Machine Learning: 06048203



Classification Performance Metrics

Part One: Confusion Matrix Basics

- You've probably heard of terms such as "false positive" or "false negative". As well as metrics like "accuracy".
- But what do these terms actually mean mathematically?

- Imagine we've developed a test or model to detect presence of a virus infection in a person based on some biological feature.
- We could treat this as a Logistic Regression, predicting:
 - O Not Infected (Tests Negative)
 - 1 Infected (Tests Positive)

- It is unlikely our model will perform perfectly. This means there 4 possible outcomes:
 - Infected person tests positive.
 - Healthy person tests negative.

- It is unlikely our model will perform perfectly. This means there 4 possible outcomes:
 - Infected person tests positive.
 - Healthy person tests negative.
 - Note, these are the outcomes we want! But it is unlikely our test is perfect...

- It is unlikely our model will perform perfectly. This means there 4 possible outcomes:
 - Infected person tests positive.
 - Healthy person tests negative.
 - Infected person tests negative.
 - Healthy person tests positive.

- Based off these 4 possibilities, there are many error metrics we can calculate.
- First, let's start by visualizing these four possibilities as a matrix.

Confusion Matrix

ACTUAL

PREDICTE HEALTHY

HEALTHY

Confusion Matrix

ACTUAL

PREDICTE INFECTED TRUE POSITIVE

HEALTHY

Confusion Matrix

ACTUAL

INFECTED HEALTHY INFECTED TRUE **POSITIVE** PREDICTE **HEALTHY** TRUE **NEGATIVE**

Confusion Matrix

ACTUAL

INFECTED HEALTHY INFECTED TRUE **FALSE** POSITIVE POSITIVE **PREDICTE HEALTHY** TRUE **NEGATIVE**

Confusion Matrix

ACTUAL

INFECTED HEALTHY

PREDICTE
D

INFECTED TRUE FALSE POSITIVE
POSITIVE
TRUE NEGATIVE

POSITIVE
POSITIVE
NEGATIVE

What is accuracy?

ACTUAL

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

- Accuracy:
 - How often is the model correct?

$$Acc = (TP+TN)/Total$$

Calculating accuracy:

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| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

(4+93)/100 = 97% Accuracy

- Accuracy:
 - How often is the model correct?

$$Acc = (TP+TN)/Total$$

Is this a good value for accuracy?

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

ACTUAL

Accuracy:

 How often is the model correct?

Acc = (TP+TN)/Total

(4+93)/100 = 97% Accuracy

The accuracy paradox...

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| | | INFECTED | HEALTHY |
|------------|----------|----------|---------|
| PREDICTE - | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

(4+93)/100 = 97% Accuracy

- Accuracy:
 - How often is the model correct?

$$Acc = (TP+TN)/Total$$

• Imagine we always report back "healthy"

ACTUAL

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

• Imagine we always report back "healthy"

ACTUAL

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 0 | 0 |
| D | HEALTHY | 5 | 95 |

PREDICTE

Imagine we always report back "healthy"

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|---|----|---|----|--|
| | | _ | | |

| | INFECTED | HEALTHY |
|----------|----------|---------|
| INFECTED | 0 | О |
| HEALTHY | 5 | 95 |

(0+95)/100 = 95% Accuracy

- Accuracy:
 - How often is the model correct?

95% accuracy for a model that always returns "healthy"!

 You may be thinking, "The numbers here are arbitrary, we just happen to get good accuracy in this made up case. Real world data would reflect poor accuracy if a model always returned the same result".

- This is the accuracy paradox!
 - Any classifier dealing with imbalanced classes has to confront the issue of the accuracy paradox.
 - Imbalanced classes will always result in a distorted accuracy reflecting better performance than what is truly warranted.

- Imbalanced classes are often found in real world data sets.
 - Medical conditions can affect small portions of the population.
 - Fraud is not common (e.g. Real vs. Fraud credit card usage).

- If a class is only a small percentage (n%), then a classifier that always predicts the majority class will always have an accuracy of (1-n).
- In our previous example we saw infected were only 5% of the data.
- Allowing the accuracy to be 95%.

- This means we shouldn't solely rely on accuracy as a metric!
- This is where precision, recall, and fl-score will come in.
- Let's explore these other metrics in the next lecture.

Classification Performance Metrics

Part Two: Precision and Recall

- We already know how to calculate accuracy and its associated paradox.
- Let's explore three more metrics that can help give a clearer picture of performance:
 - Recall (a.k.a. sensitivity)
 - Precision
 - F1-Score

• Let's begin with recall.

ACTUAL

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

• Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

Let's begin with recall.

ACTUAL

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

Recall = (TP)/Total Actual Positives

• Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

• Let's begin with recall.

| | | ACTUAL | |
|----------|----------|----------|---------|
| | | INFECTED | HEALTHY |
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

Recall = (TP)/5

• Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

• Let's begin with recall.

| | ACTUAL | | |
|----------|----------|----------|---------|
| | | INFECTED | HEALTHY |
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

Recall =

(4)/5

• Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

• Let's begin with recall.

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| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 4 | 2 |
| D | HEALTHY | 1 | 93 |

Recall = 0.8

• Recall:

 How many relevant cases are found?

 What's the recall if we always classify as "healthy"?

ACTUAL

| | | INFECTED | HEALTHY |
|----------|----------|----------|---------|
| PREDICTE | INFECTED | 0 | Ο |
| D | HEALTHY | 5 | 95 |

Recall = (TP)/Total Actual Positives

- Recall:
 - How many relevant cases are found?

 What's the recall if we always classify as "healthy"?

ACTUAL

| PREDICTE | |
|----------|--|
| D | |

| | INFECTED | HEALTHY |
|----------|----------|---------|
| INFECTED | 0 | 0 |
| HEALTHY | 5 | 95 |

Recall = (0)/5!

Recall:

 How many relevant cases are found?

 A recall of 0 alerts you the model isn't catching cases!

ACTUAL

| | | INFECTED | HEALTHY |
|---------------|----------|----------|---------|
| PREDICTE D | INFECTED | О | О |
| | HEALTHY | 5 | 95 |

Recall = (0)/5!

- Recall:
 - How many relevant cases are found?

Now let's explore precision.

PREDICTE

ACTUAL

| | INFECTED | HEALTHY |
|----------|----------|---------|
| INFECTED | 4 | 2 |
| HEALTHY | 1 | 93 |

Precision = (TP)/Total Predicted Positives

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted Positives

Now let's explore precision.

| | | ACTUAL | | |
|---------------|----------|----------|---------|--|
| | | INFECTED | HEALTHY | |
| PREDICTE D | INFECTED | 4 | 2 | |
| | HEALTHY | 1 | 93 | |

Precision = (TP)/Total Predicted Positives

 $\Lambda \subset T \sqcup \Lambda \sqcup$

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted
Positives

Now let's explore precision.

| | | ACTUAL | |
|---------------|----------|----------|---------|
| | | INFECTED | HEALTHY |
| PREDICTE D | INFECTED | 4 | 2 |
| | HEALTHY | 1 | 93 |

Precision = (TP)/6

 $\Lambda \subset T \cup \Lambda \cup$

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted
Positives

Now let's explore precision.

| | | ACTUAL | |
|---------------|----------|----------|---------|
| | | INFECTED | HEALTHY |
| PREDICTE D | INFECTED | 4 | 2 |
| | HEALTHY | 1 | 93 |

Precision = (TP)/6

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted Positives

Now let's explore precision.

| | | ACTUAL | |
|---------------|----------|----------|---------|
| | | INFECTED | HEALTHY |
| PREDICTE D | INFECTED | 4 | 2 |
| | HEALTHY | 1 | 93 |

Precision = (4)/6

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted Positives

Now let's explore precision.

ACTUAL

| | | INFECTED | HEALTHY |
|---------------|----------|----------|---------|
| PREDICTE D | INFECTED | 4 | 2 |
| | HEALTHY | 1 | 93 |

Precision = 0.666

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted
Positives

 What's the precision if we always classify as "healthy"?

ACTUAL

| PREDICTE | = |
|----------|---|
| D | |

| | INFECTED | HEALTHY |
|----------|----------|---------|
| INFECTED | 0 | О |
| HEALTHY | 5 | 95 |

Precision = (TP)/Total Predicted Positives

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted Positives

 What's the precision if we always classify as "healthy"?

ACTUAL

| | | INFECTED | HEALTHY |
|---------------|----------|----------|---------|
| PREDICTE D | INFECTED | 0 | 0 |
| | HEALTHY | 5 | 95 |

Precision = 0/0

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?

(TP)/Total Predicted
Positives

- Recall and Precision can help illuminate our performance specifically in regards to the relevant or positive case.
- Depending on the model, there is typically a trade-off between precision and recall, which we will explore later on with the ROC curve.

 Since precision and recall are related to each other through the numerator (TP), we often also report the F1-Score, which is the harmonic mean of precision and recall.

$$F = \frac{2 \times precision \times recall}{precision + recall}$$

 The harmonic mean (instead of the normal mean) allows the entire harmonic mean to go to zero if either precision or recall ends up being zero.

$$F = \frac{2 \times precision \times recall}{precision + recall}$$

Classification Performance Metrics

Part Three: ROC Curves

 During World War 2, Radar technology was developed to help detect incoming enemy aircraft.



 The technology was so new, the US Army wanted to develop a methodology to evaluate radar operator performance.

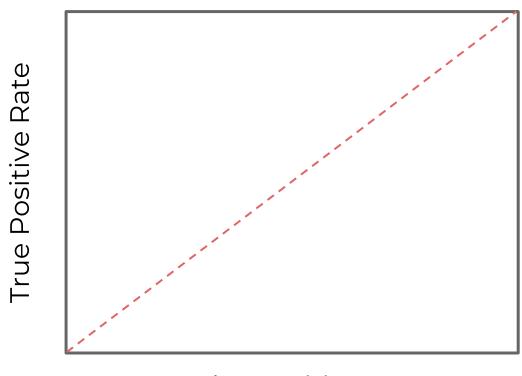


 They developed the Receiver Operator Characteristic curve.

```
True Positive Rate (TPR) = \frac{\text{True Positives (TP)}}{\text{True Positives (TP)} + \text{False Negatives (FN)}}
False Positive Rate (FPR) = \frac{\text{False Positives (FP)}}{\text{False Positives (FP)} + \text{True Negatives (TN)}}
\frac{\text{Positive Rate (FPR)}}{\text{False Positives (FP)}} = \frac{\text{False Positives (FP)}}{\text{False Positives (FP)} + \text{True Negatives (TN)}}
```

False Positive Rate

 They developed the Receiver Operator Characteristic curve.

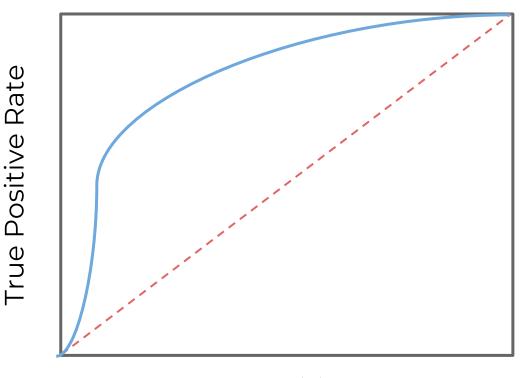


False Positive Rate

 They developed the Receiver Operator Characteristic curve.

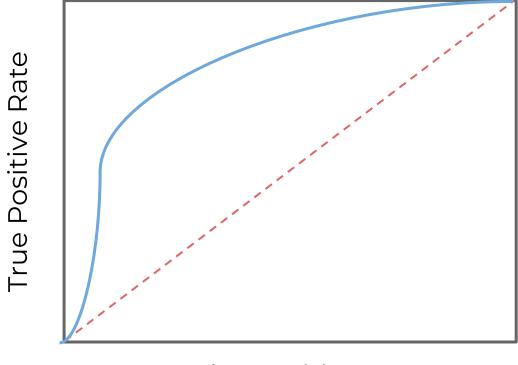


 $False\ Positive\ Rate\ (FPR) = \frac{False\ Positives\ (FP)}{False\ Positives\ (FP) + True\ Negatives\ (TN)}$



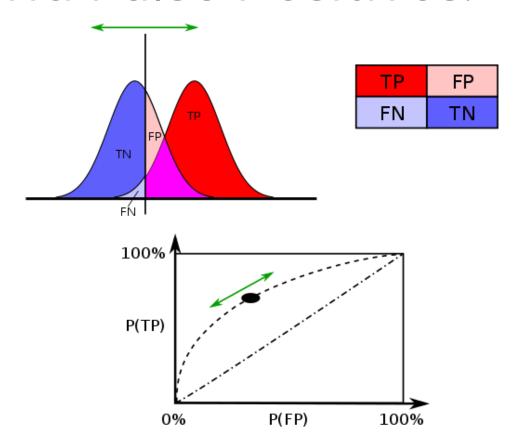
False Positive Rate

 There can be a trade-off between True Positives and False Positives.

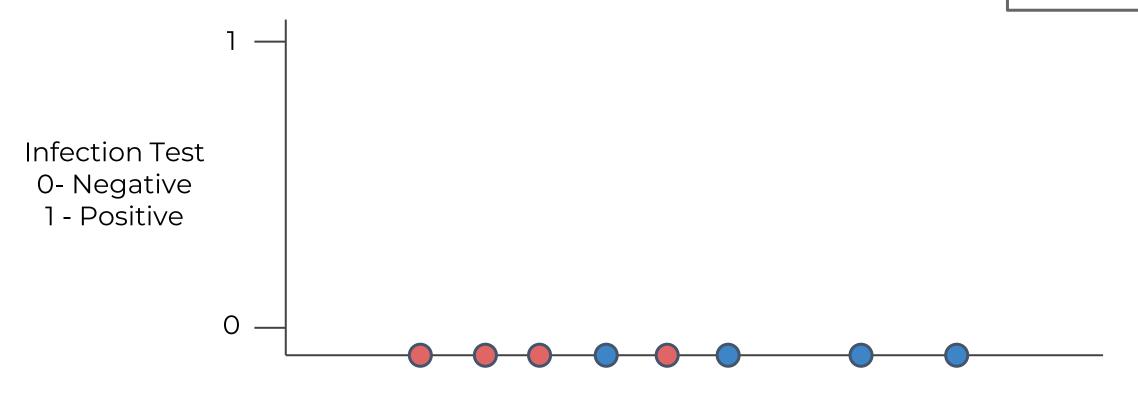


False Positive Rate

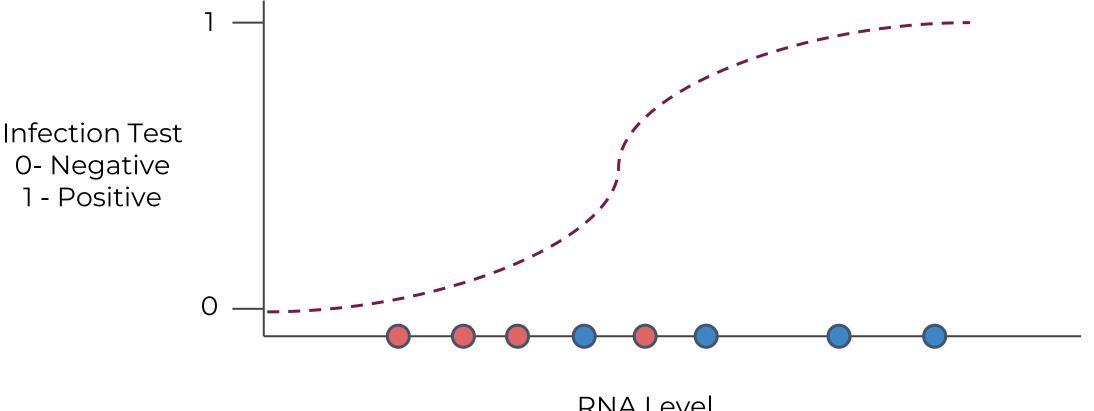
 There can be a trade-off between True Positives and False Positives.



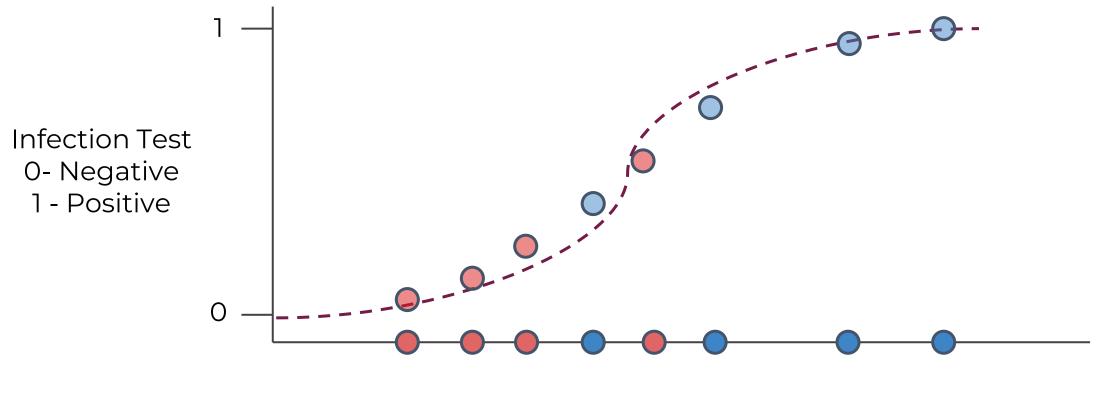
• Our previous infection test.



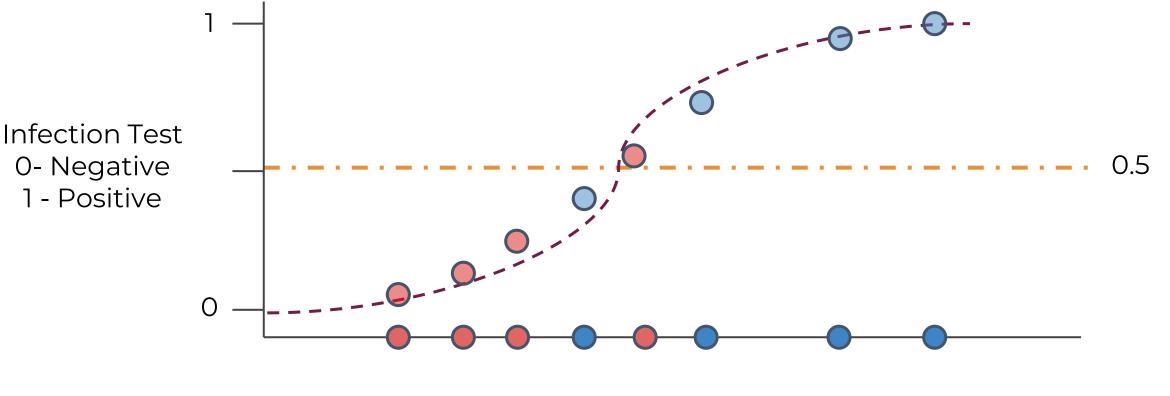
• Fit logistic regression model.



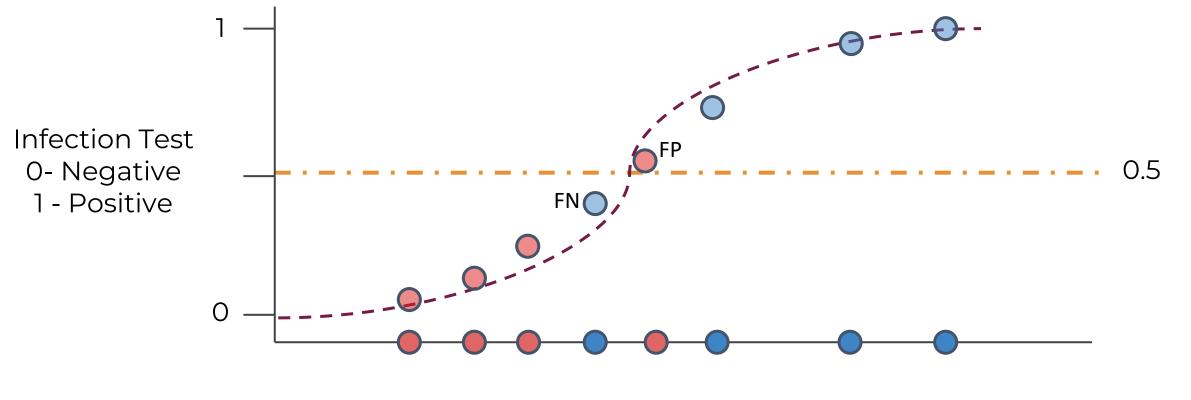
• Given X we predict 0 or 1.

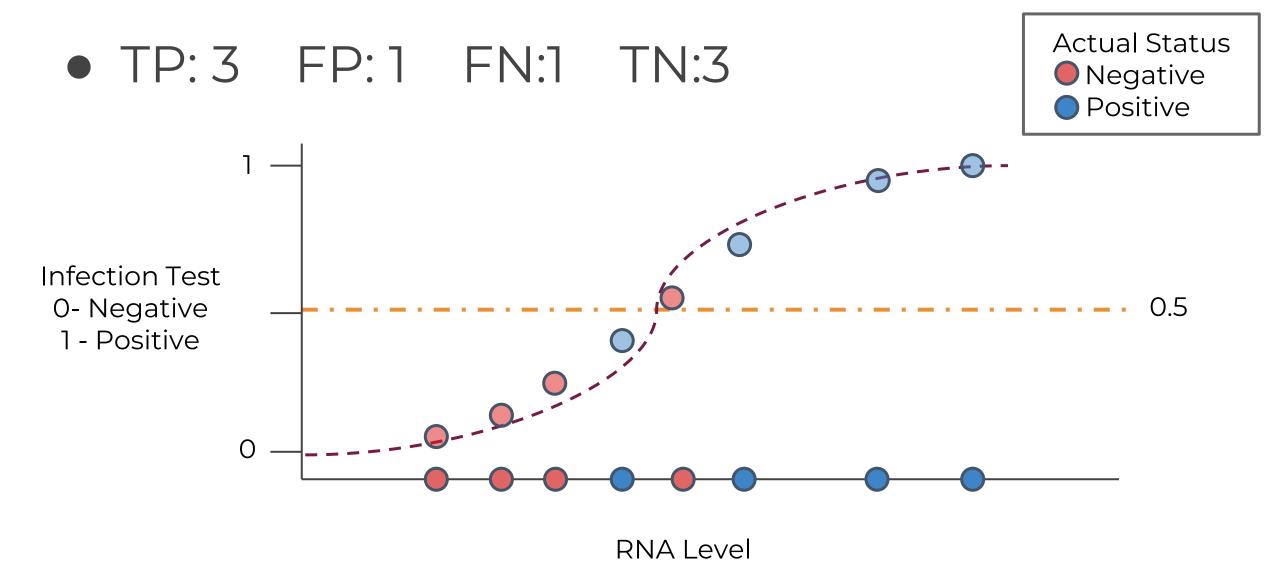


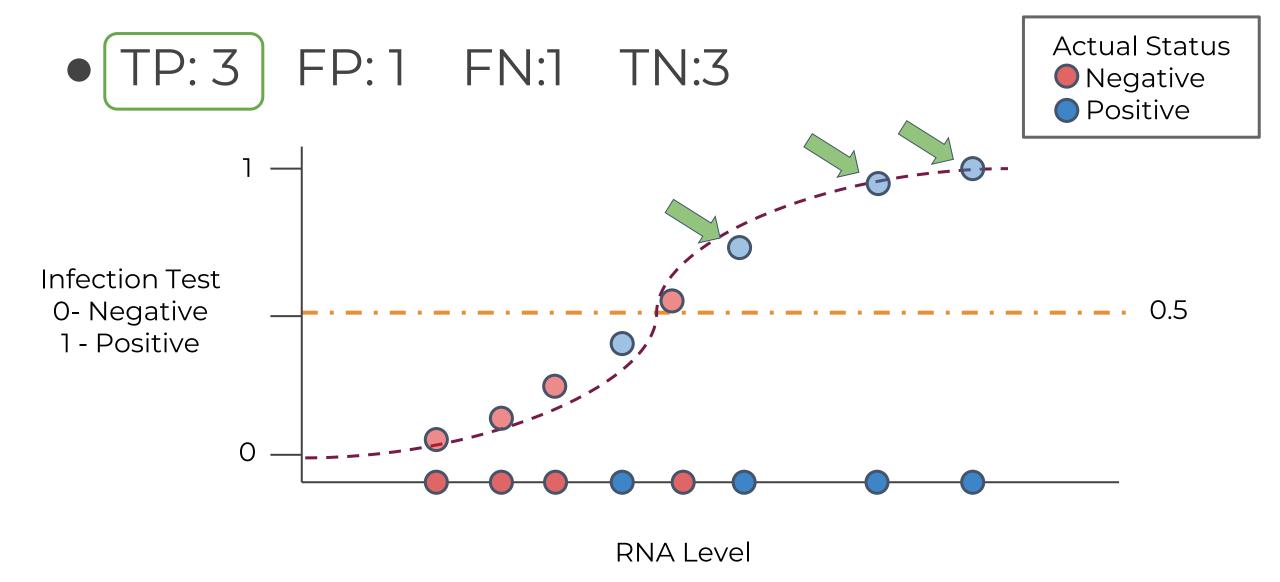
• Default is to choose 0.5 as cut-off.

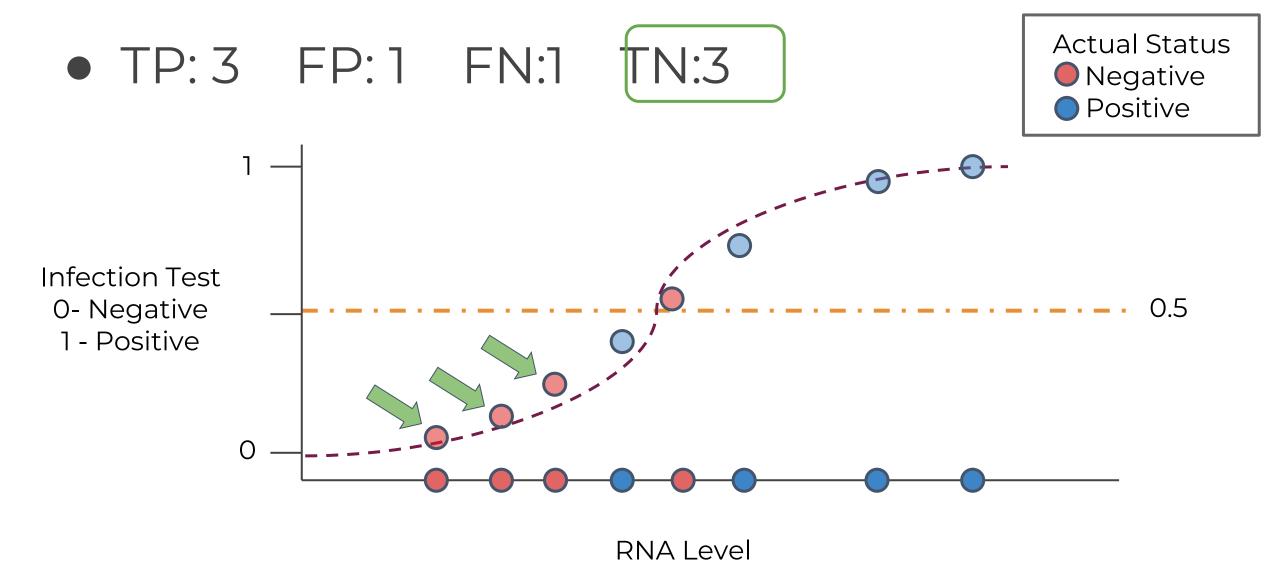


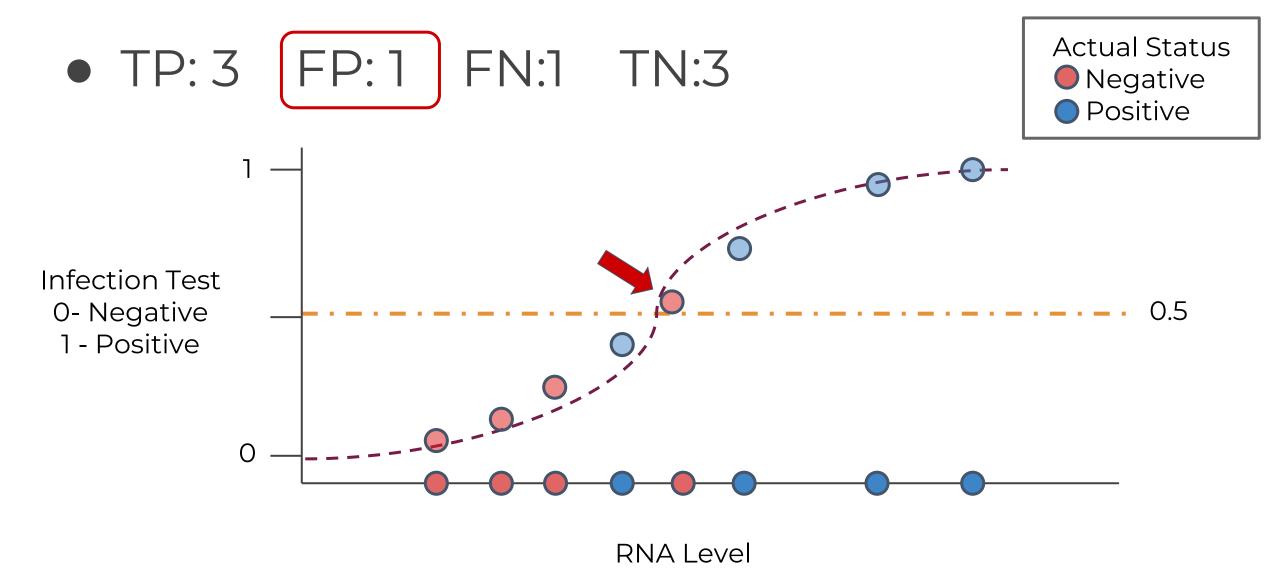
How many TP vs FP?

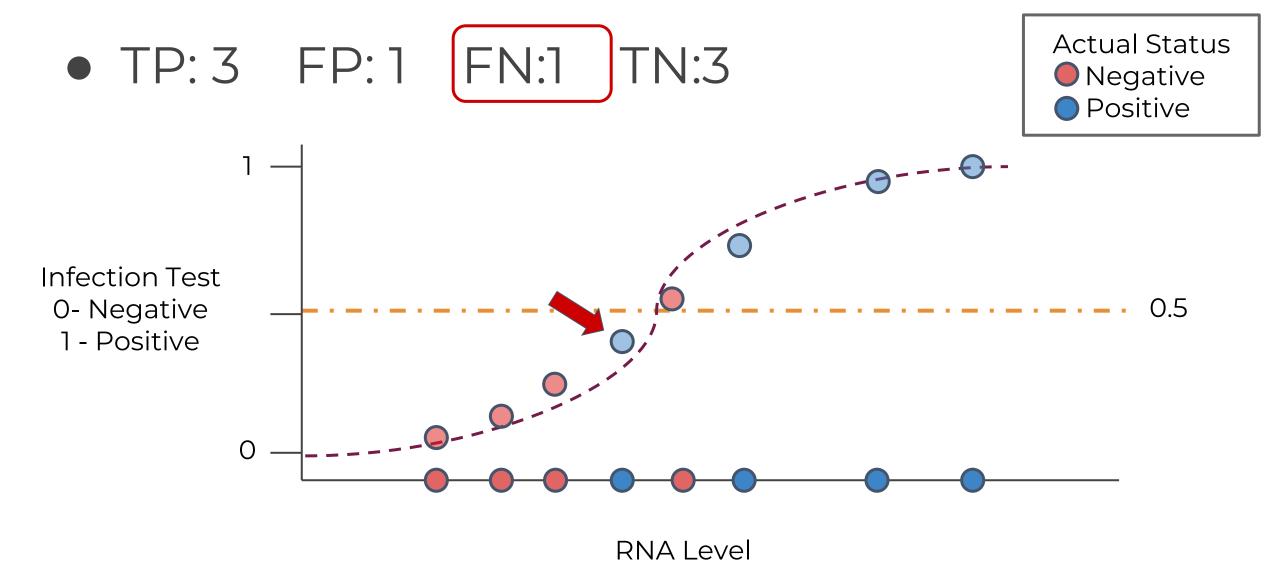




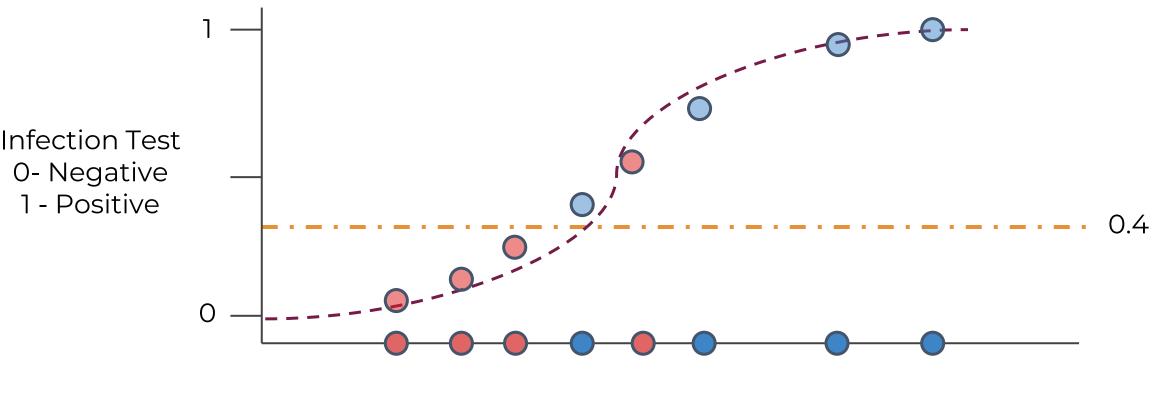


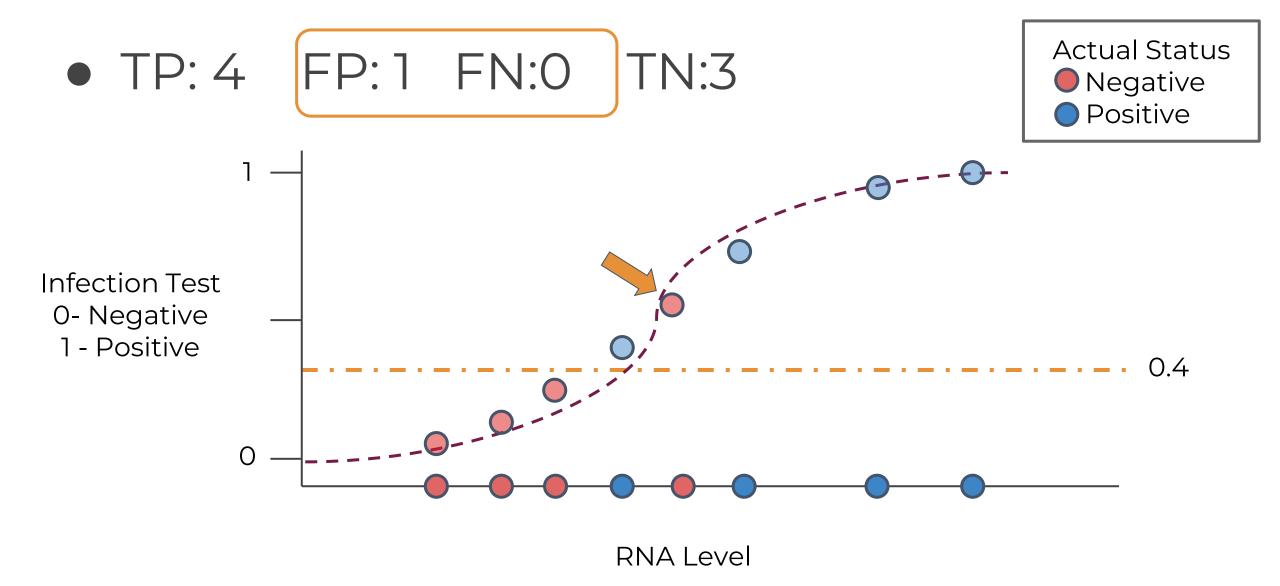






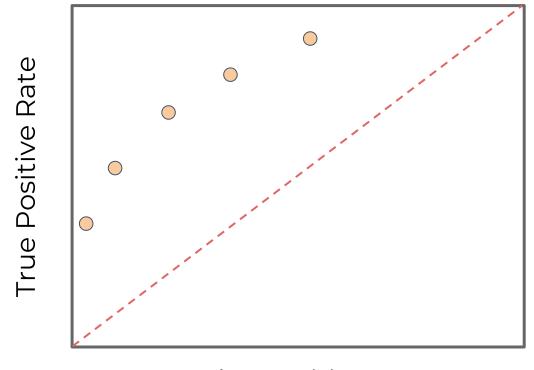
What if we lowered the cut-off?





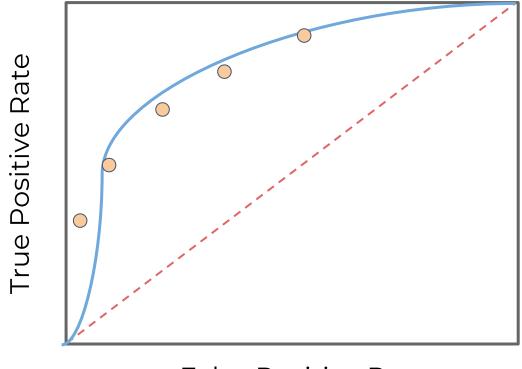
- In certain situations, we gladly accept more false positives to reduce false negatives.
- Imagine a dangerous virus test, we would much rather produce false positives and later do more stringent examination than accidentally release a false negative!

 Chart the True vs. False positives for various cut-offs for the ROC curve.



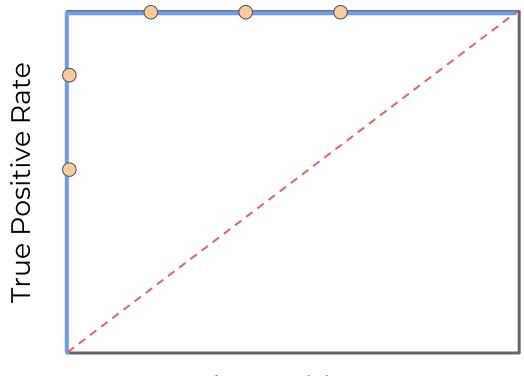
False Positive Rate

 By changing the cut-off limit, we can adjust our True vs. False Positives!



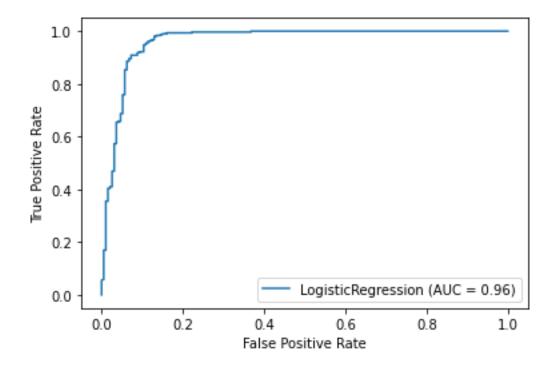
False Positive Rate

- A perfect model would have a zero FPR.
- Random guessing is the red line.

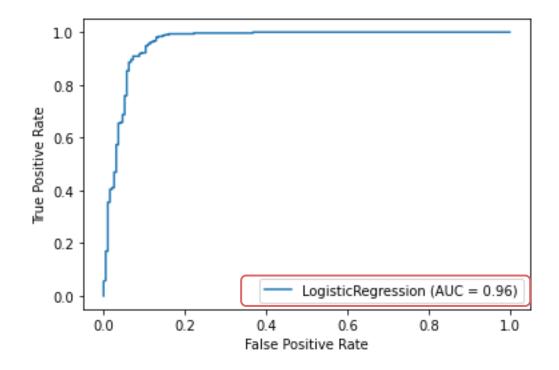


False Positive Rate

 Realistically with smaller data sets the ROC curves are not as smooth.



 AUC - Area Under the Curve, allows us to compare ROCs for different models.



Can also create precision vs. recall curves:

