

Big Data Computing

Master's Degree in Computer Science

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- We discussed 2 main methods to approach classification tasks:
 - Logistic Regression
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We need a robust evaluation framework to assess models performance

Evaluation Metrics for Machine Learning

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Evaluation Metrics for Machine Learning

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- There are different metrics for clustering, regression, classification, etc.
- Some metrics, such as precision-recall, may be useful for multiple tasks
- We have already talked about quality metrics for clustering and regression
- We now discuss performance metrics for **classification**

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- It is used when the output can be of two or more types of classes
- It is not a performance measure as such, but almost all of the performance metrics are based on it
- **Example:** binary classification task to predict whether a patient has cancer (class label=**1**) or not (class label=**0**)

Confusion Matrix: Example

		PREDICTED	
		POSITIVES (1)	NEGATIVES (0)
ACTUAL	POSITIVES (1)		
	NEGATIVES (0)		

Confusion Matrix: True Positives (TP)

		PREDICTED	
		POSITIVES (1)	NEGATIVES (0)
ACTUAL	POSITIVES (1)	TRUE POSITIVES (TP)	
	NEGATIVES (0)		

True Positives (TP)

The actual class of the data point is 1 (True) and the predicted is also 1 (True)

A patient actually has cancer (1) and the model predicts he has cancer (1)

Confusion Matrix: True Negatives (TN)

		PREDICTED	
		POSITIVES (1)	NEGATIVES (0)
ACTUAL	POSITIVES (1)		
	NEGATIVES (0)		TRUE NEGATIVES (TN)

True Negatives (TN)

The actual class of the data point is **0** (False) and the predicted is also **0** (False)

A patient has NO cancer (**0**) and the model predicts he has NO cancer (**0**)

Confusion Matrix: False Positives (FP)

		PREDICTED	
		POSITIVES (1)	NEGATIVES (0)
ACTUAL	POSITIVES (1)		
	NEGATIVES (0)	FALSE POSITIVES (FP)	

False Positives (FP)

The actual class of the data point is **0** (False) and the predicted is **1** (True)

A patient has NO cancer (**0**) and yet the model diagnosed him with cancer (**1**)

Confusion Matrix: False Negatives (FN)

		PREDICTED	
		POSITIVES (1)	NEGATIVES (0)
ACTUAL	POSITIVES (1)		FALSE NEGATIVES (FN)
	NEGATIVES (0)		

False Negatives (FN)

The actual class of the data point is **1** (True) and the predicted is **0** (False)

A patient actually has cancer (**1**) and yet the model predicts he has NO cancer (**0**)

Confusion Matrix: Example

		PREDICTED	
		POSITIVES (1)	NEGATIVES (0)
ACTUAL	POSITIVES (1)	TRUE POSITIVES (TP)	FALSE NEGATIVES (FN)
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- We might want to minimize either FP or FN

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Misclassifying an actual cancerous patient will be a much more severe and harmful mistake than the other way around!

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- Suppose the model classifies an important non-spam email as spam
- This is pretty worst than classifying a spam email as non-spam since in that case, we can still go ahead and manually delete it
- So, in this case minimizing FP is more important than minimizing FN

Accuracy

The number of **correct** predictions **over all** the predictions made

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$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

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- **Example:**
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 - 97% accuracy would indicate a very good performing model

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 - A trivial model which always predict the majority class (i.e., no cancer) will still classify 95 patients correctly
 - Even though the model is terrible at predicting cancer, its accuracy is 95%

Precision or Positive Predicted Value (PPV)

The number of correctly predicted positive instances over all the positive predictions made

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 - $TP = 5 \rightarrow \text{Precision} = 5/100 = \mathbf{5\%}$

Recall or Sensitivity or True Positive Rate (TPR)

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If the goal is to **minimize FN**, we want to **maximize Recall** (close to 1) without hurting Precision too much

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If the goal is to **minimize FN**, we want to **maximize Recall** (close to 1) without hurting Precision too much

If the goal is to **minimize FP**, we want to **maximize Precision** (close to 1) without hurting Recall too much

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- One way of doing this is through **Precision-Recall curve**
 - Plot of Recall (x) vs. Precision (y)
- Compute precision-recall pairs for different probability thresholds
 - Figure out the desired trade-off threshold from the plot

Specificity or True Negative Rate (TNR)

The number of correctly predicted negative instances over all the actually negative existing instances

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 - $TN + FP = 0 + 95 = 95$ (as the model only predicts the **positive** class label)

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 - $TN + FP = 0 + 95 = 95$ (as the model only predicts the **positive** class label)
 - $TN = 0 \rightarrow \text{Specificity} = 0/95 = 0\%$

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- **Example**: 100 credit card transactions of which 97 are legitimate and 3 fraudulent, and a classifier predicting everything as fraudulent

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		FRAUD (1)	LEGIT (0)
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$$\text{Avg} = \frac{\text{Precision} + \text{Recall}}{2} \approx 52\%$$

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Too "good" for such a bad model!

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 - Mitigate the impact of large outliers and aggravate the impact of small ones

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$$\text{F1-score}(P, R) = \frac{2PR}{P + R}$$

F1 Score

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$$\text{F1-score}(P, R) = \frac{2 * 3 * 100}{103} \approx 5.8\%$$

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- F1 Score is an **effective** evaluation metric in the following scenarios:
 - When both FP and FN errors are equally harmful
 - When TN is high

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- This may be acceptable whenever TN are sort of innumerable (e.g., in information retrieval)
- MCC is much **more informative** than F1 Score because it considers and balances all the 4 categories of the confusion matrix

$$\text{MCC} = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

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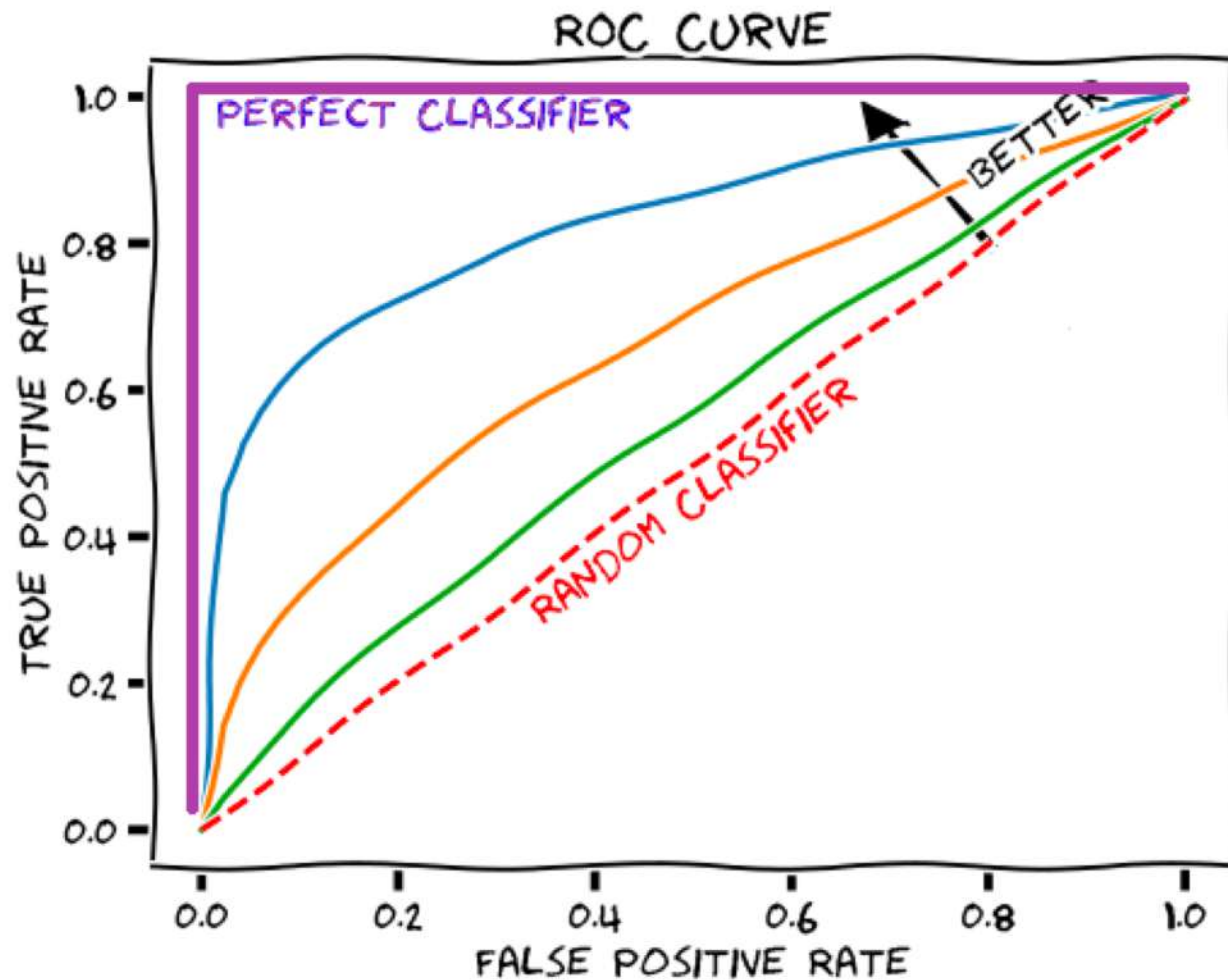
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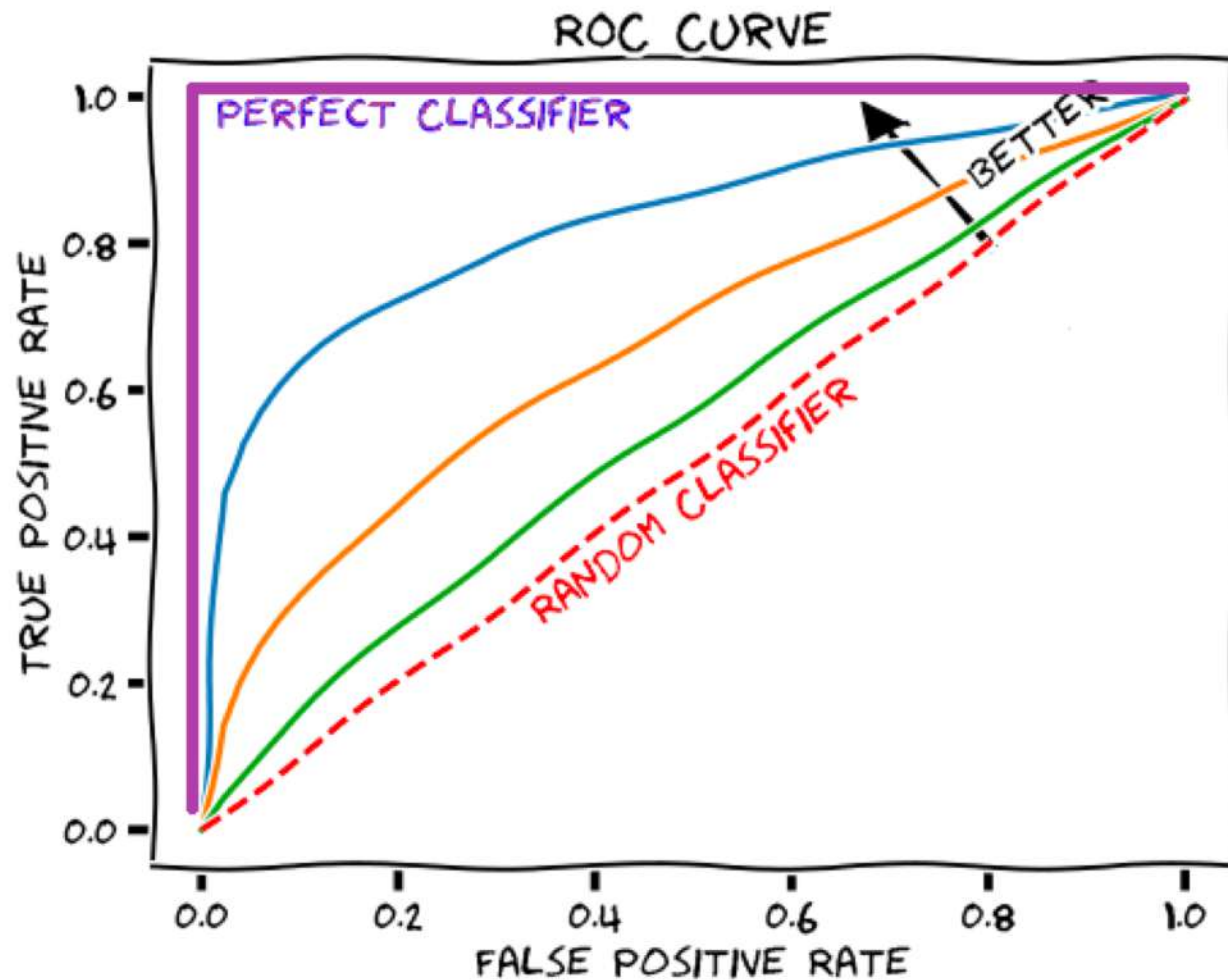
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- FPR is also known as Fall-Out (or 1-Specificity)

ROC Curve: Example



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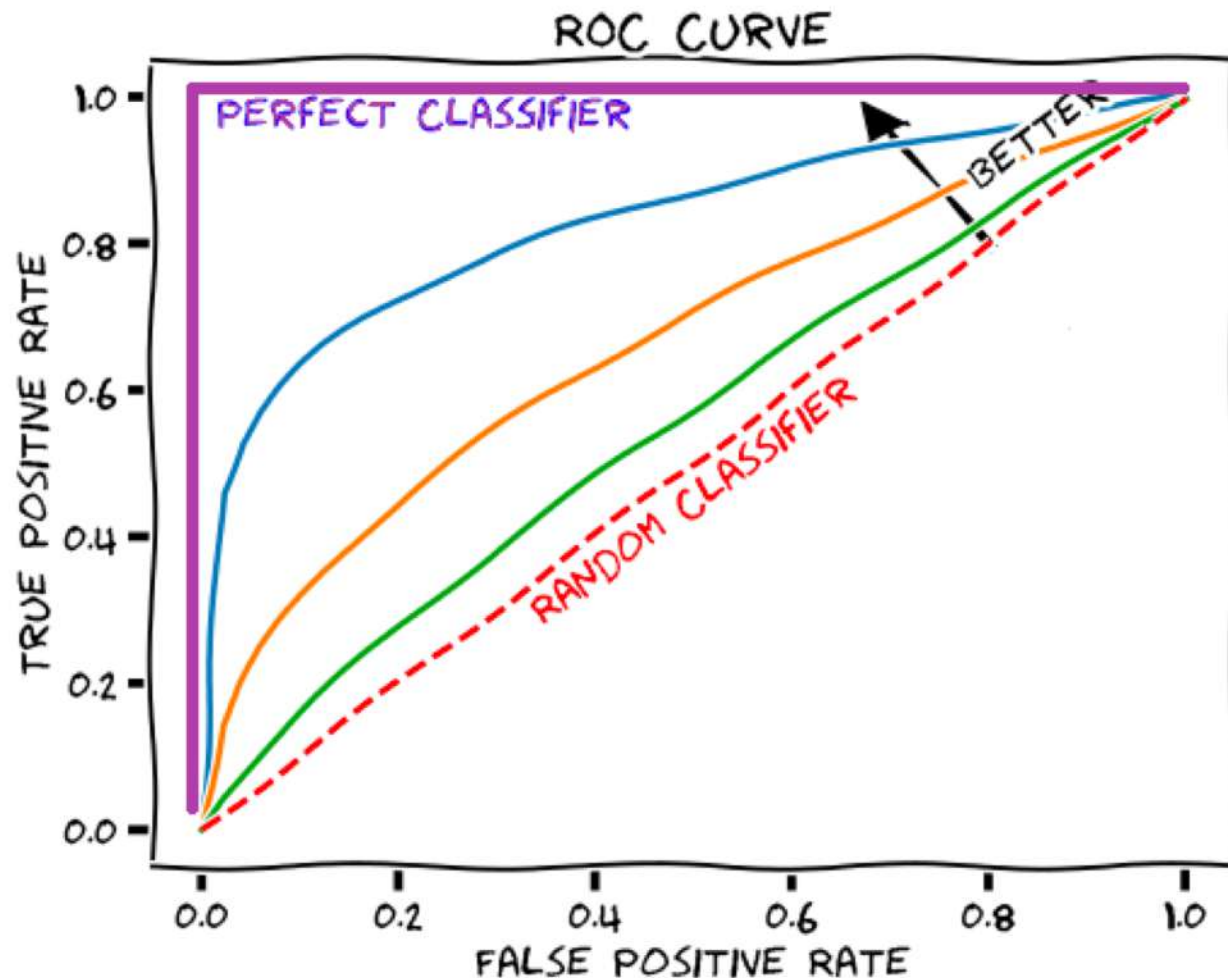
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No False Positives at all

ROC Curve: Example

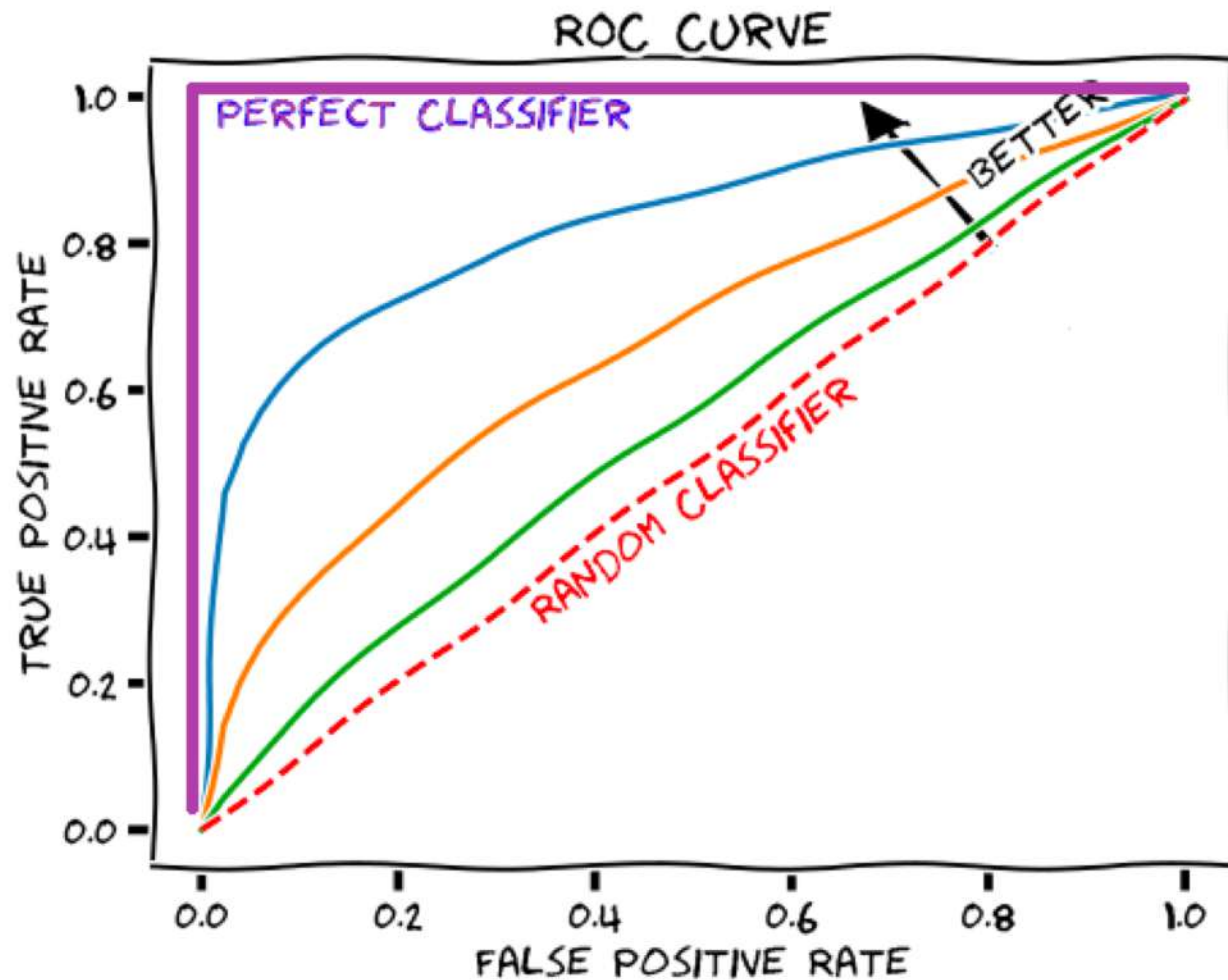


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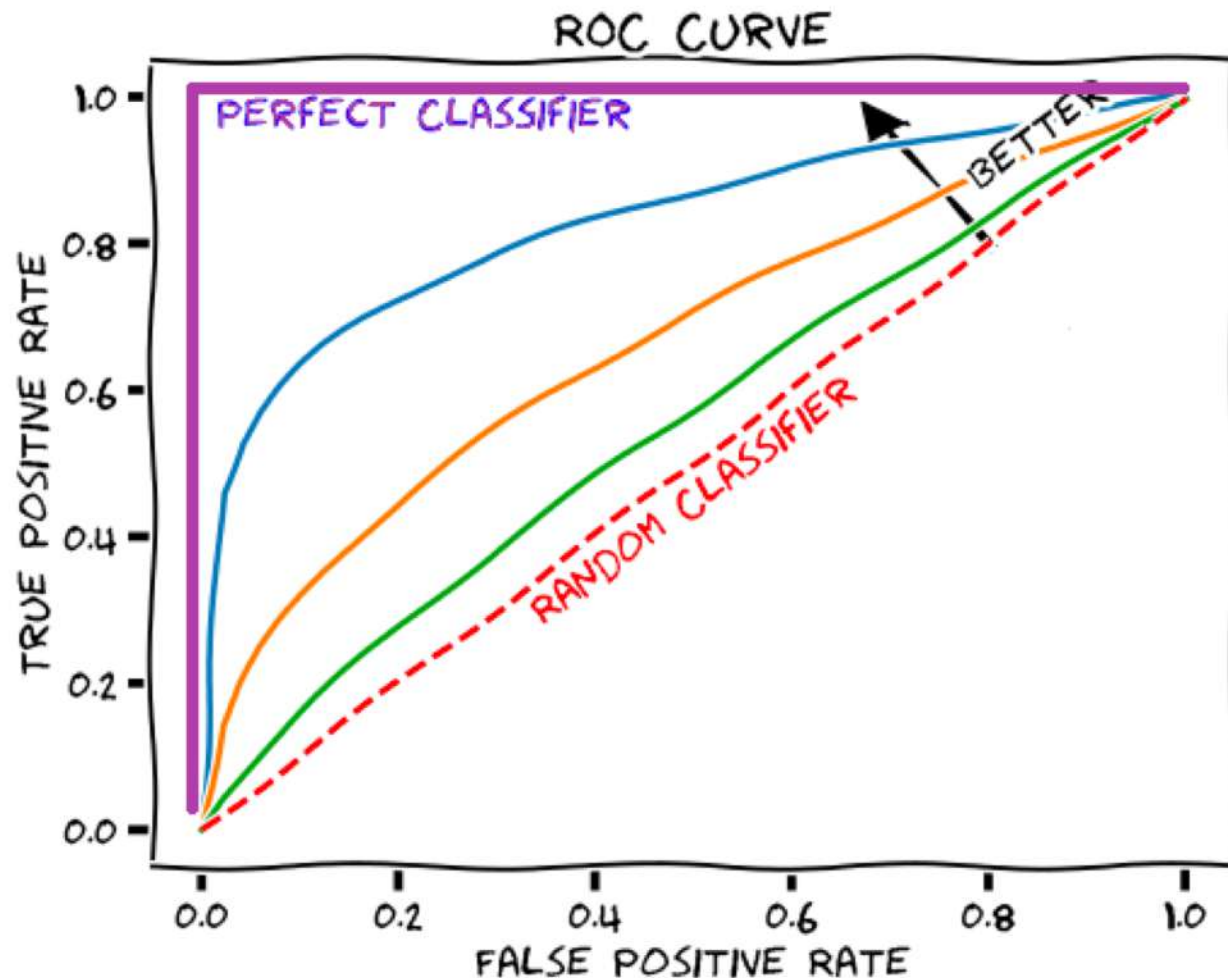
No True Positives either

ROC Curve: Example



(1, 1) represents a classifier which **always** predicts the **positive** class

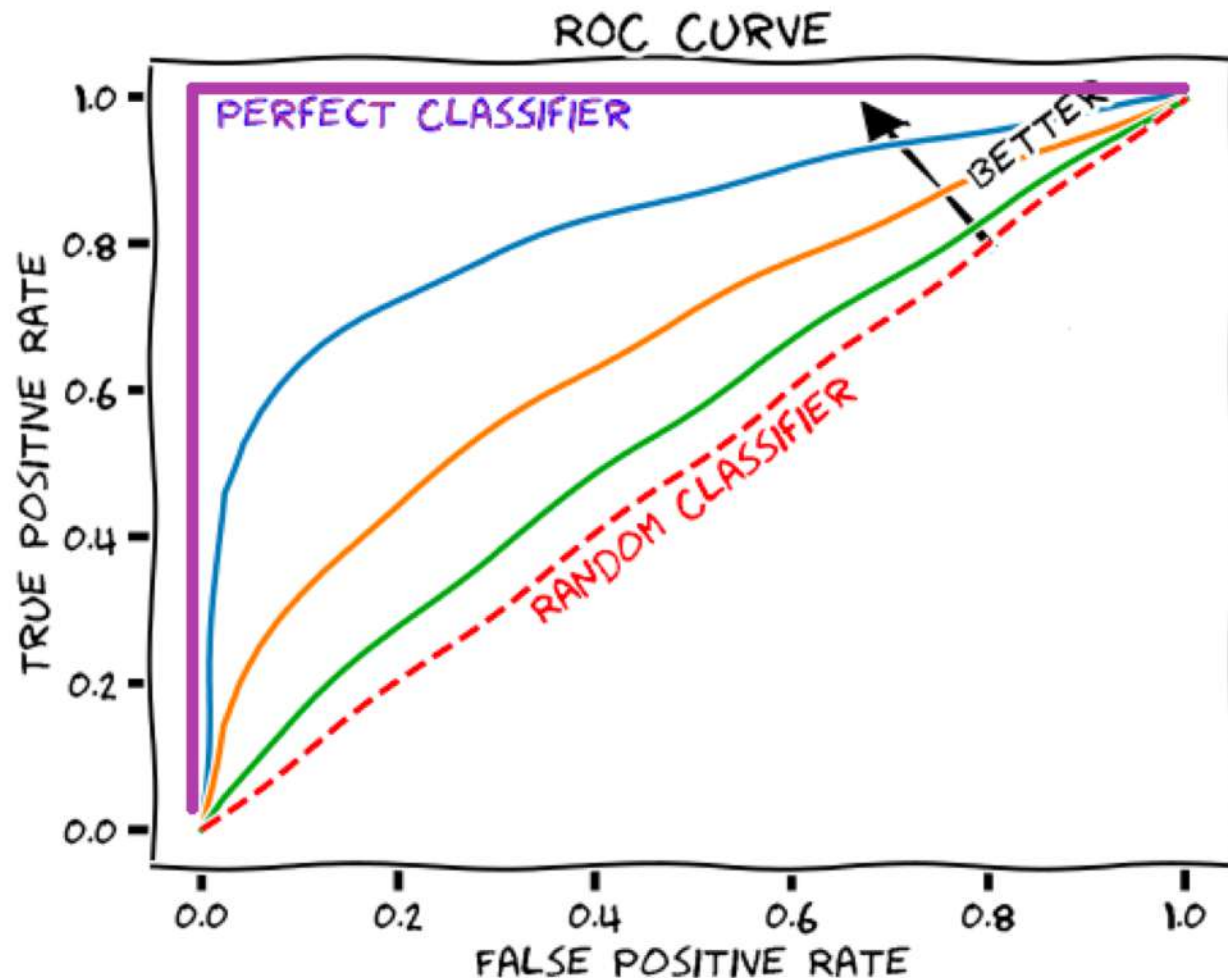
ROC Curve: Example



(1, 1) represents a classifier which **always** predicts the **positive** class

No False Negatives at all

ROC Curve: Example

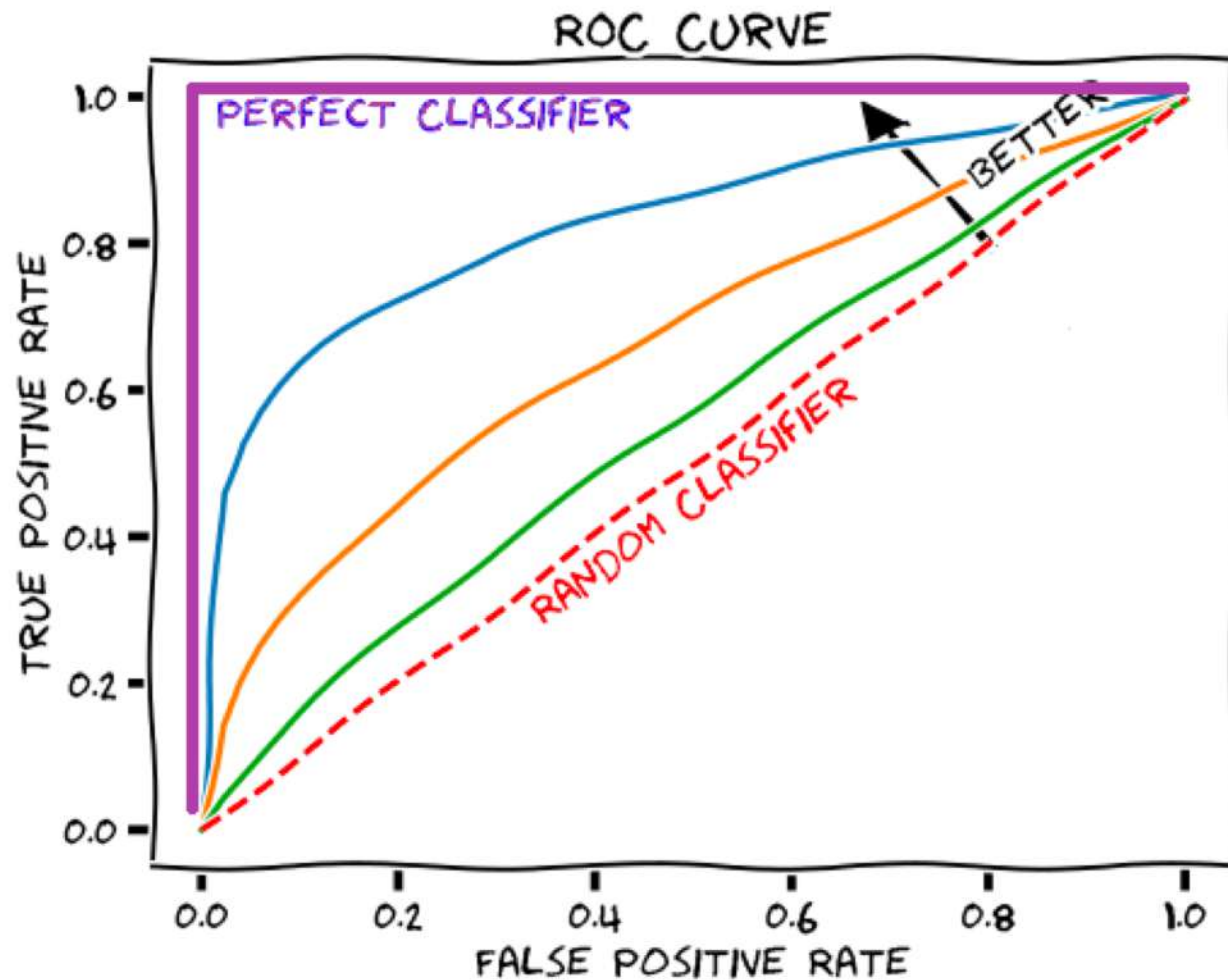


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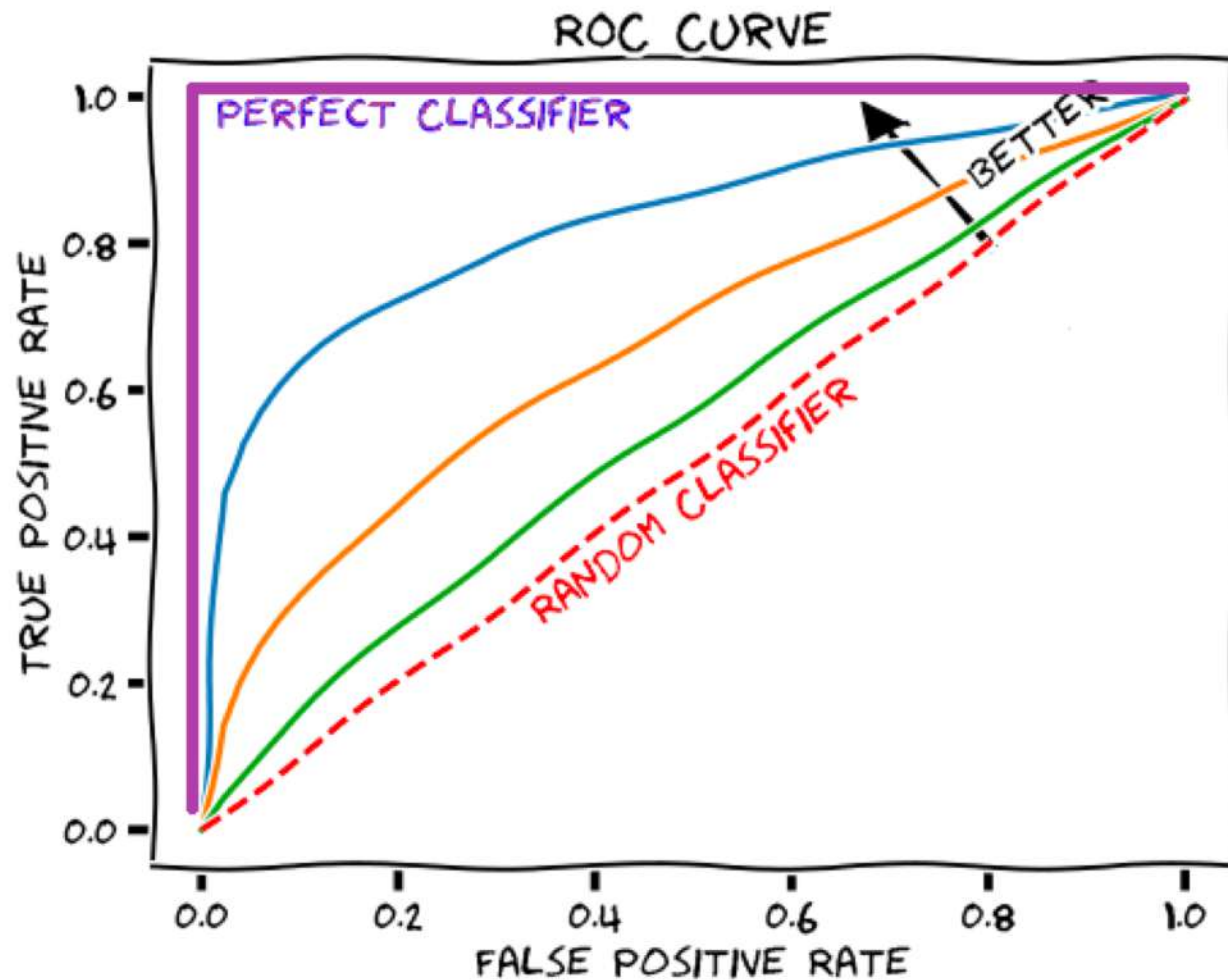
High False Positives

ROC Curve: Example



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ROC Curve: Example

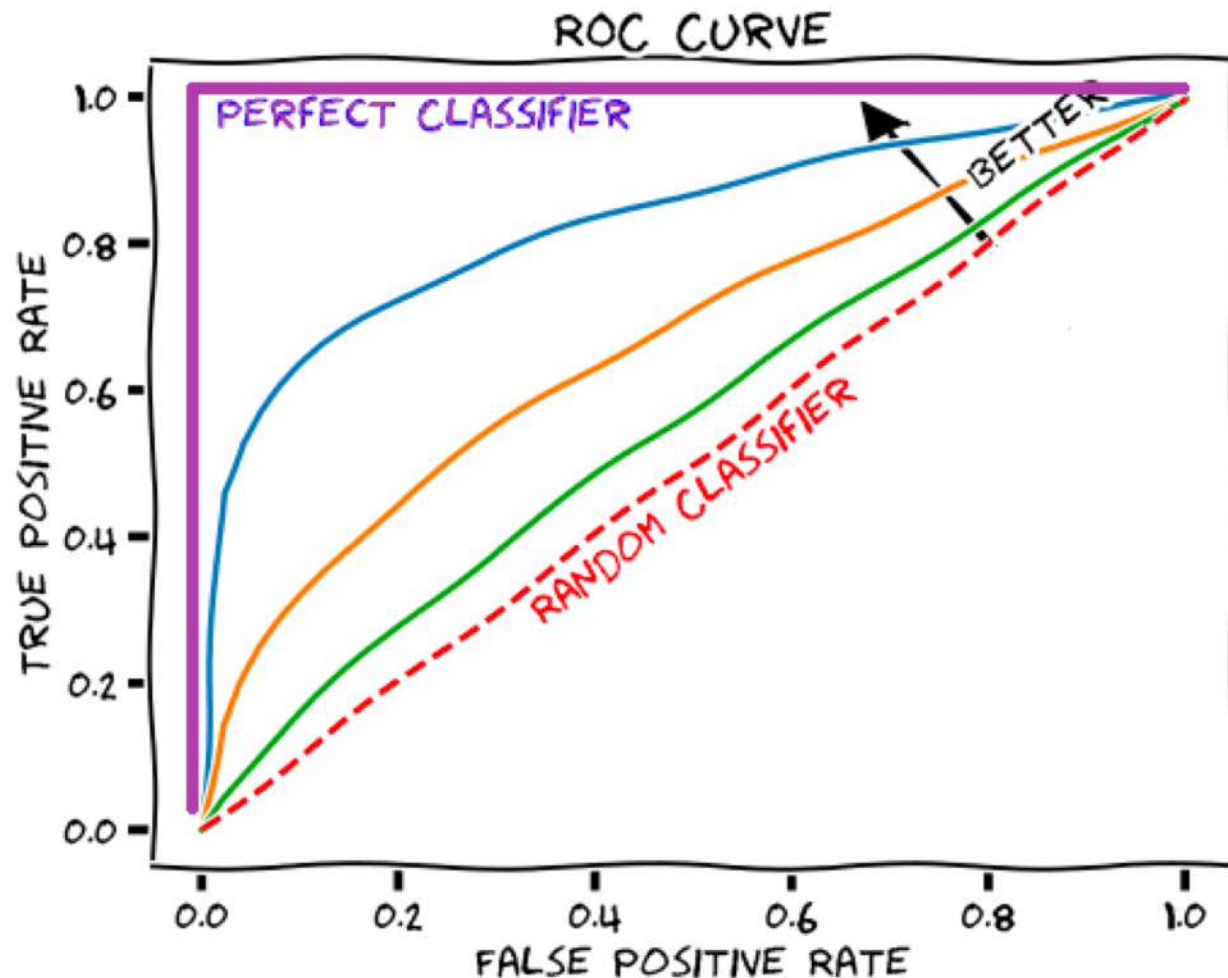


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100% Sensitivity

ROC Curve: Example



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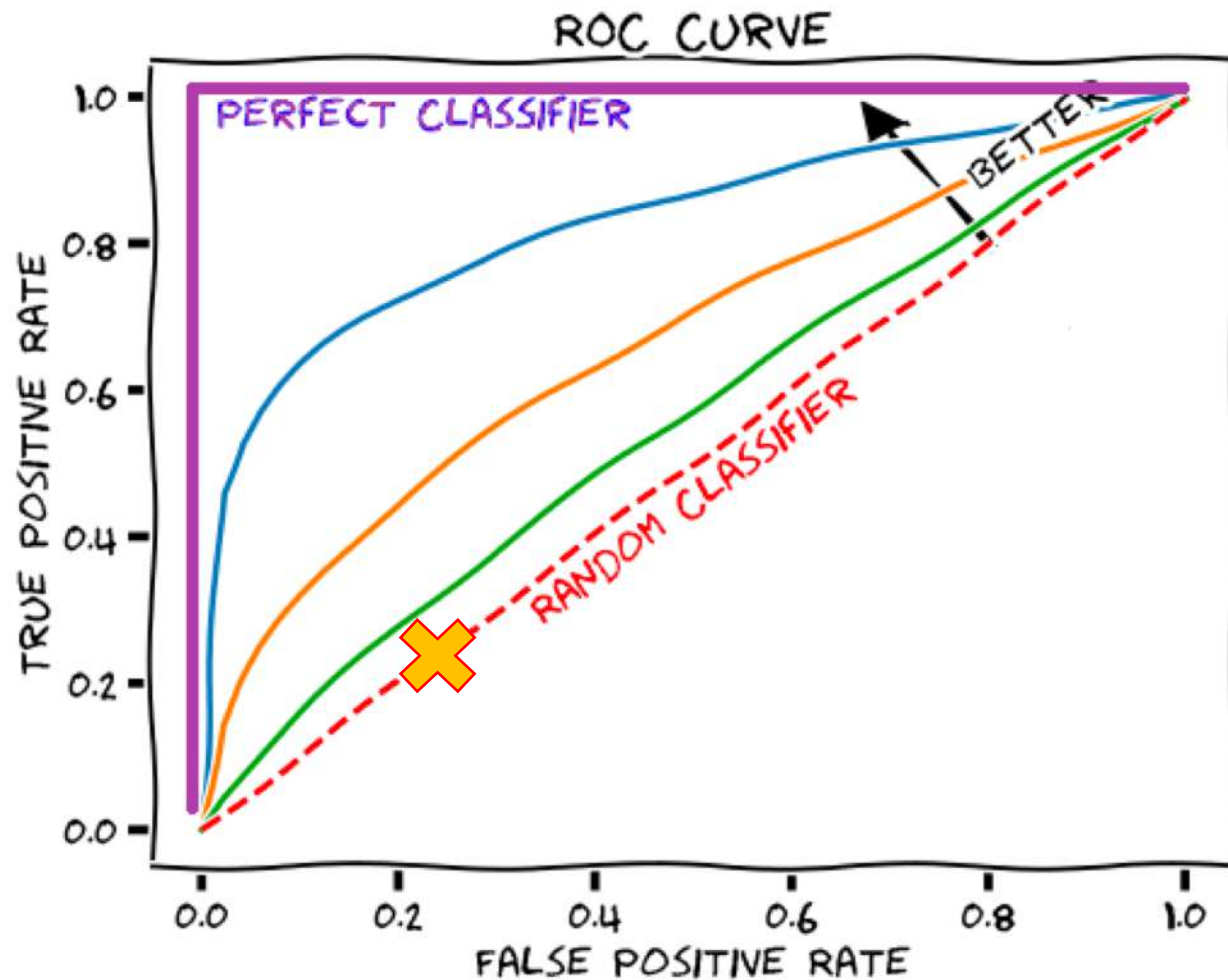
No False Negatives at all

100% Sensitivity

No False Positives at all

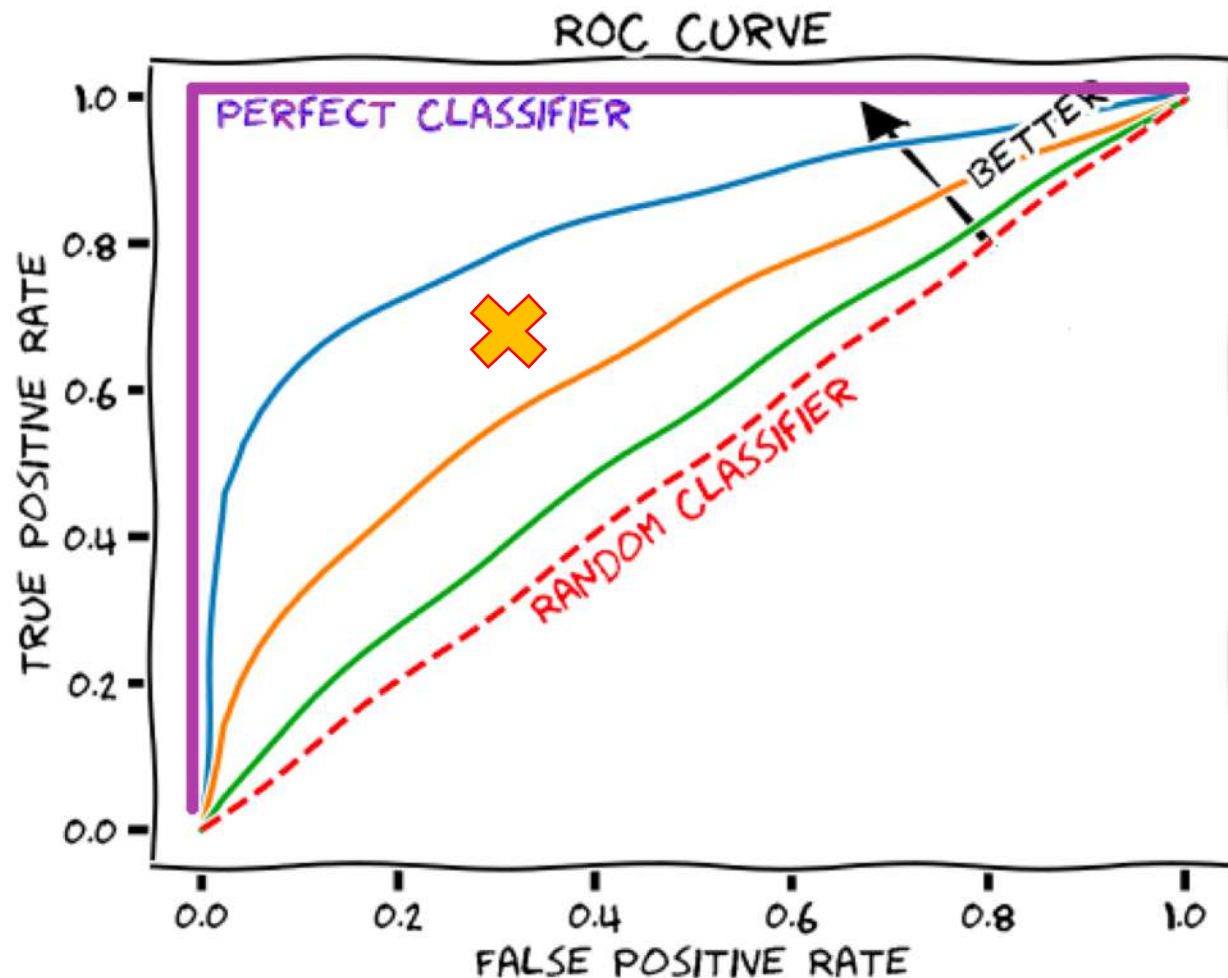
100% Specificity

ROC Curve: Example



Any random guess will result into a point along the diagonal line (**no-discrimination**)

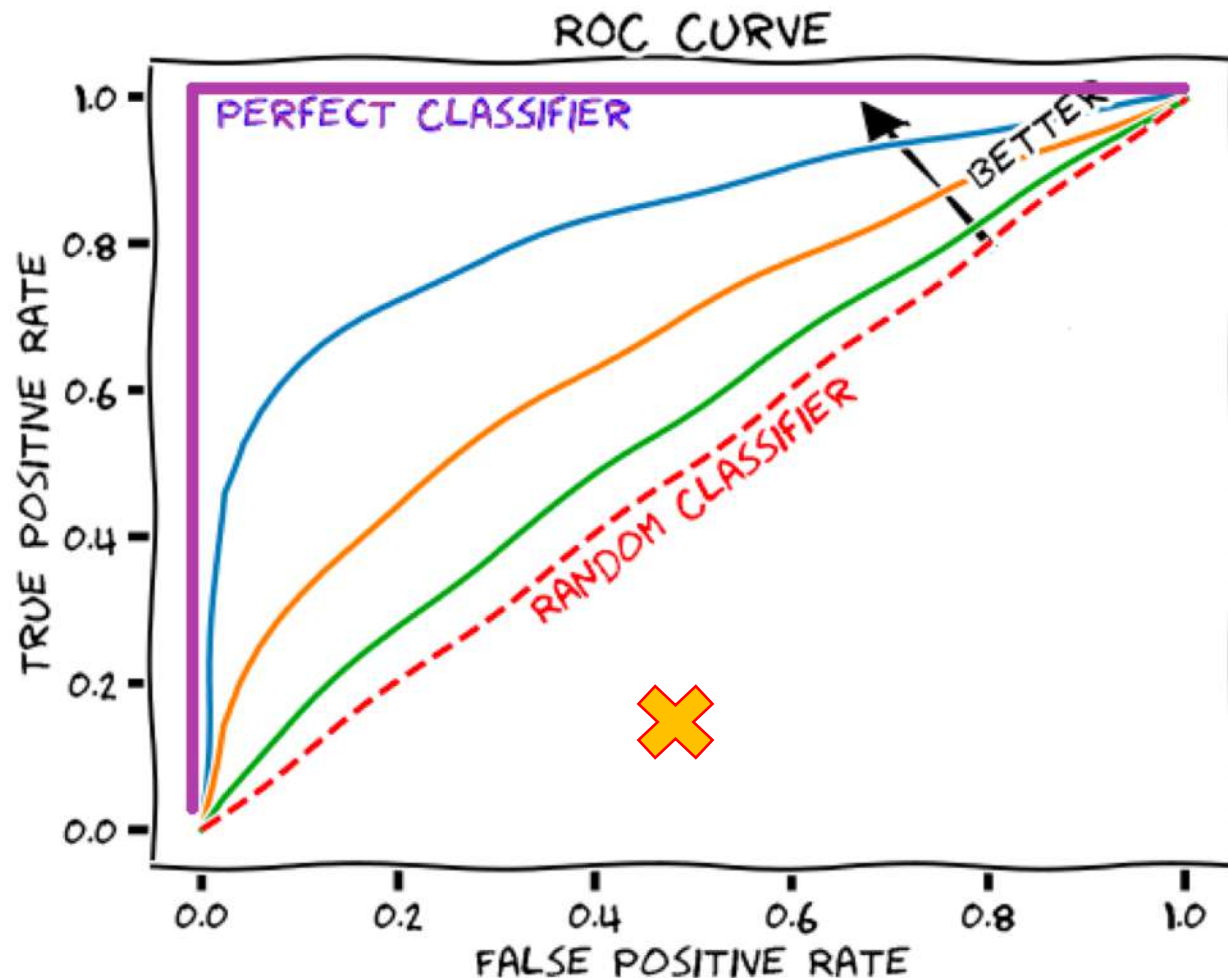
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- If the proportion of positive to negative instances changes in a test set, the ROC curves won't change (class skew independence)
- This is because the metrics TPR and FPR used for ROC are independent of the class distribution (as opposed to, for instance, accuracy)

ROC Curve: How to Compute Data Points

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- Suppose we have a logistic regression classifier
- We can evaluate its performance using several different values of classification thresholds (e.g., $p=0.1$, $p=0.2$, ..., $p=0.9$)
- For each threshold value, we can compute the corresponding (FPR, TPR) coordinate in the ROC space
- In practice, though, we typically use a single, aggregated score from the ROC curve, i.e., its **Area Under the Curve (AUC)**

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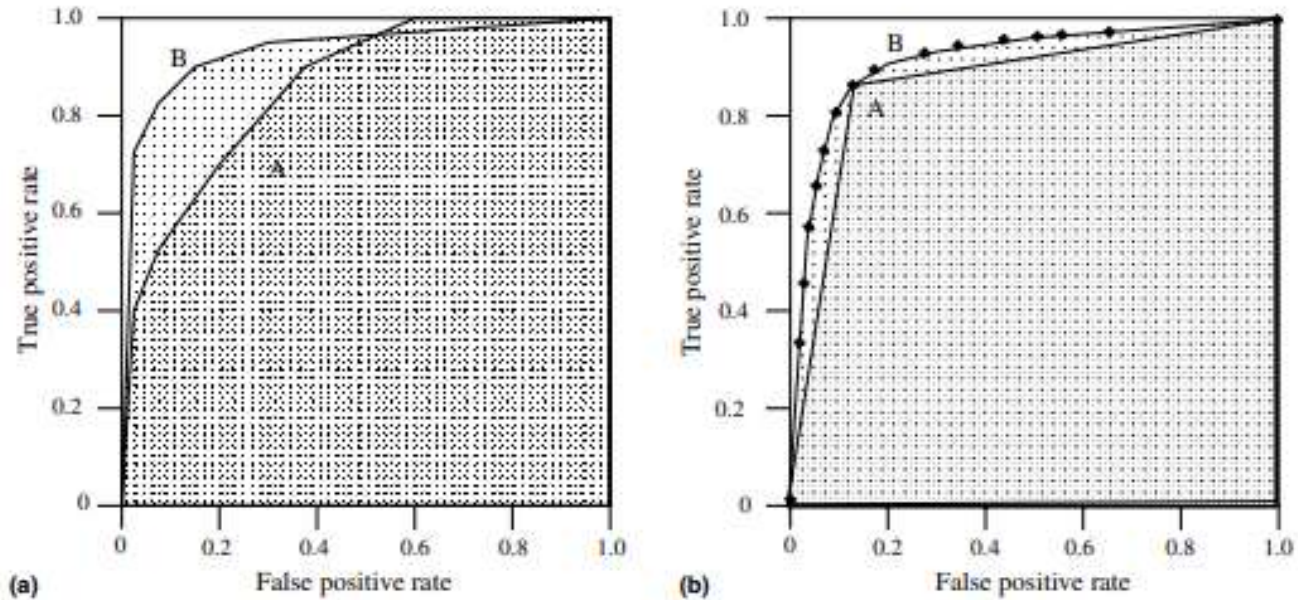
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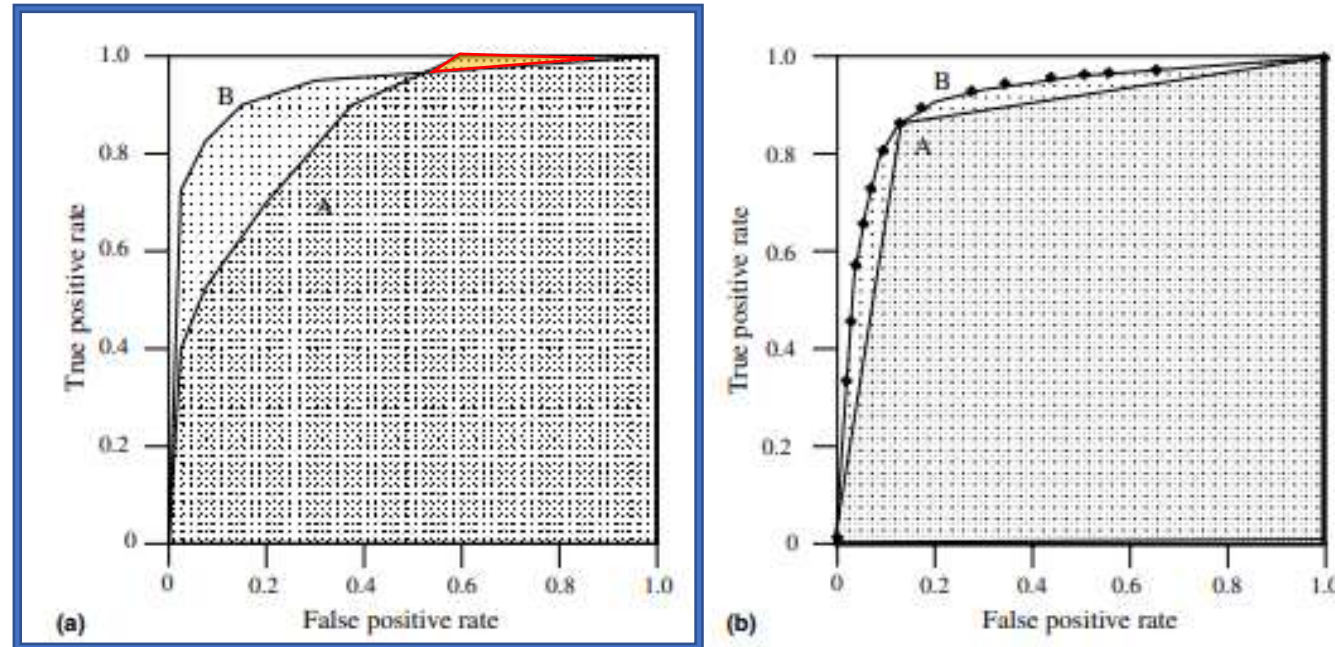
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- The AUC of a ROC curve is a portion of the unit-square surface
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- The random classifier lies along the diagonal line and has ROC AUC = 0.5
- Any realistic and useful classifier should have ROC AUC > 0.5

ROC AUC: Area Under the ROC Curve

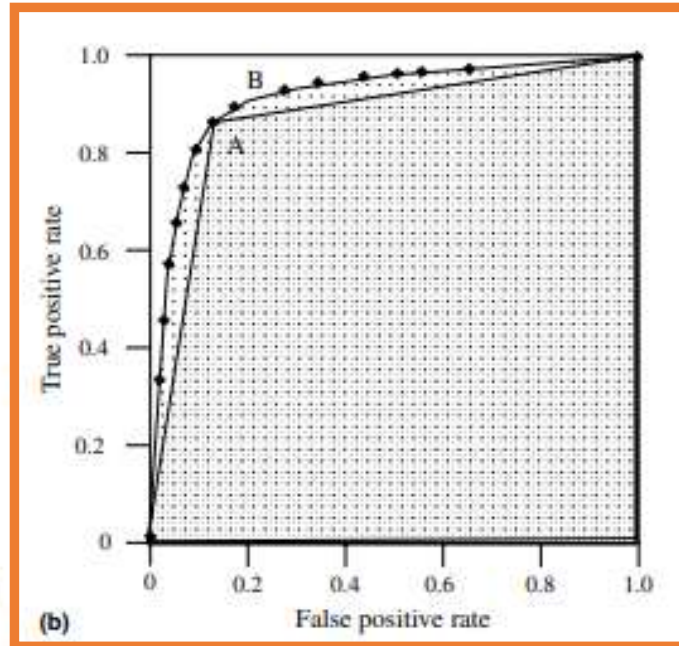
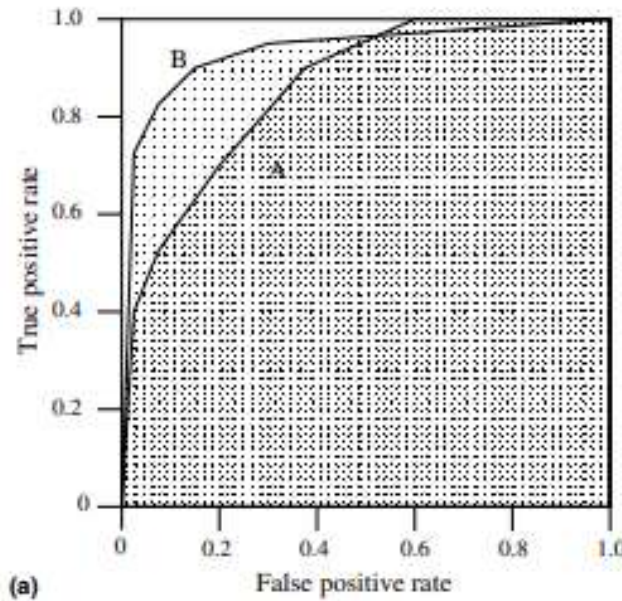


ROC AUC: Area Under the ROC Curve



Classifier B has a greater ROC AUC than classifier A, although the latter may outperform the former at some specific threshold (e.g., at $FPR = 0.6$ A is performing better than B)

ROC AUC: Area Under the ROC Curve



B is a scoring classifier (e.g., logistic regression predicting class probabilities)
A is a binary classifier which directly predicts the class label

ROC AUC: Advantages

2 main reasons why ROC AUC is a desirable evaluation metric

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classification-threshold-invariant

measures the quality of the model's predictions irrespective of what classification threshold is chosen

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- The metrics we discussed are **offline** metrics as opposed to **online** metrics which are what we ultimately want to measure
 - e.g., In online advertising, we want to show ads that get clicked to increase the **revenue** (**online** metric): we measure the "accuracy" of our click model in predicting the **click probability** first (**offline** metric)
- Offline metrics should represent a **good proxy** of the online metric(s) we are ultimately interested in

Take-Home Message of Today

- Several well-known **offline** evaluation metrics for classification models

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Take-Home Message of Today

- Several well-known **offline** evaluation metrics for classification models
- Some of them make sense only under specific circumstances (e.g., when class labels are uniform and balanced)
- Evaluation metrics can be extended to the case of multi-class although things get more complex
- Offline metrics usually do not coincide with the online metrics we aim to optimize but they must be good **proxies** of those