt.title(class_labels[i])
        plt.tight_layout()
        plt.show()
```

```
In [37]: plot_calibration_curve(y, pred)
```

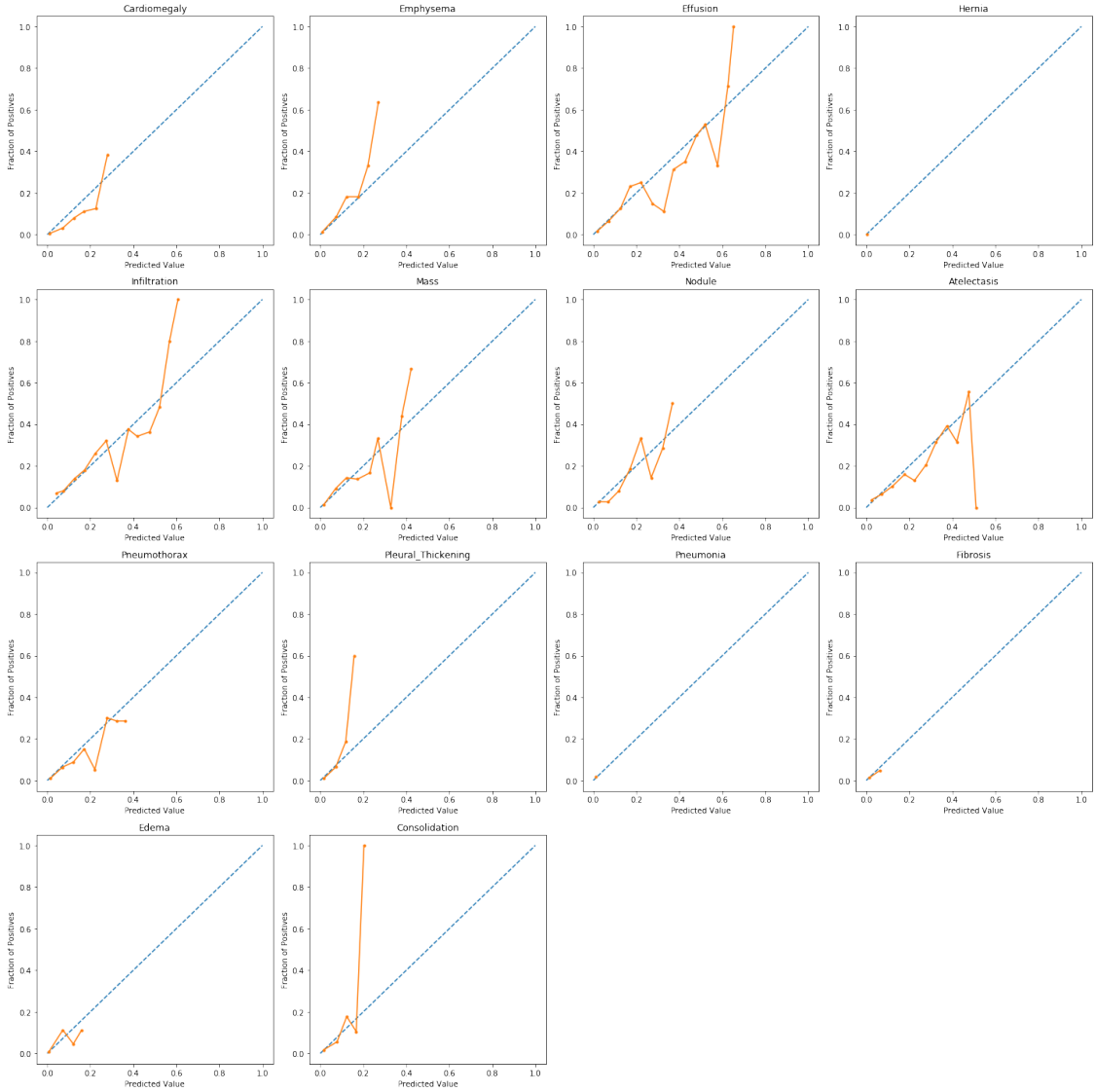


As the above plots show, for most predictions our model's calibration plot does not resemble a well calibrated plot. How can we fix that?...

Thankfully, there is a very useful method called Platt scaling which works by fitting a logistic regression model to our model's scores. To build this model, we will be using the training portion

of our dataset to generate the linear model and then will use the model to calibrate the predictions for our test portion.

```
In [38]: from sklearn.linear_model import LogisticRegression as LR

         y_train = train_results[class_labels].values
         pred_train = train_results[pred_labels].values
         pred_calibrated = np.zeros_like(pred)

         for i in range(len(class_labels)):
             lr = LR(solver='liblinear', max_iter=10000)
             lr.fit(pred_train[:, i].reshape(-1, 1), y_train[:, i])
             pred_calibrated[:, i] = lr.predict_proba(pred[:, i].reshape(-1, 1))[:,1]

In [39]: plot_calibration_curve(y[:,], pred_calibrated)
```



2 That's it!

Congratulations! That was a lot of metrics to get familiarized with. We hope that you feel a lot more confident in your understanding of medical diagnostic evaluation and test your models correctly in your future work :)