PRINCIPLES OF MACHINE LEARNING
IN MEDICINE

Evaluation of Binary Classifiers

09/05/2022

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Docentship Demo Lecture

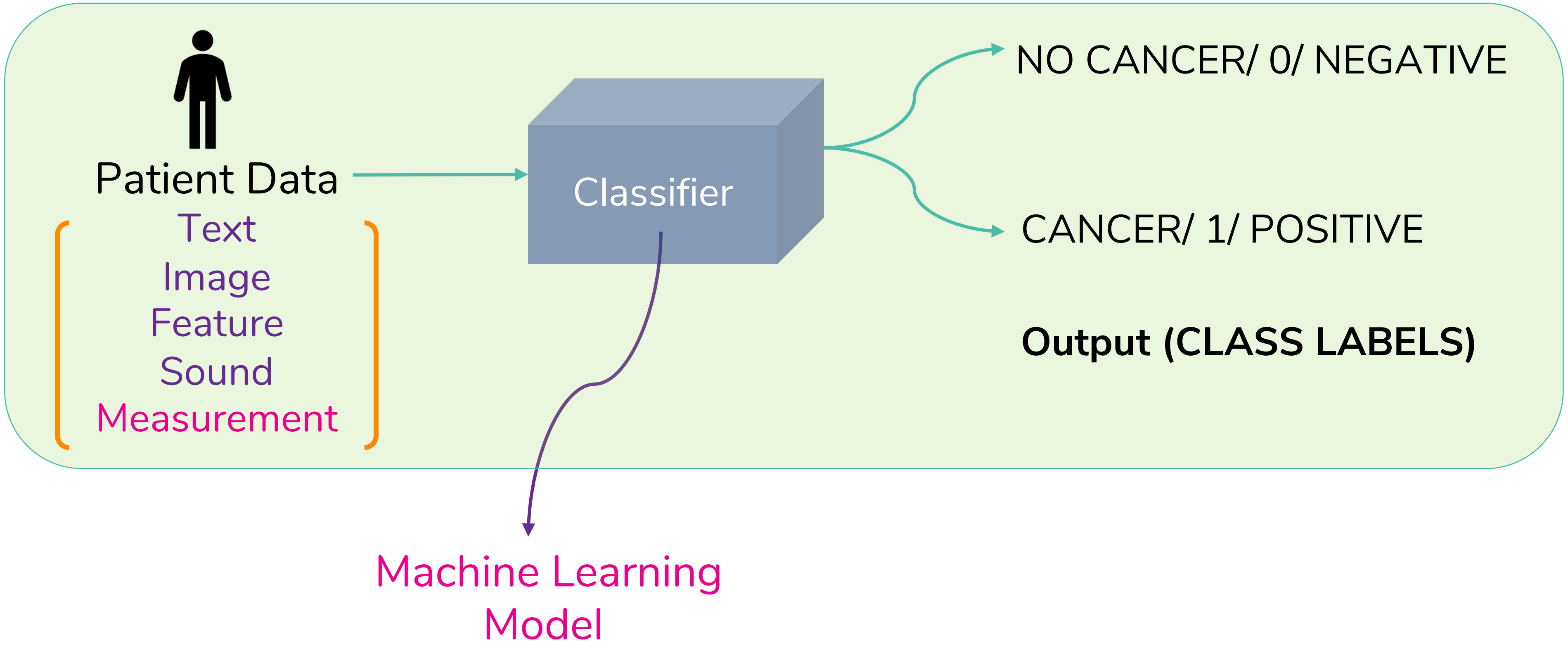
In this lecture

Overview of

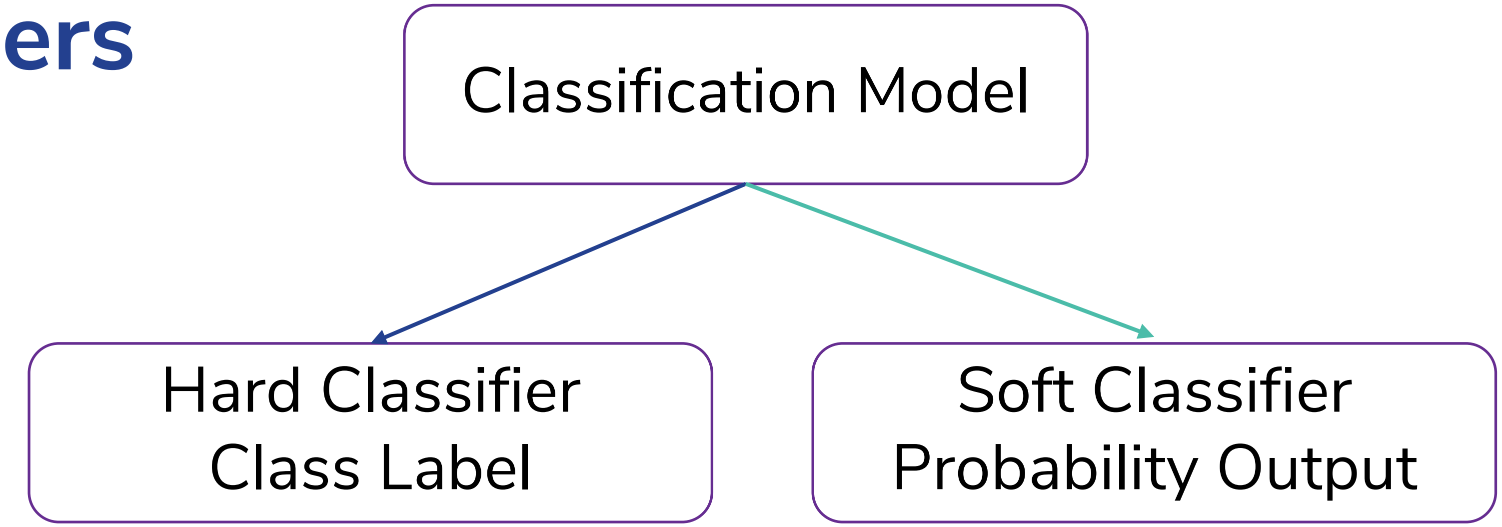
- **Binary classifiers**
  - Discrete vs probabilistic classifiers
- **Comparing different machine learning algorithms**
- **Performance metrics**
  - Accuracy
  - Confusion matrix
  - Balanced Accuracy
  - ROC AUC
  - Precision Recall AUC

Binary Classifiers

- classifying the data into two groups
- **a large number of medical studies are based on classification models**



Types of Binary Classifiers



e.g. for Binary classification
(class labels: 0, 1)

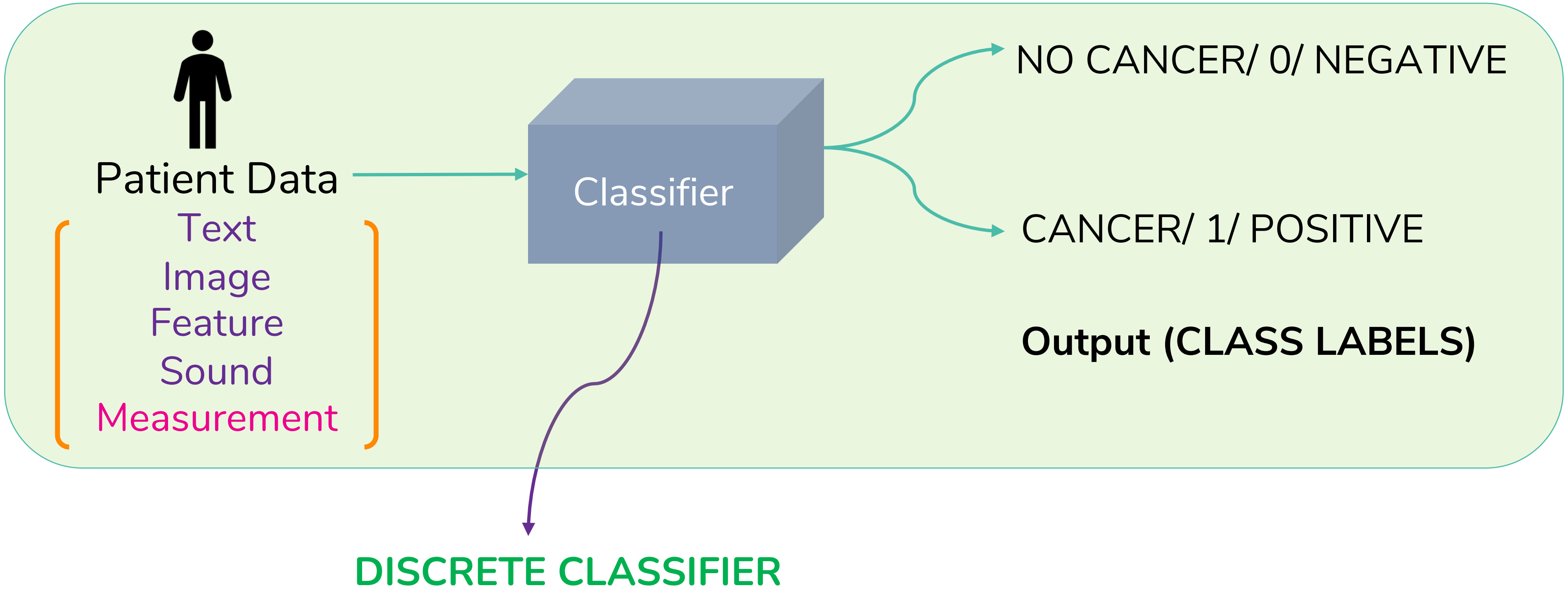
Output: 0 or 1

e.g. for Binary classification (class labels: 0,1)

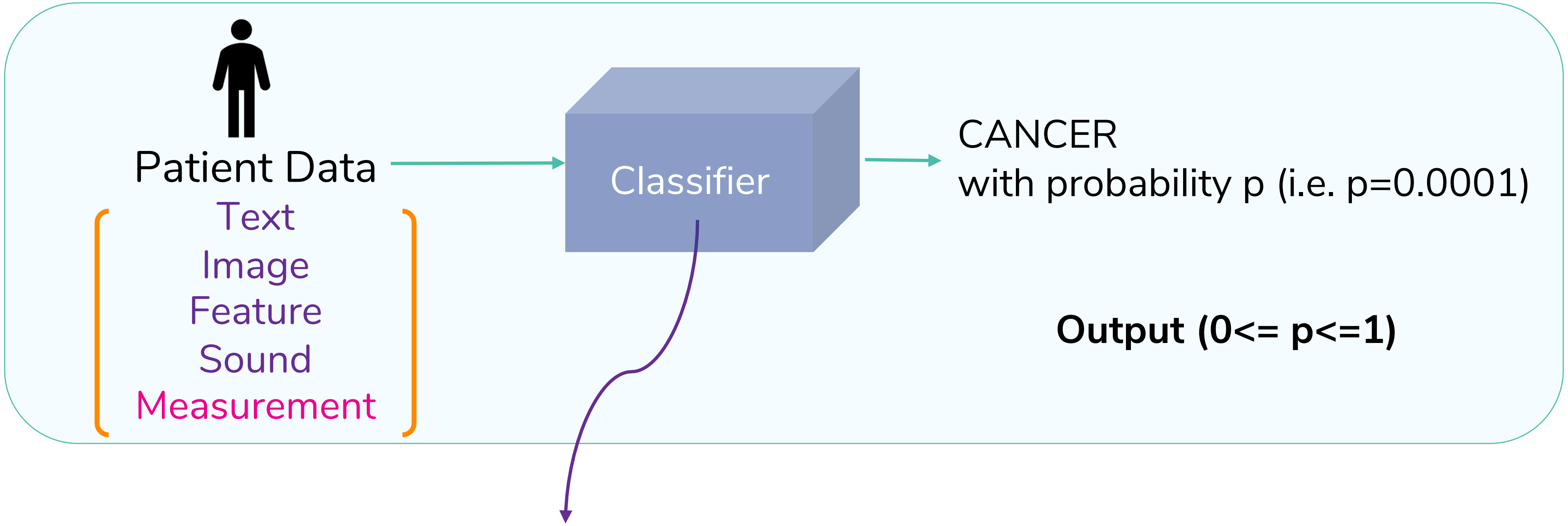
Output:
P(input=class 0)= p
P(input=class 1)= 1-p

Threshold the output to obtain hard decisions

Hard (Discrete) Classifier

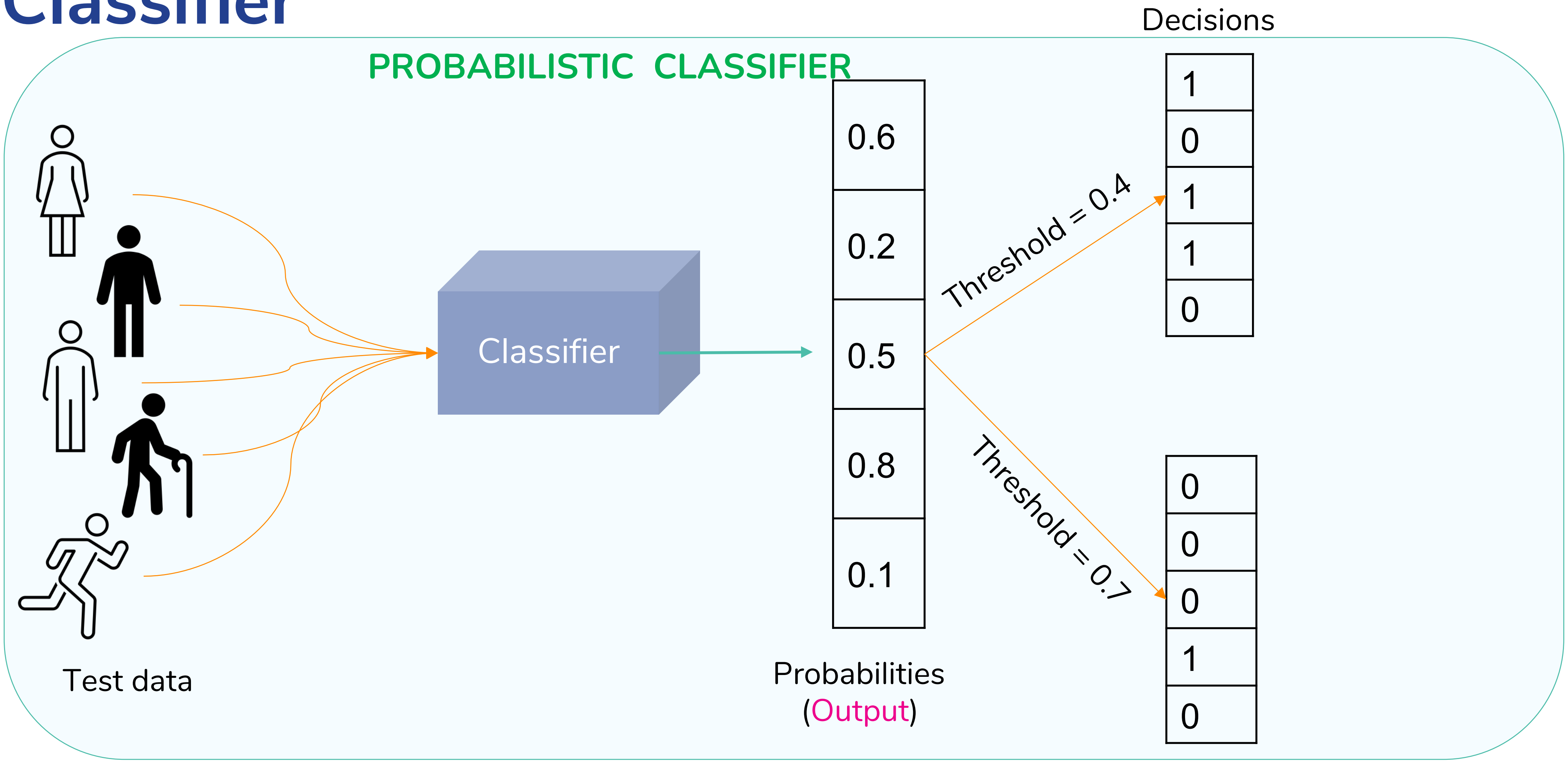


Soft (Probabilistic) Classifier

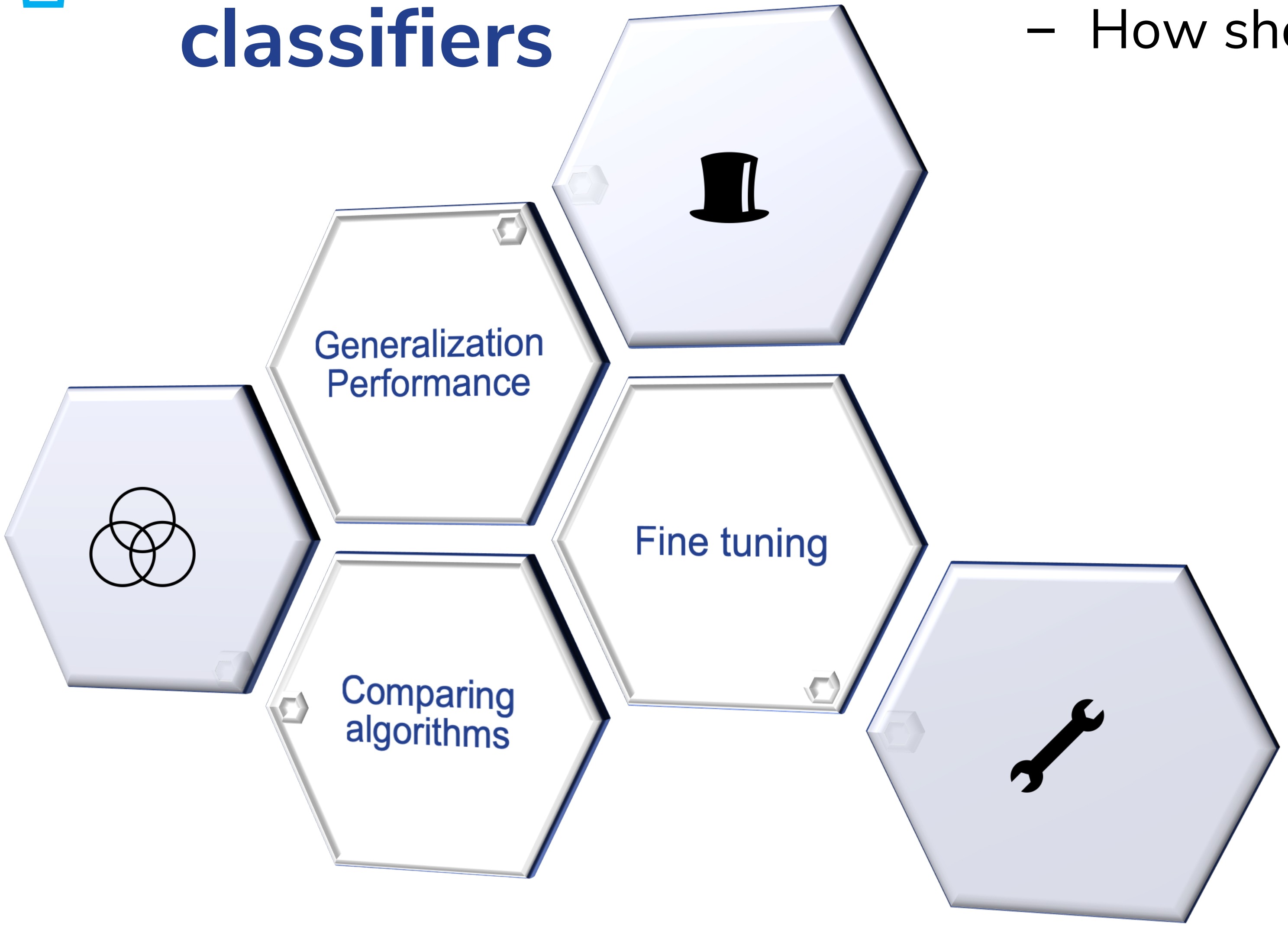


PROBABILISTIC CLASSIFIER

Soft (Probabilistic) Classifier



Performance of classifiers



- The most important task
- How should we evaluate

Performance Metrics

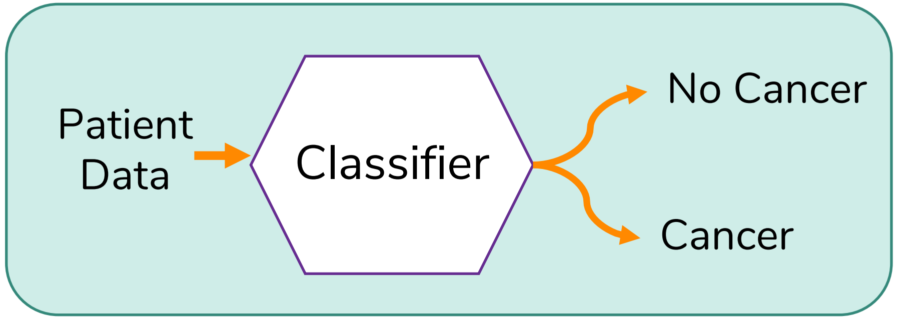
Compare predicted labels and true labels

OR

interpret the predicted probabilities

1. Confusion Martix
2. False positive rate | Type-I error
3. False negative rate | Type-II error
4. True negative rate | Specificity
5. Negative predictive value
6. False discovery rate
7. True positive rate | Recall | Sensitivity
8. Positive predictive value | Precision
9. Accuracy
10. F beta score
11. F1 score
12. F2 score
13. Cohen Kappa
14. Matthews correlation coefficient
15. ROC curve
16. ROC AUC score
17. Precision-Recall curve
18. PR AUC | Average precision
19. Log loss
20. Brier score
21. Cumulative gain chart
22. Lift curve | Lift chart
23. Kolmogorov-Smirnov plot
24. Kolmogorov Smirnov statistics
25. Balanced Accuracy

Confusion matrix



ACTUAL

If patient have cancer or not

PREDICTION *what our model predicted*

	have cancer	doesn't have cancer
have cancer	number of **TP**	number of **FP**
doesn't have cancer	number of **FN**	number of **TN**

True positive (TP
False positive (FP)- Type 1 error
True negative (TN)
False negative (FN) – Type2 error

Image: https://www.analyticsvidhya.com/blog/2020/10/confusion-matrix-is-no-more-a-confusion/

Accuracy

		ACTUAL If patient have cancer or not	
		have cancer	doesn't have cancer
PREDICTION what our model predicted	have cancer	number of **TP**	number of **FP**
	doesn't have cancer	number of **FN**	number of **TN**

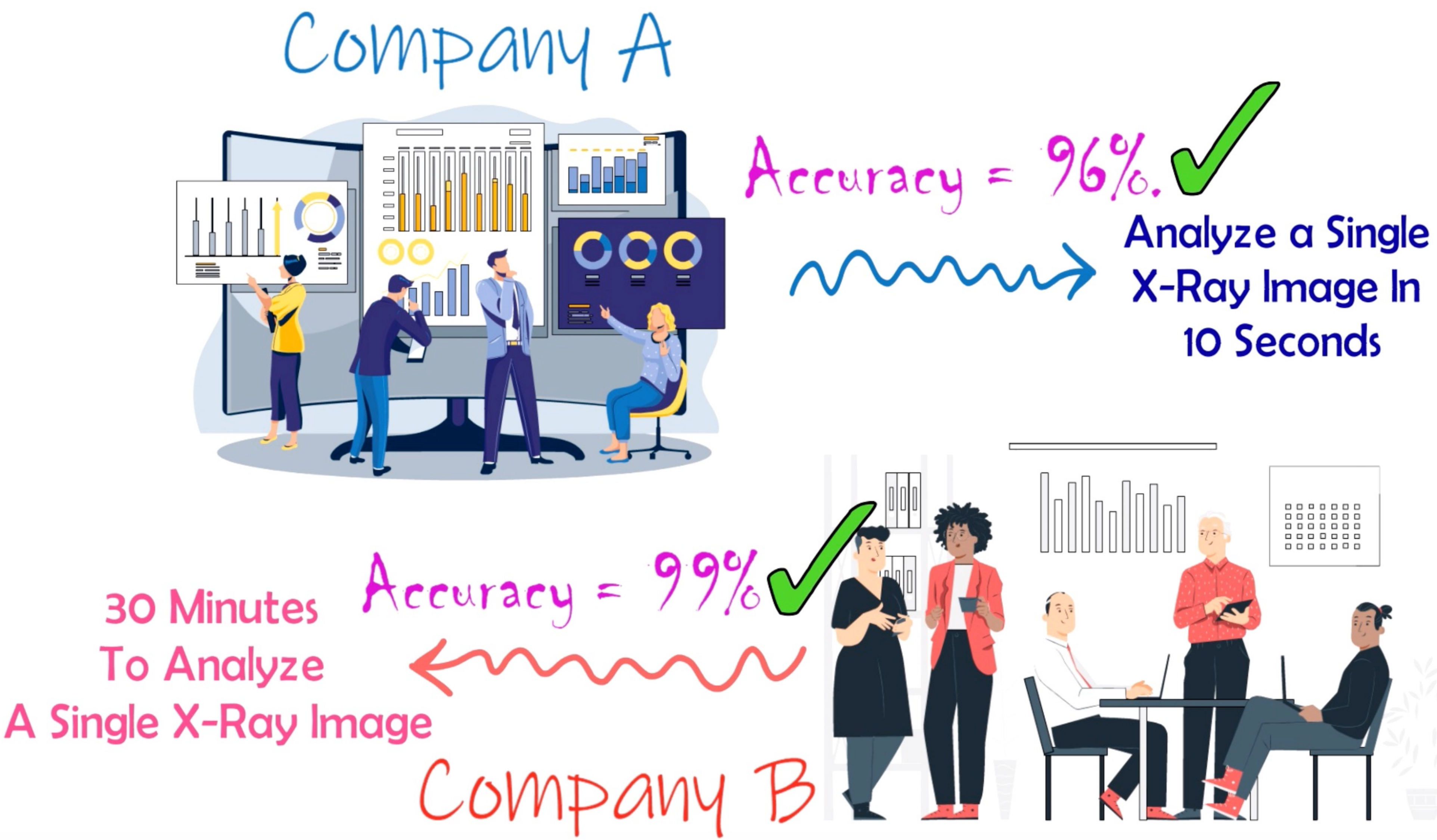
$$ACCURACY = \frac{Number\ of\ correct\ predictions}{Total\ number\ of\ predictions} = \frac{TP + TN}{TP + TN + FN + FP}$$

Image: https://www.analyticsvidhya.com/blog/2020/10/confusion-matrix-is-no-more-a-confusion/

Example

[Click for video]

What would you do?



Click for video

What would you do?

Company A

Accuracy = 96%.

Analyze a Single X-Ray Image In 10 Seconds

9 sec

~~30 Minutes~~

To Analyze A Single X-Ray Image

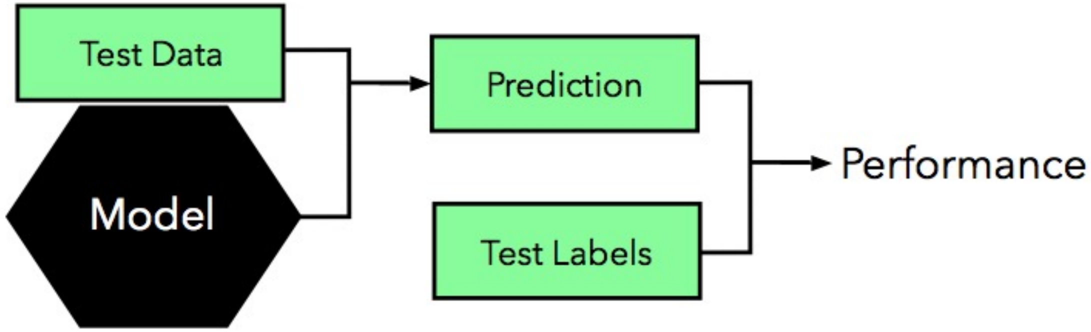
Accuracy = 99%

Company B

What should we do? – Should not decide yet

Image: https://www.123rf.com/

Fair Comparison



– **Use the same test set**

- Otherwise test would be biased

– **Collect a diverse and big data**

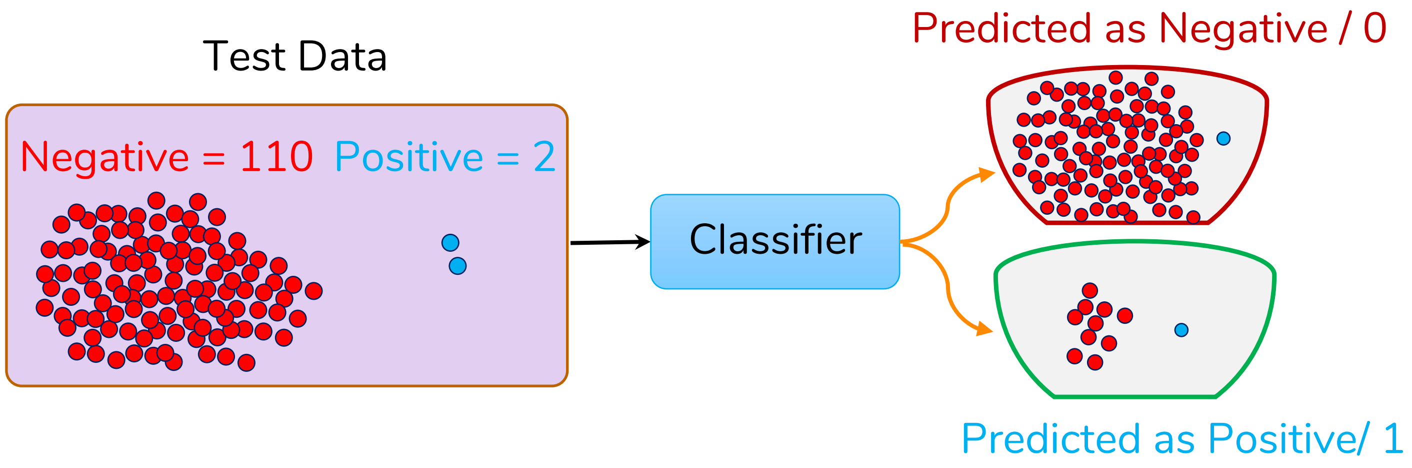
- Test data should be representative of the real life problem

– **Use other metrics than accuracy**

Image: https://sebastianraschka.com/

ACCURACY PARADOX

Test Data



Negative = No pneumonia
Positive = pneumonia

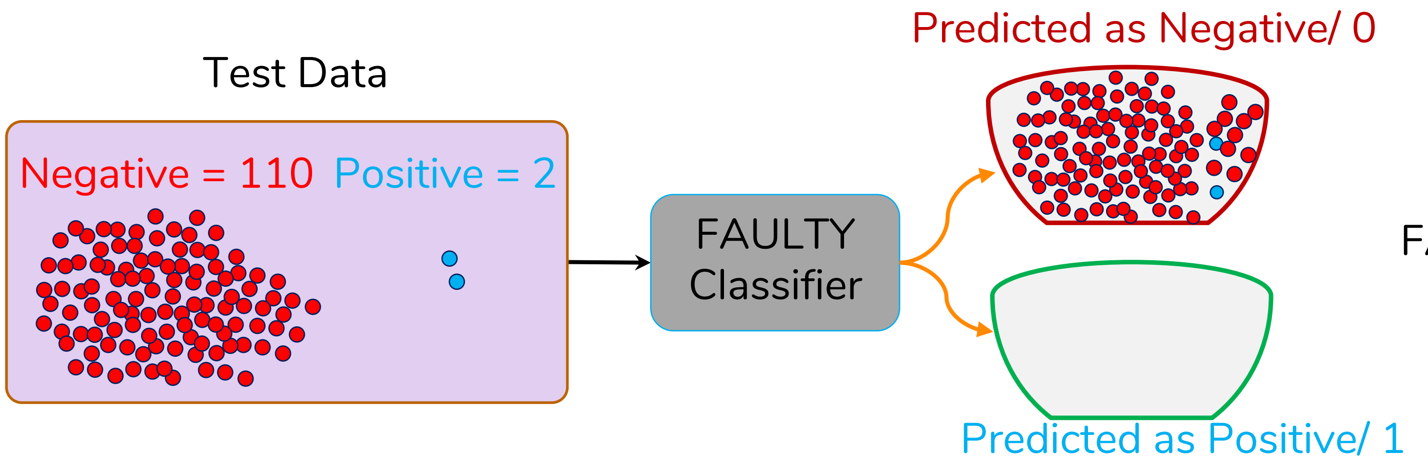
		Actual	
		Positive	Negative
Predicted	Positive	1	10
	Negative	1	100

Confusion Matrix

False Positive Rate	0.091
Accuracy	0.901

Recall/True Positive Rate (FP/N)	0.5
Precision (TP/(TP+FP))	0.091

ACCURACY PARADOX



FAULTY MODEL

Negative = No pneumonia
Positive = pneumonia

		Actual	
		Positive	Negative
Predicted	Positive	0	0
	Negative	2	110

Confusion Matrix

Accuracy= 110/112=0.98

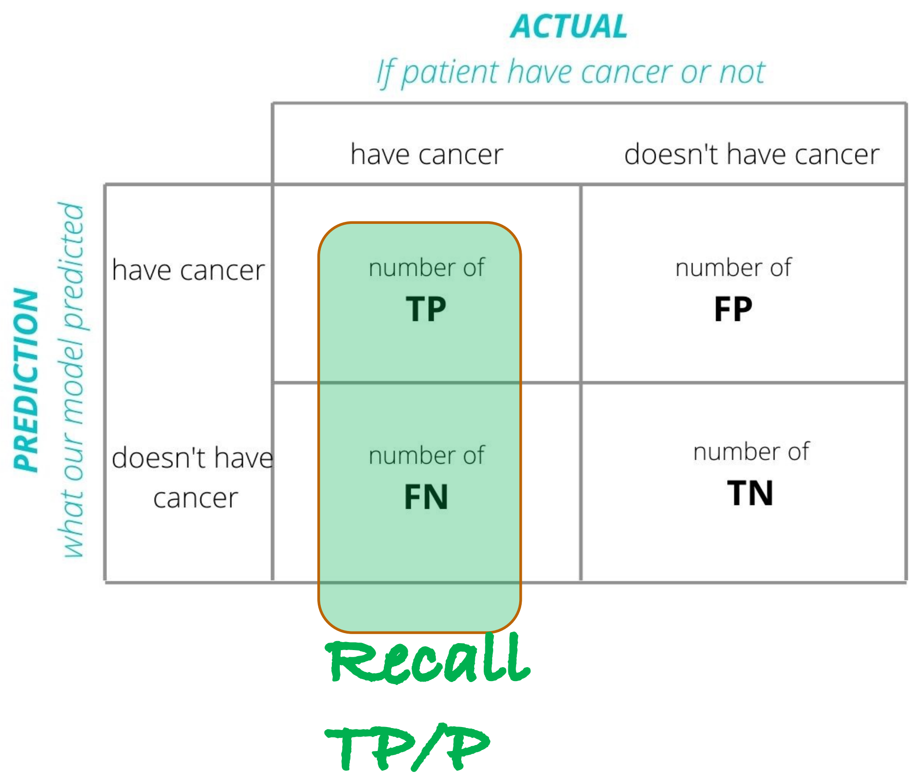
More Metrics Derived from Confusion Matrix

- Sensitivity (Recall or True positive rate)
- Specificity (True negative rate)
- False positive rate (FPR)
- Precision

- Recall – Specificity → Balanced Accuracy
- Recall – FPR → ROC AUC
- Precision –Recall → PR AUC

Recall & True Negative Rate

- Sensitivity (Recall or True positive rate)
- Specificity (True negative rate)



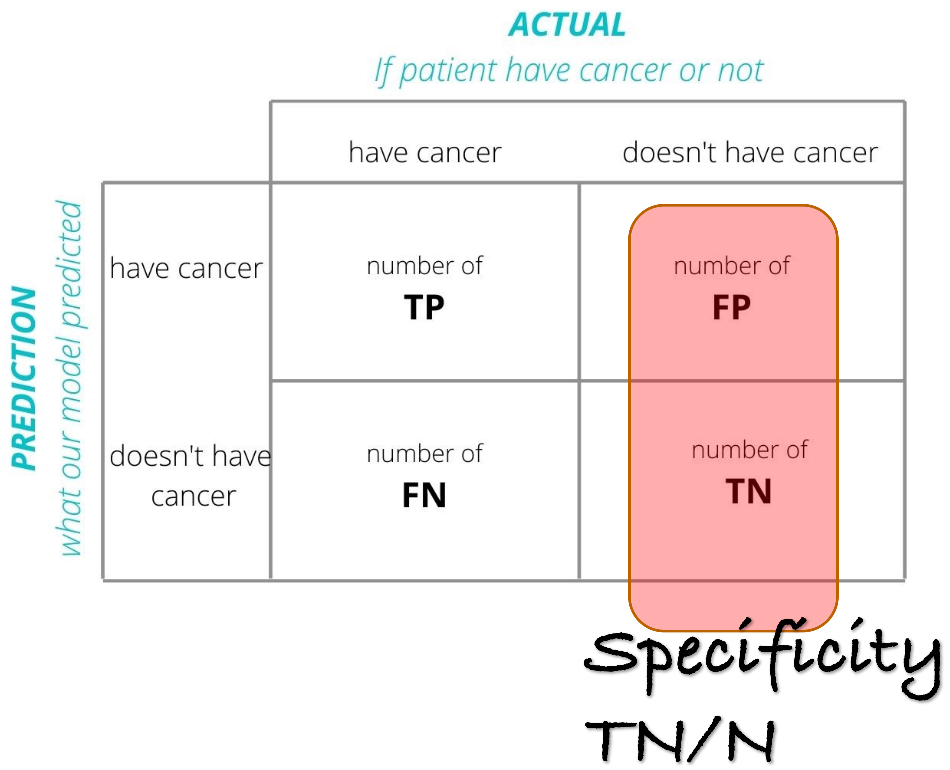


Image: https://www.analyticsvidhya.com/blog/2020/10/confusion-matrix-is-no-more-a-confusion/

False Positive Rate & Precision

ACTUAL
If patient have cancer or not

PREDICTION *what our model predicted*	have cancer	doesn't have cancer
have cancer	number of **TP**	number of **FP**
doesn't have cancer	number of **FN**	number of **TN**

False Positive Rate
FP/N

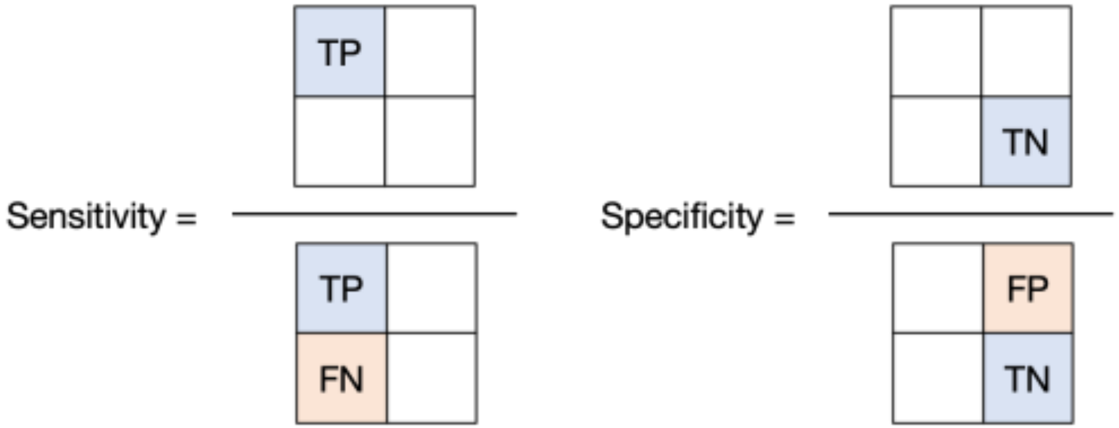
ACTUAL
If patient have cancer or not

PREDICTION *what our model predicted*	have cancer	doesn't have cancer
have cancer	number of **TP**	number of **FP**
doesn't have cancer	number of **FN**	number of **TN**

Precision
TP/(TP+FP)

Image: Wikipedia
Image: https://www.analyticsvidhya.com/blog/2020/10/confusion-matrix-is-no-more-a-confusion/

Balanced accuracy



$$Balanced\ accuracy = \frac{Sensitivity + Specificity}{2}$$

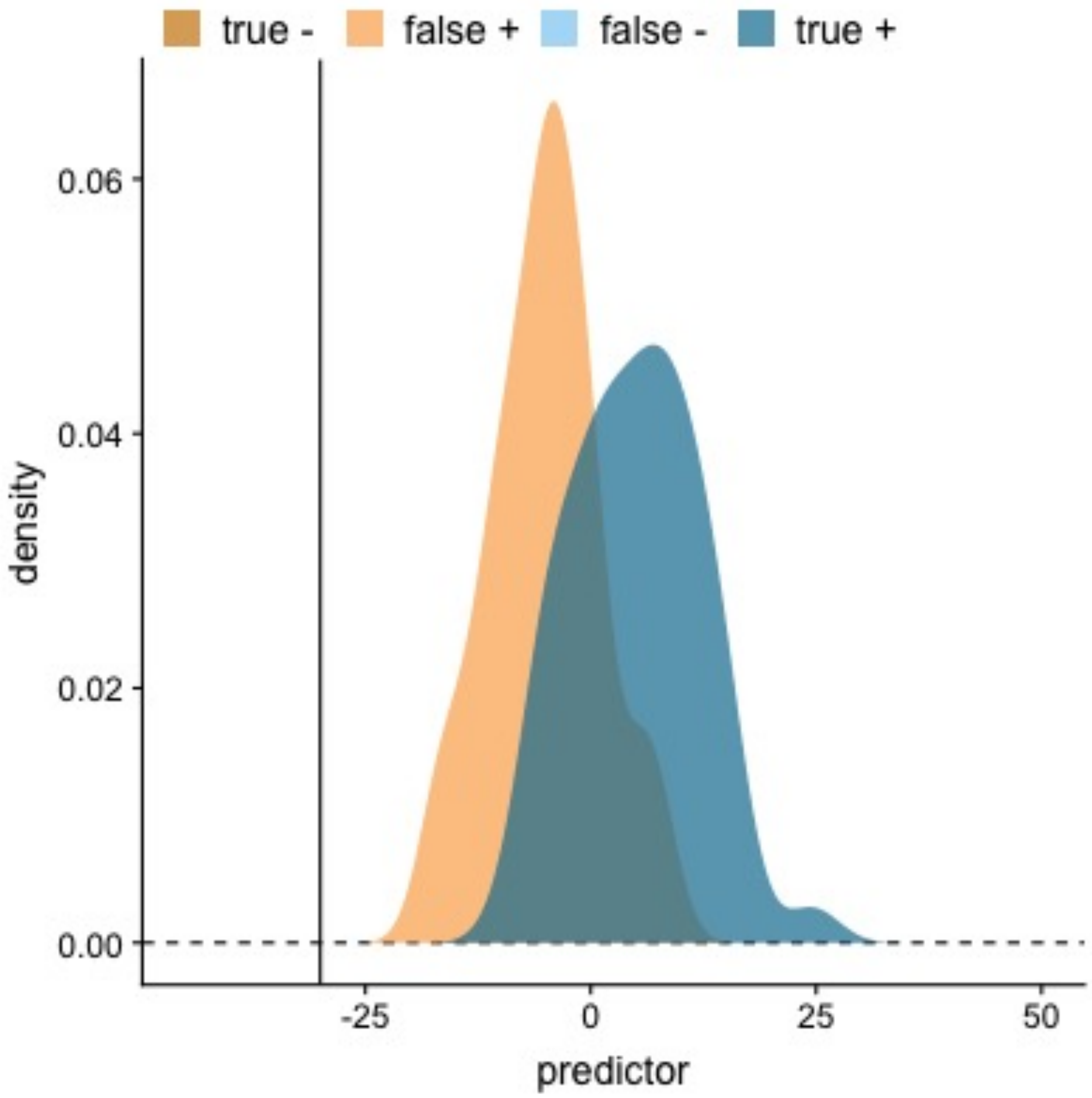
		Actual	
		Positive	Negative
Predicted	Positive	1	10
	Negative	1	100

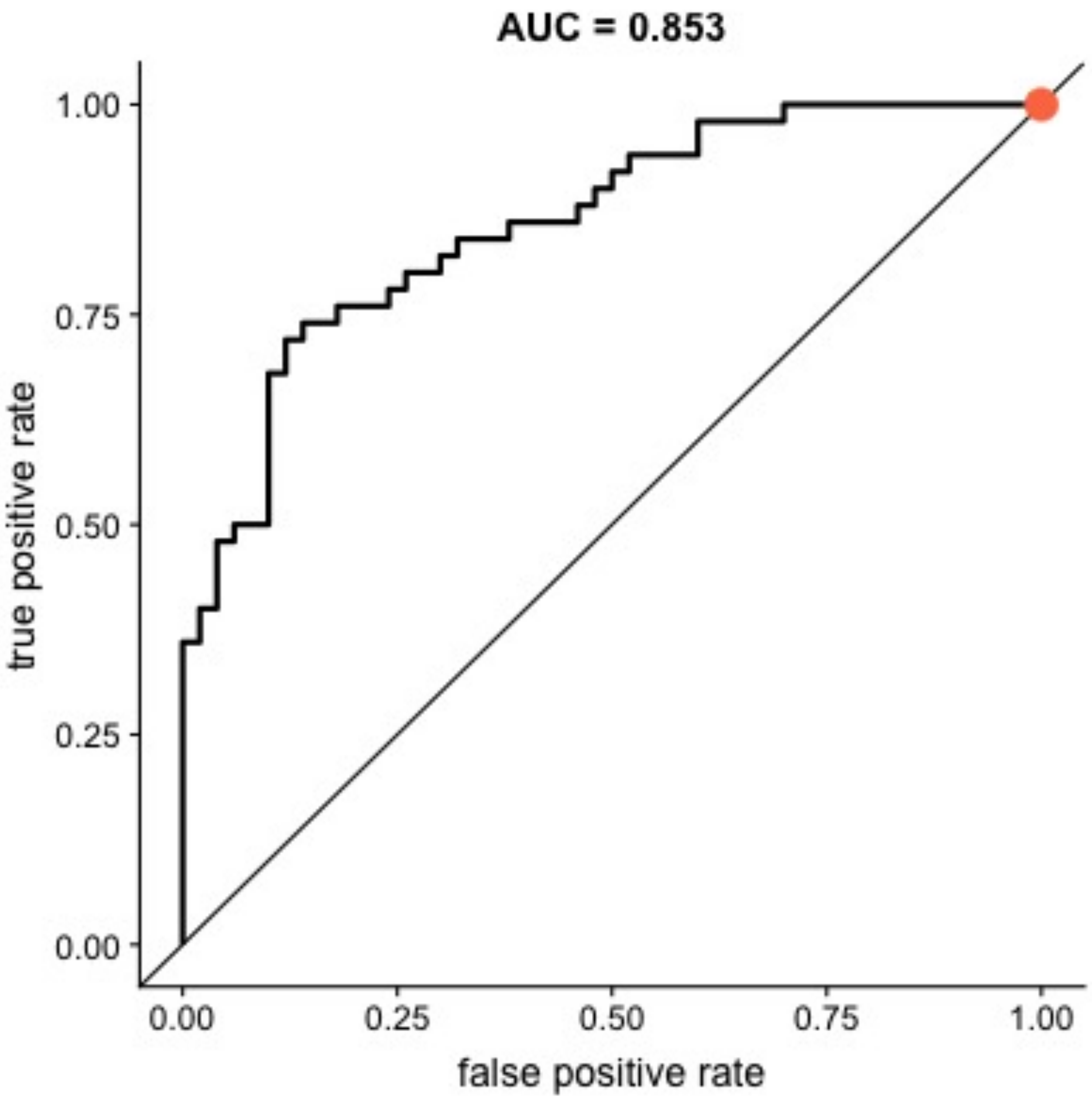
Recall/True Positive Rate	0.5
False Positive Rate	0.091
Precision	0.091
Accuracy	0.901
Balanced Accuracy	**0.45**

https://statisticaloddsandends.wordpress.com/2020/01/23/what-is-balanced-accuracy/

ROC Curve –ROC-AUC

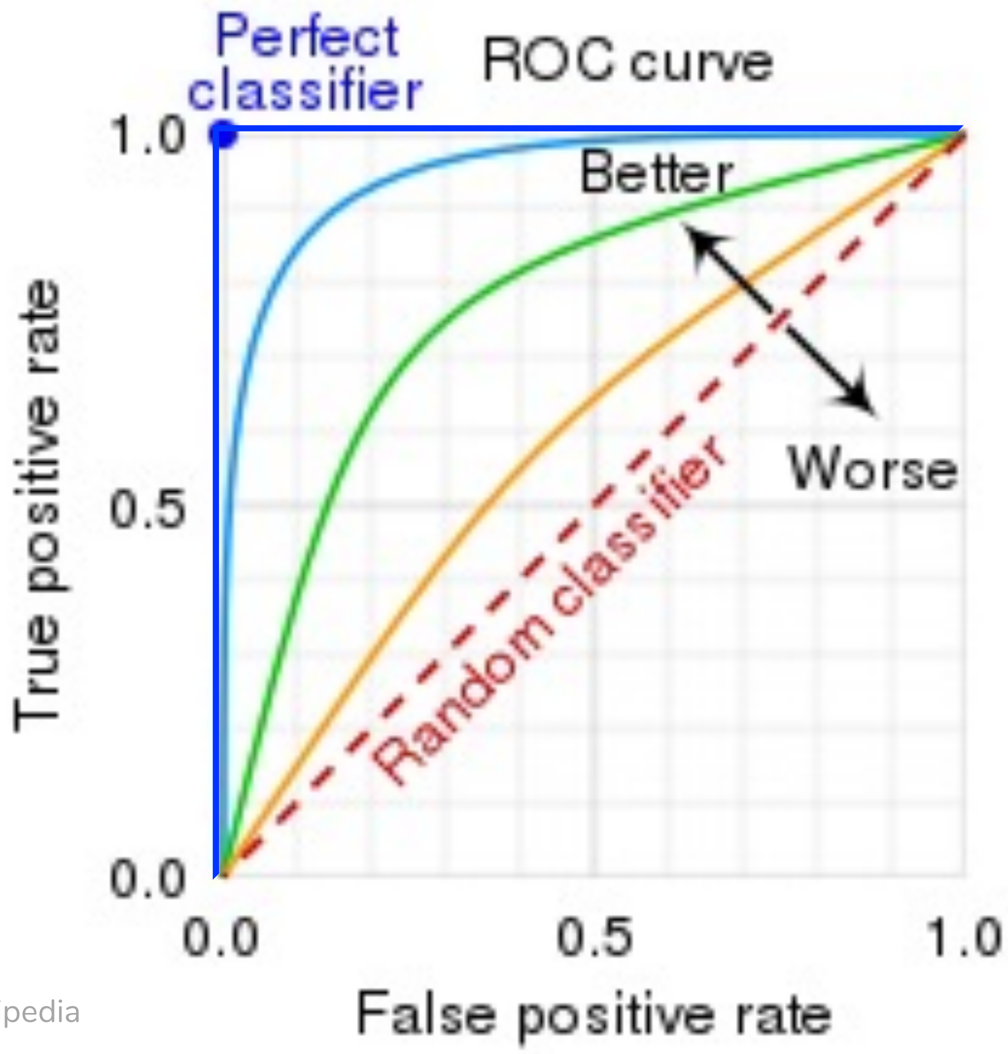
Receiver Operating Characteristic curve





https://github.com/dariyasydykova/open_projects

ROC Curves and ROC AUC



wikipedia

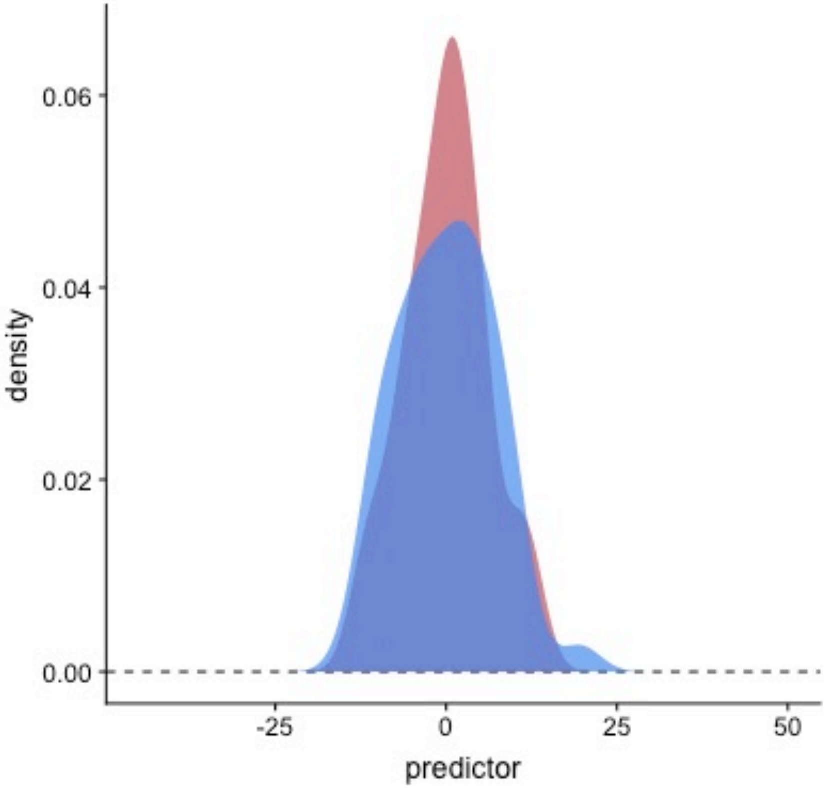
- A receiver operating characteristic curve, or **ROC curve**: Recall(TPR) vs FPR
- The **ROC-AUC** : Area under the ROC curve → summarizes classifier performance
- **ROC-AUC=0.5 → random classifier**
- **ROC-AUC= 1.0 → perfect classifier**
- More informative than accuracy for imbalanced data
- **Excessively optimistic for highly imbalanced set**

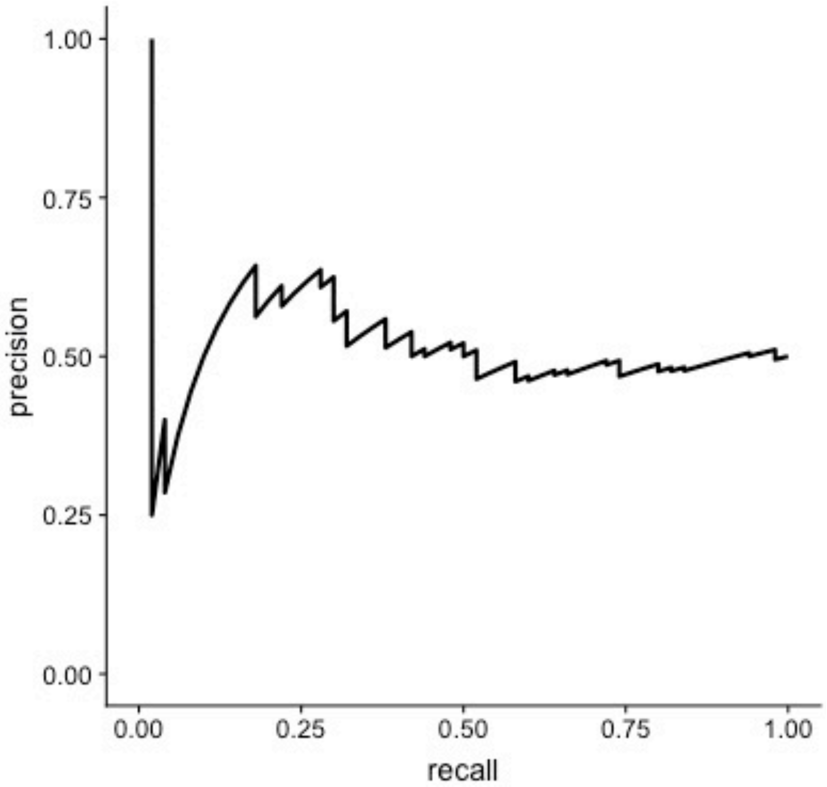
(# of negative samples)>>(# of positive samples)

Precision-Recall(PR) Curve and Area Under PR Curve

- For soft-classifiers
- Precision vs Recall

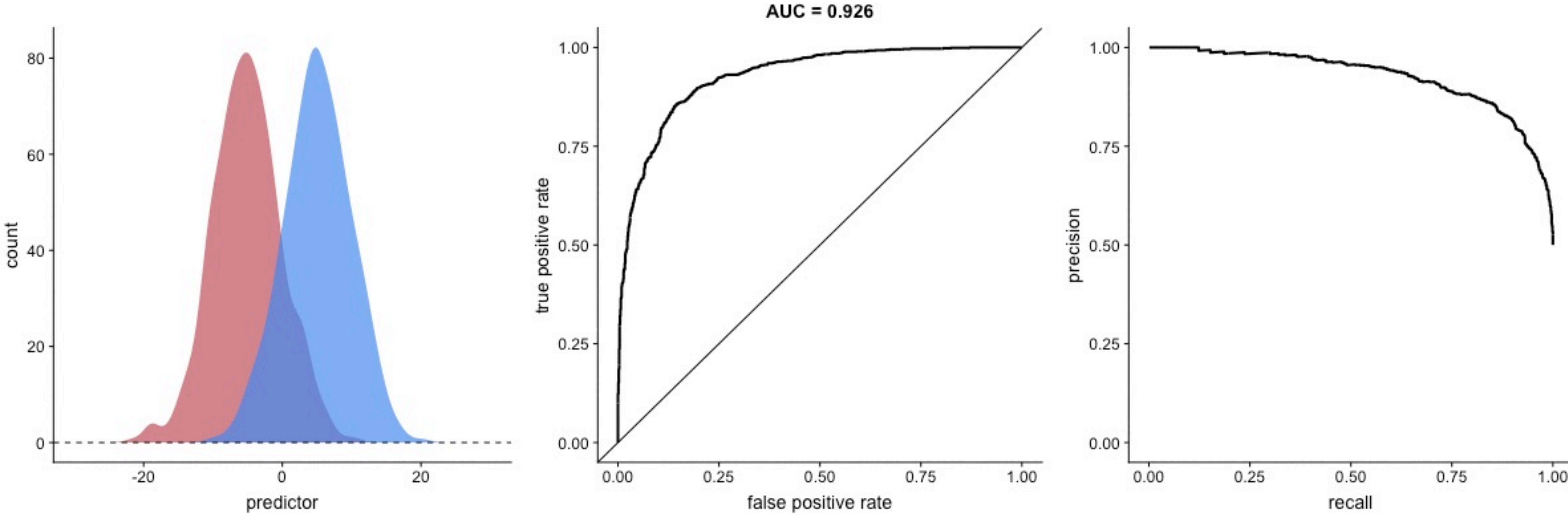
- Area Under the Precision-Recall Curve: summarizes the PR Curve (AP: Average Precison, AUCPR, AUPRC)





ROC vs PR Curve

- When data is imbalanced, the ROC-AUC might not reflect the true performance of the classifier
- PR AUC would be the metric to use if the focus of the model is to identify correctly as many positive samples as possible.



https://github.com/dariyasydykova/open_projects

Summary

– Fair comparison

- Use same test data

– Metrics

- Accuracy (might be misleading)
- Balanced Accuracy
- ROC-AUC (if both classes are equally important)
- PR-AUC (if focusing to identify positive samples)

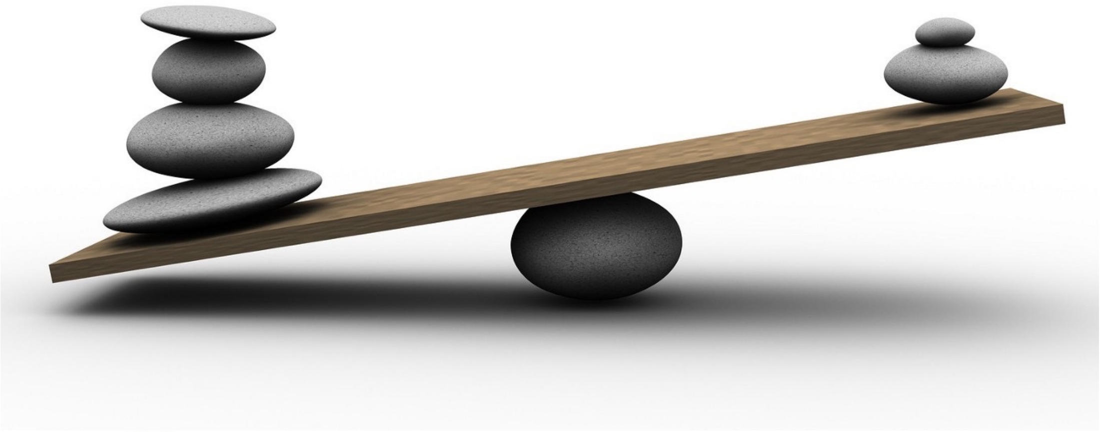


Image: https://towardsdatascience.com/having-an-imbalanced-dataset-here-is-how-you-can-solve-it -1640568947eb

Evaluation of Binary Classifiers

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09/05/2022

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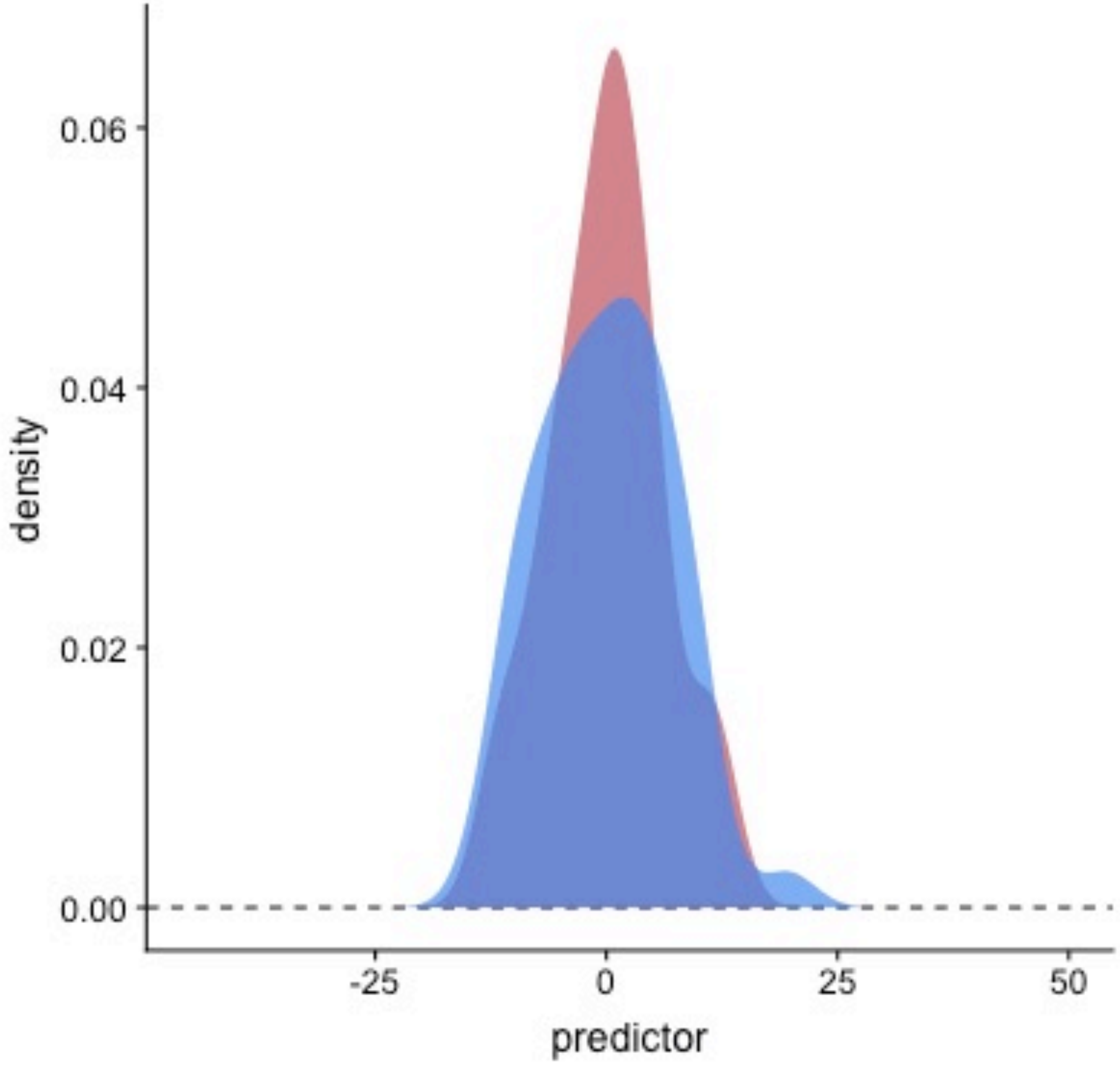
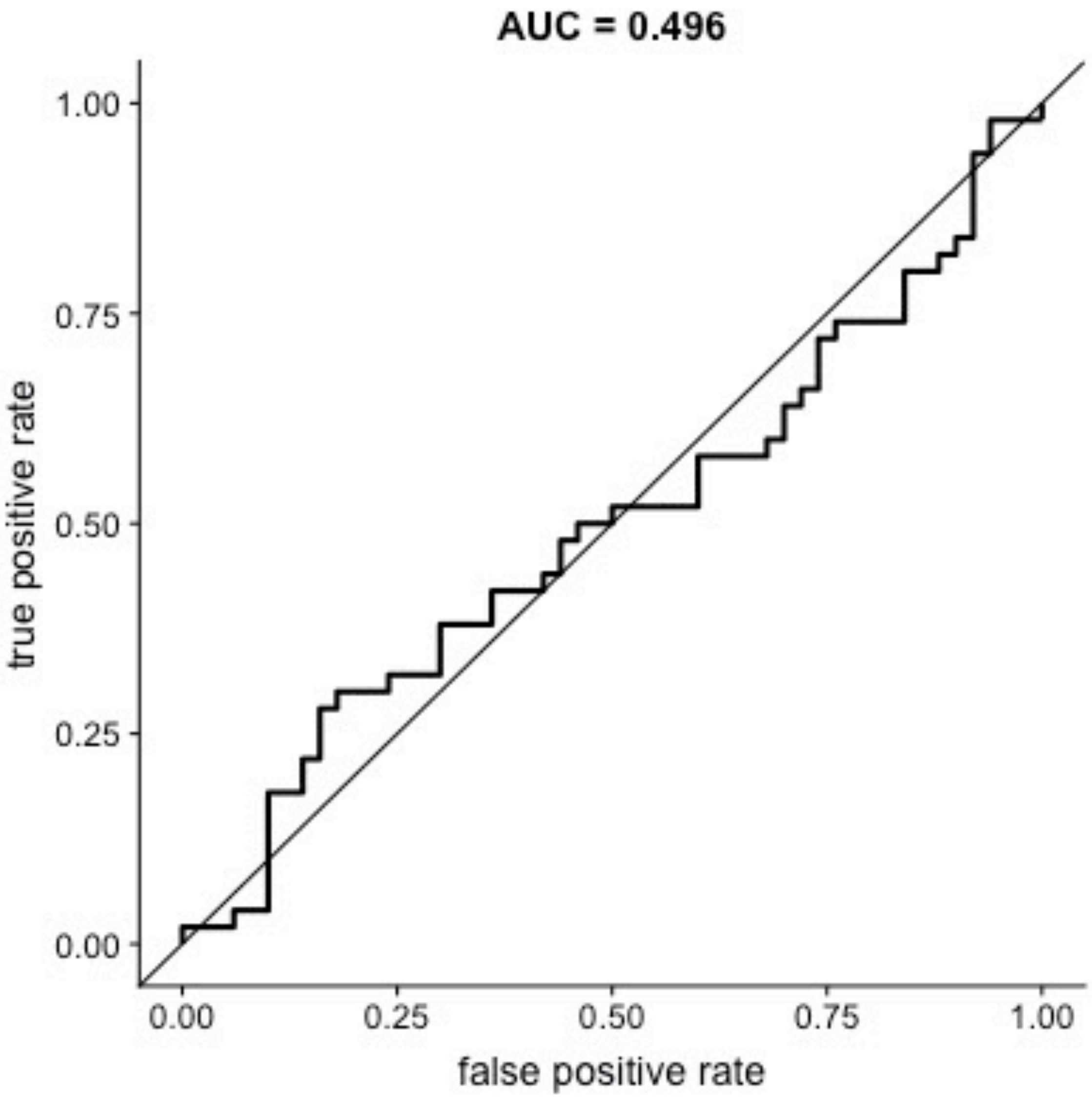
https://www.neslihan.ai/demo/lecture.pdf

ROC Curve –ROC-AUC





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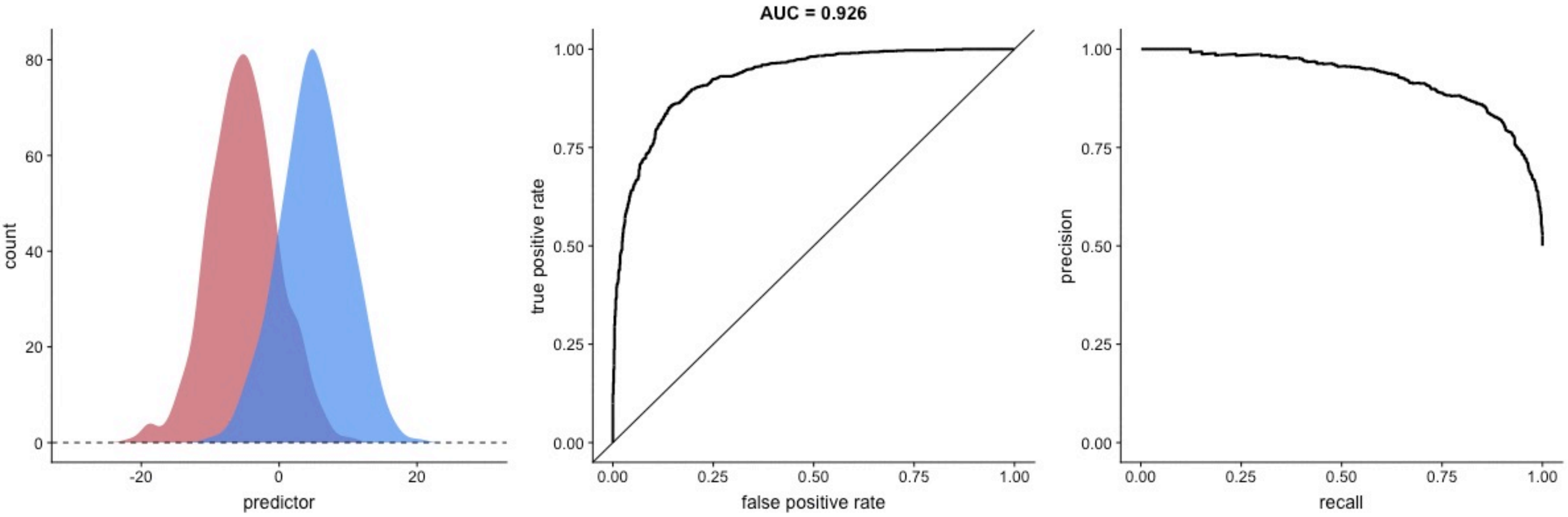
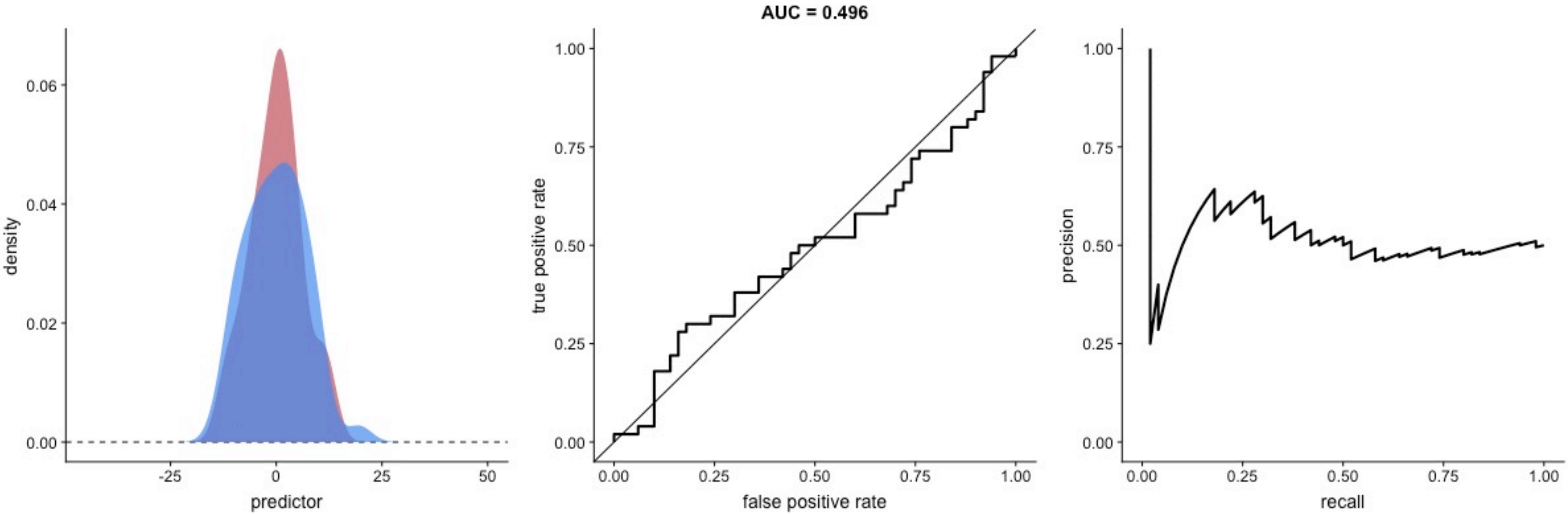
ROC vs PR



count
80
60
40
20
0
-20
0
20
predictor
AUC = 0.926
true positive rate
1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
false positive rate
precision
1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
recall

ROC vs PR


AUC = 0.496
density
0.06
0.04
0.02
0.00
-25
0
25
50
predictor
true positive rate
1.00
0.75
0.50
0.25
0.00
false positive rate
precision
recall

Binary Classifiers

- classifying the data into two groups
- **a large number of medical studies are based on classification models**