Big Data Computing

Master's Degree in Computer Science

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Recap from Last Lectures

- 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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- 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**

Confusion Matrix

- It is one of the most intuitive and easiest metrics used for finding the correctness and accuracy of the model
- 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:**
  - An image classifier trained over a quite balanced dataset of 60% pictures of dogs and 40% pictures of cats
  - 97% accuracy would indicate a very good performing model

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- **Example:**
  - In our cancer detection setting, only 5 out of 100 people have cancer
  - 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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Total positive predictions

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  - TP = 5 → Precision = 5/100 = **5%**

Recall or Sensitivity or True Positive Rate (TPR)

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$$\text{Recall} = \frac{TP}{\boxed{TP + FN \quad \text{Total actually positives}}}$$

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  - TP = 5 → Recall = 5/5 = **100%**

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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 instaces

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  - TN + FP = 0 + 95 = 95 (as the model only predicts the positive class label)
  - TN = 0 → 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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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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$$\boxed{\text{F1-score}(P, R) = \frac{2PR}{P+R}}$$

F1 Score

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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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- 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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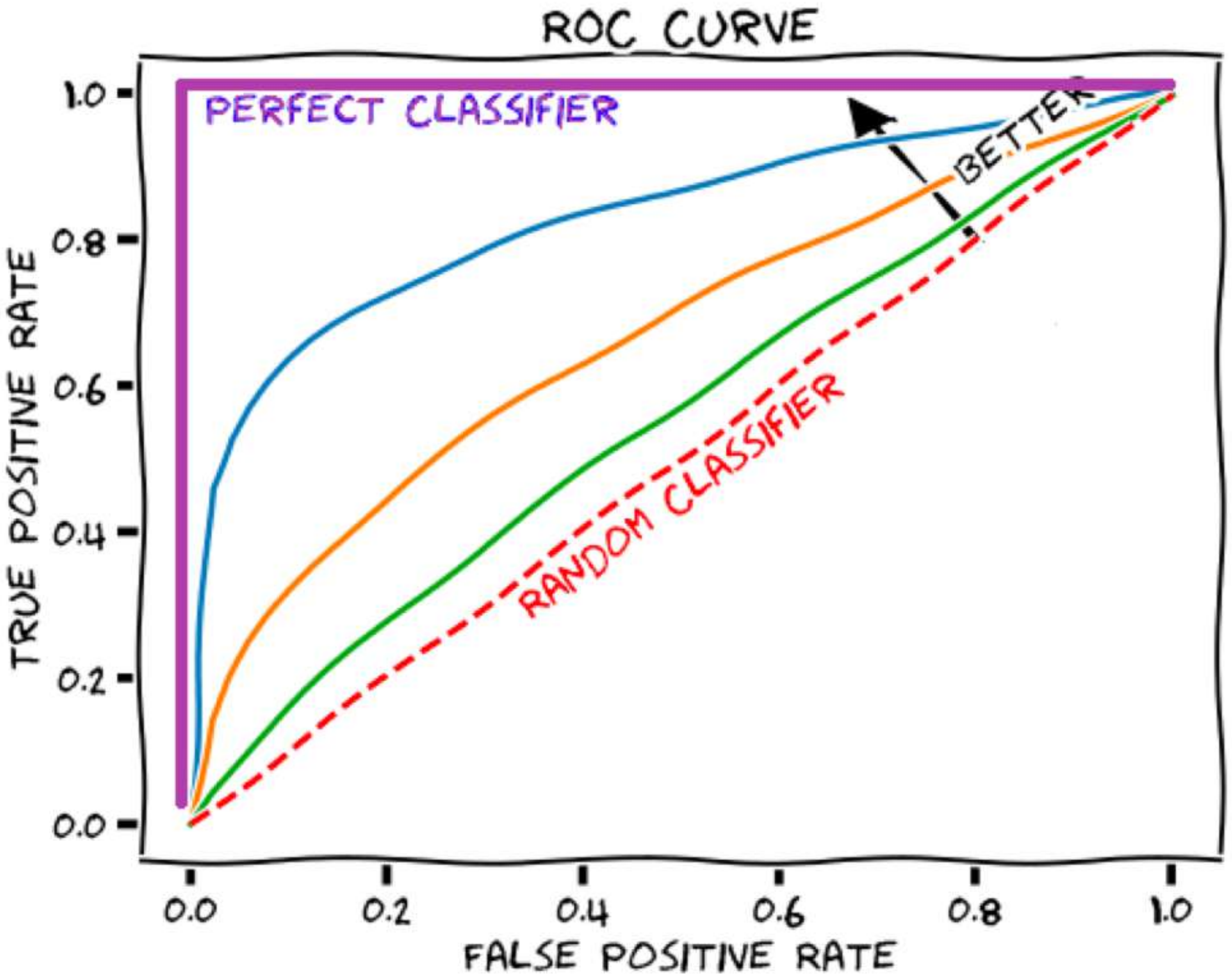
- TPR is equivalent to Recall (or Sensitivity)
- FPR is also known as Fall-Out (or 1-Specificity)

ROC Curve: Example



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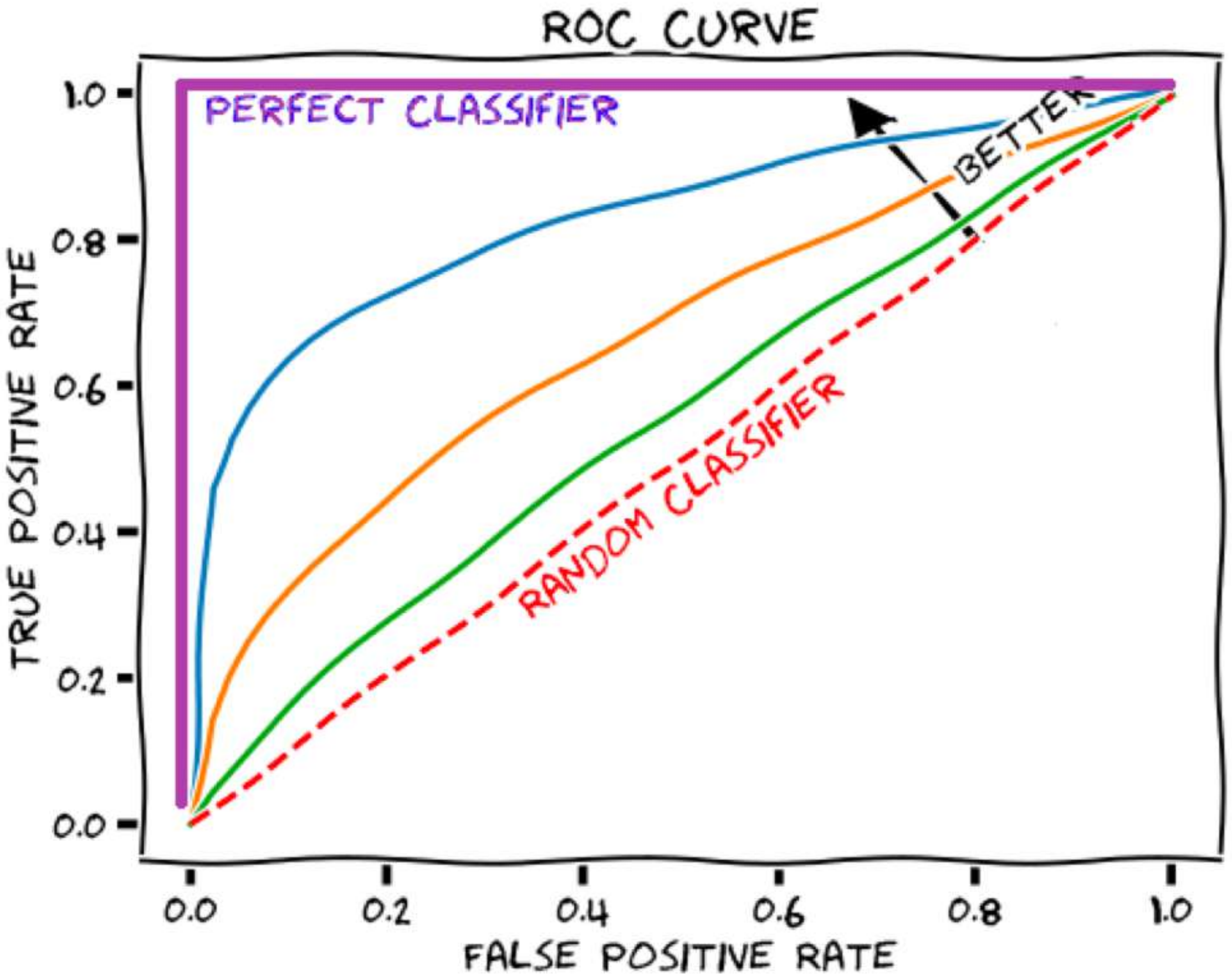

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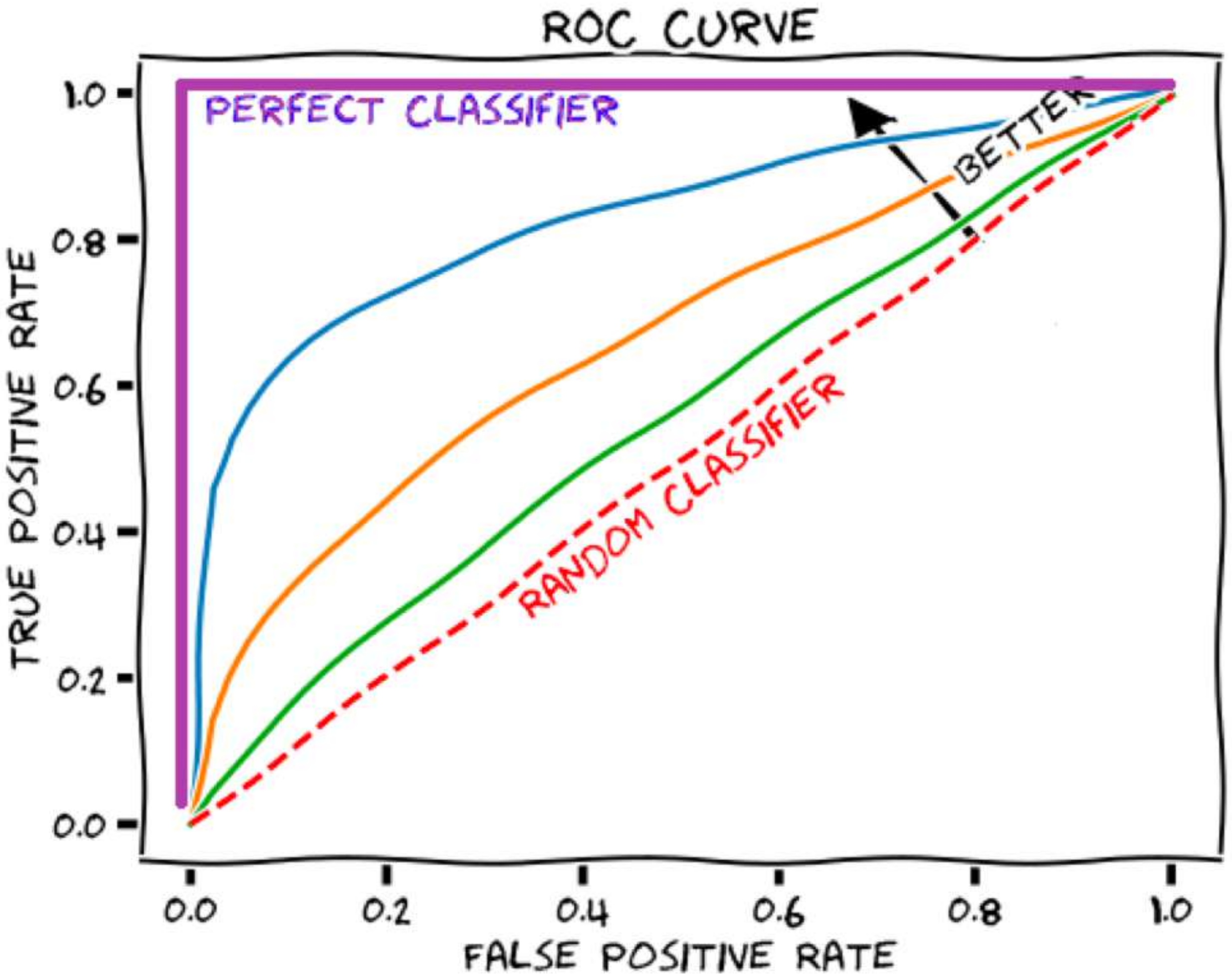

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No True Positives either

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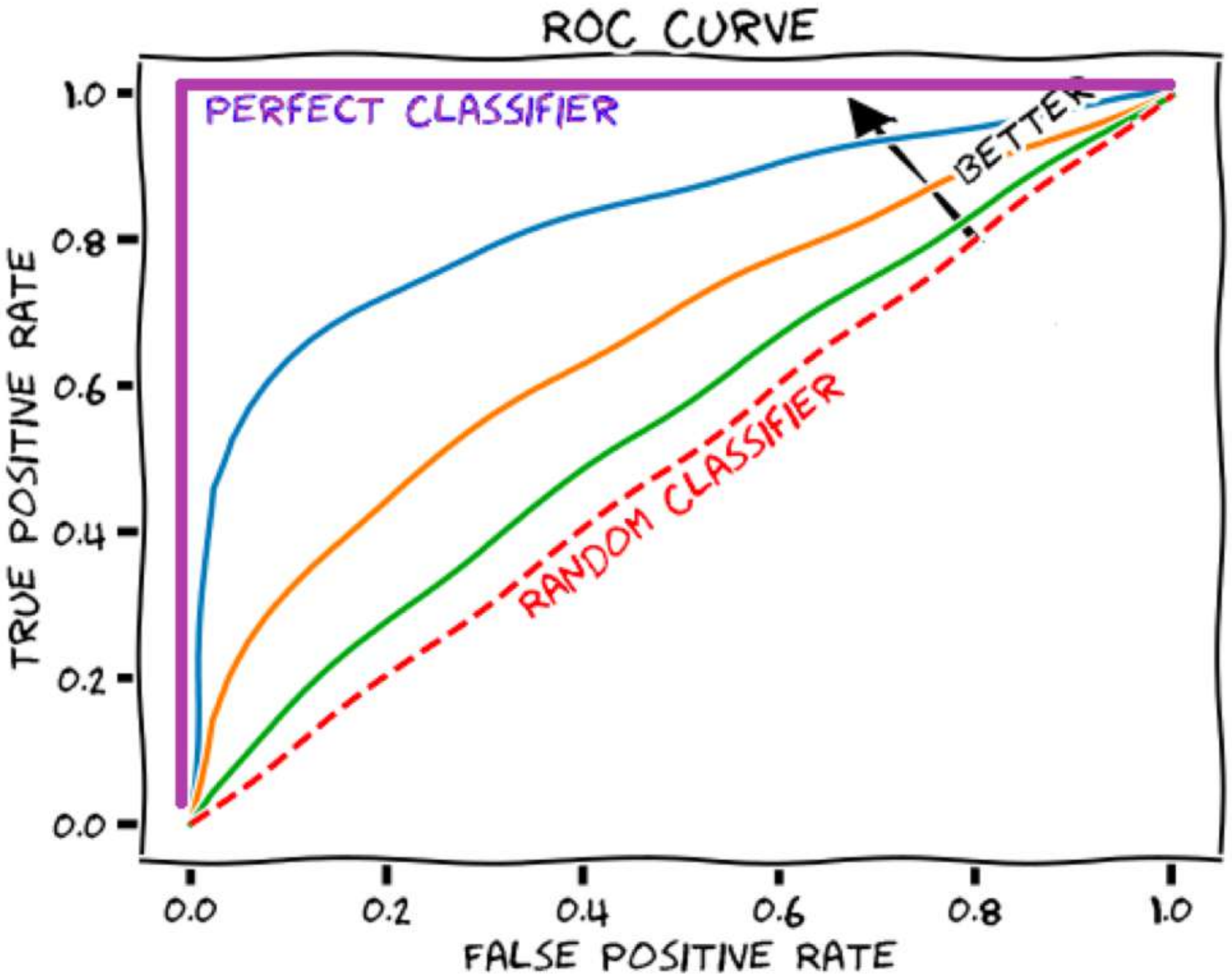

(1, 1) represents a classifier which **always** predicts the **positive** class

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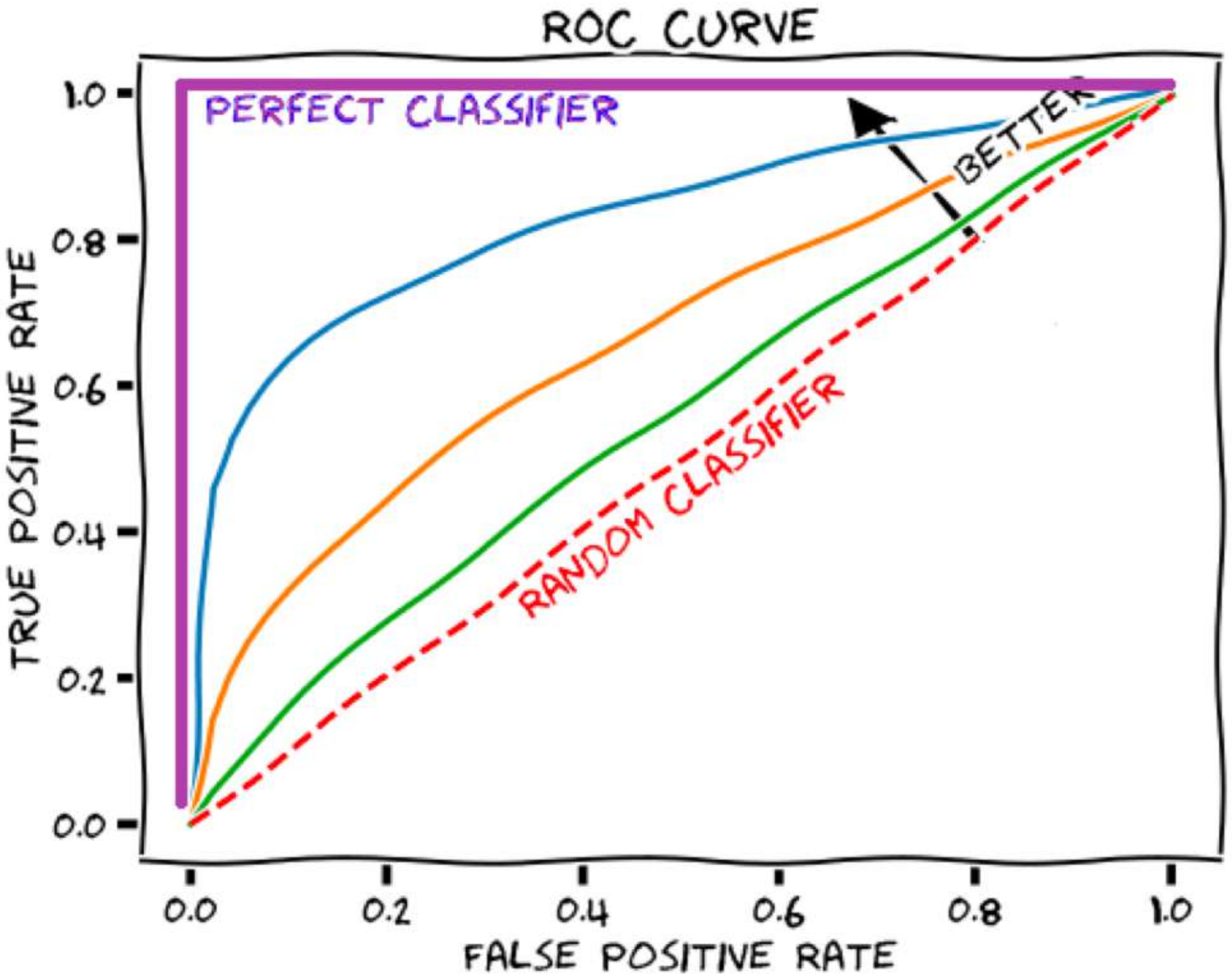

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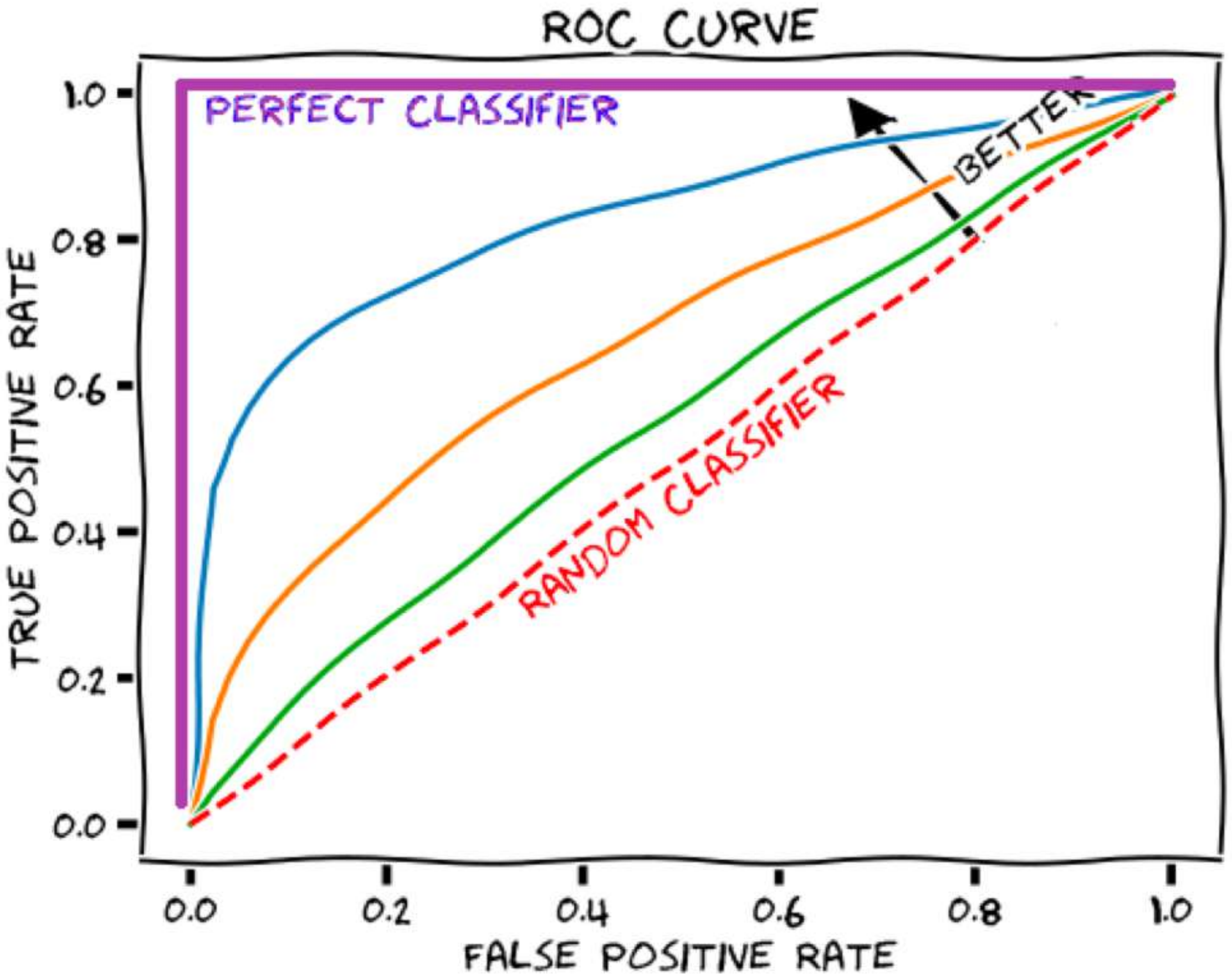

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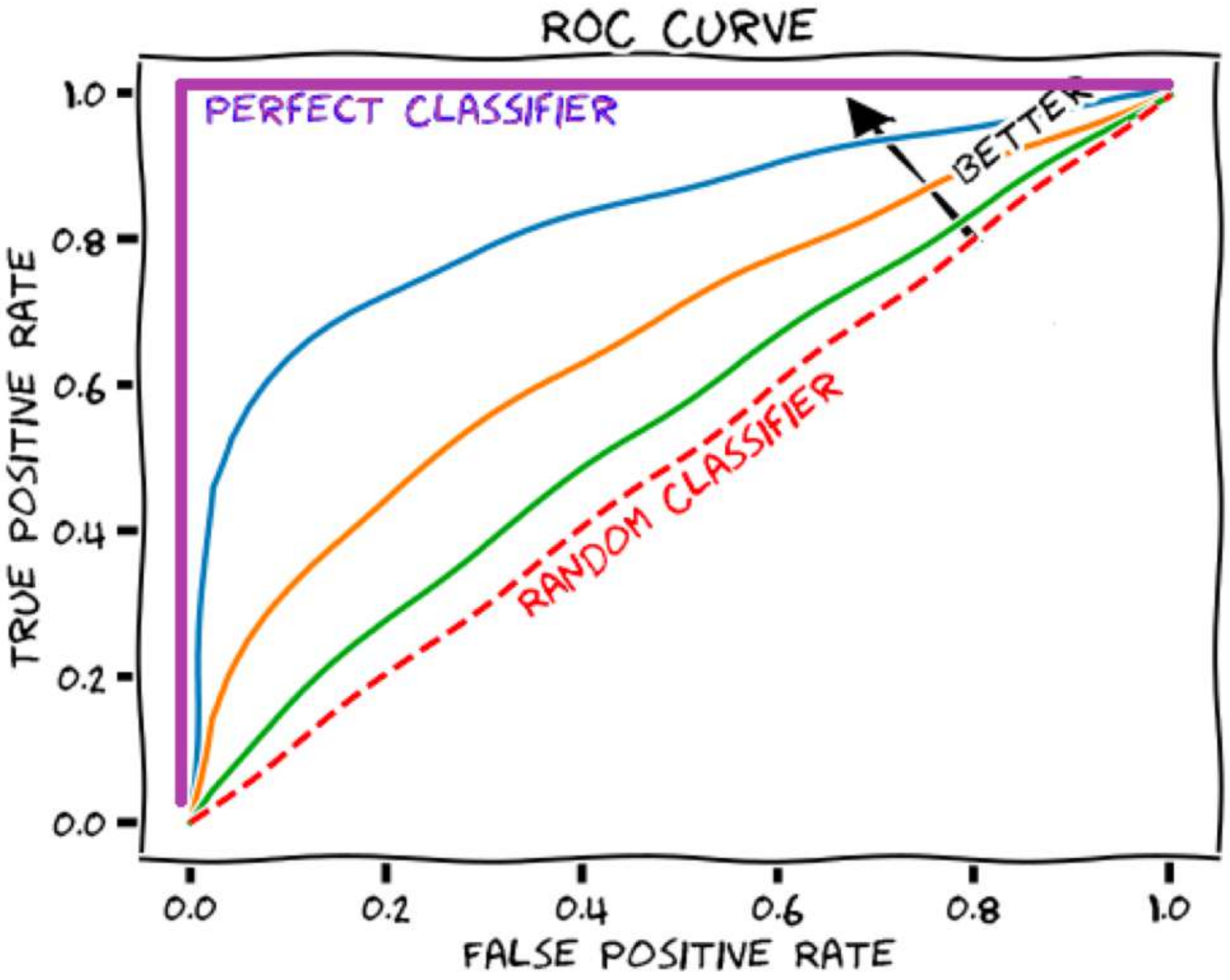

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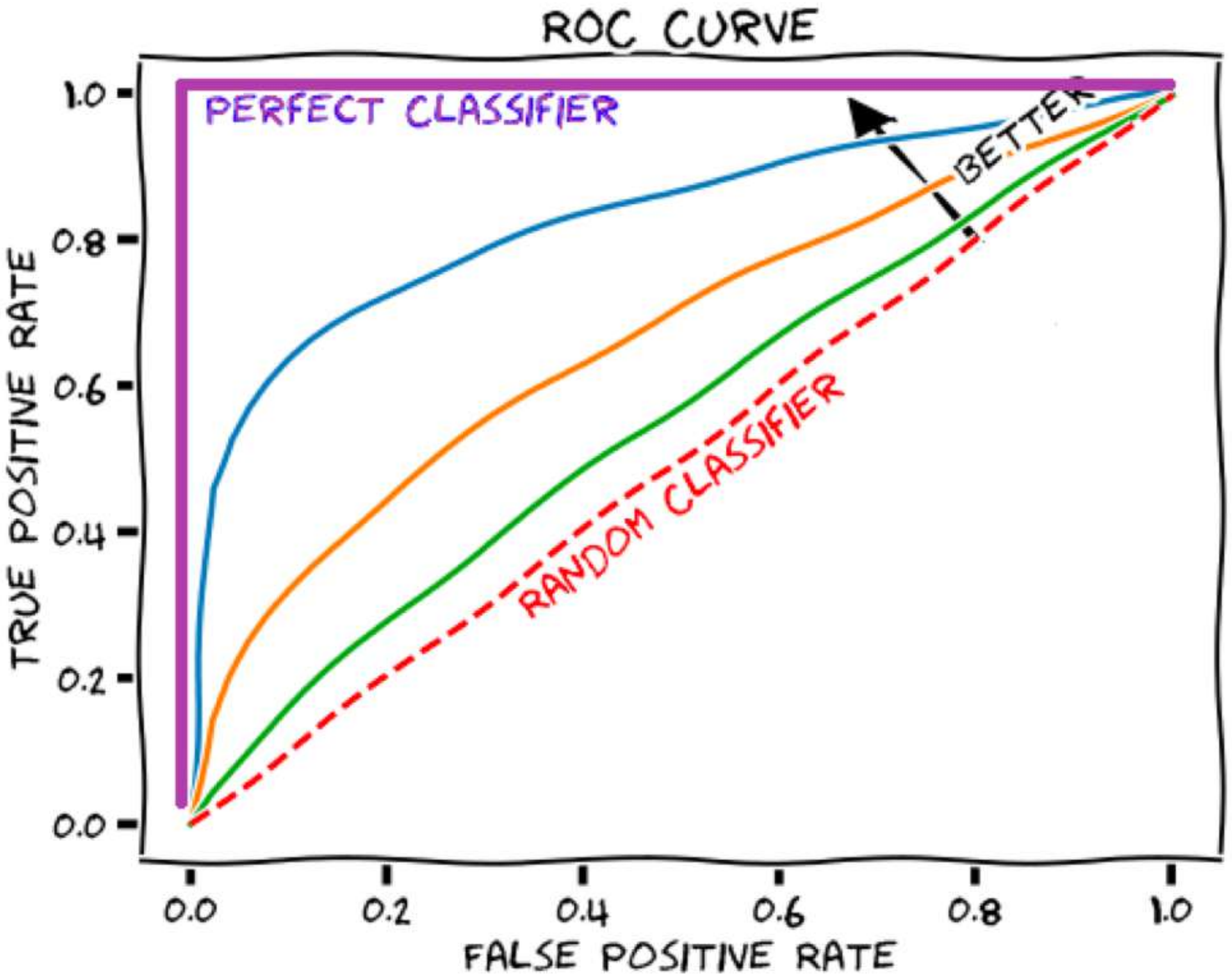

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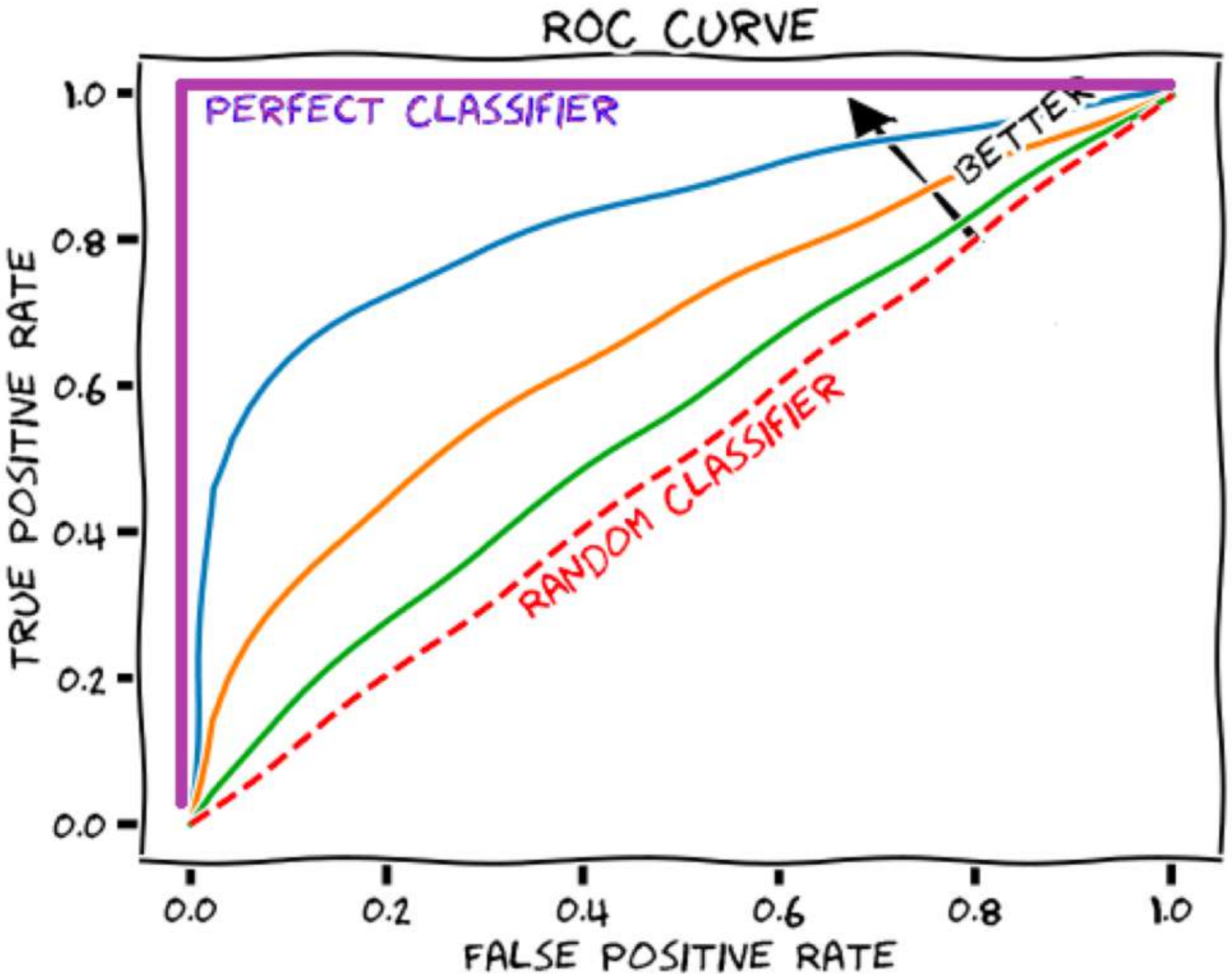

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100% Specificity

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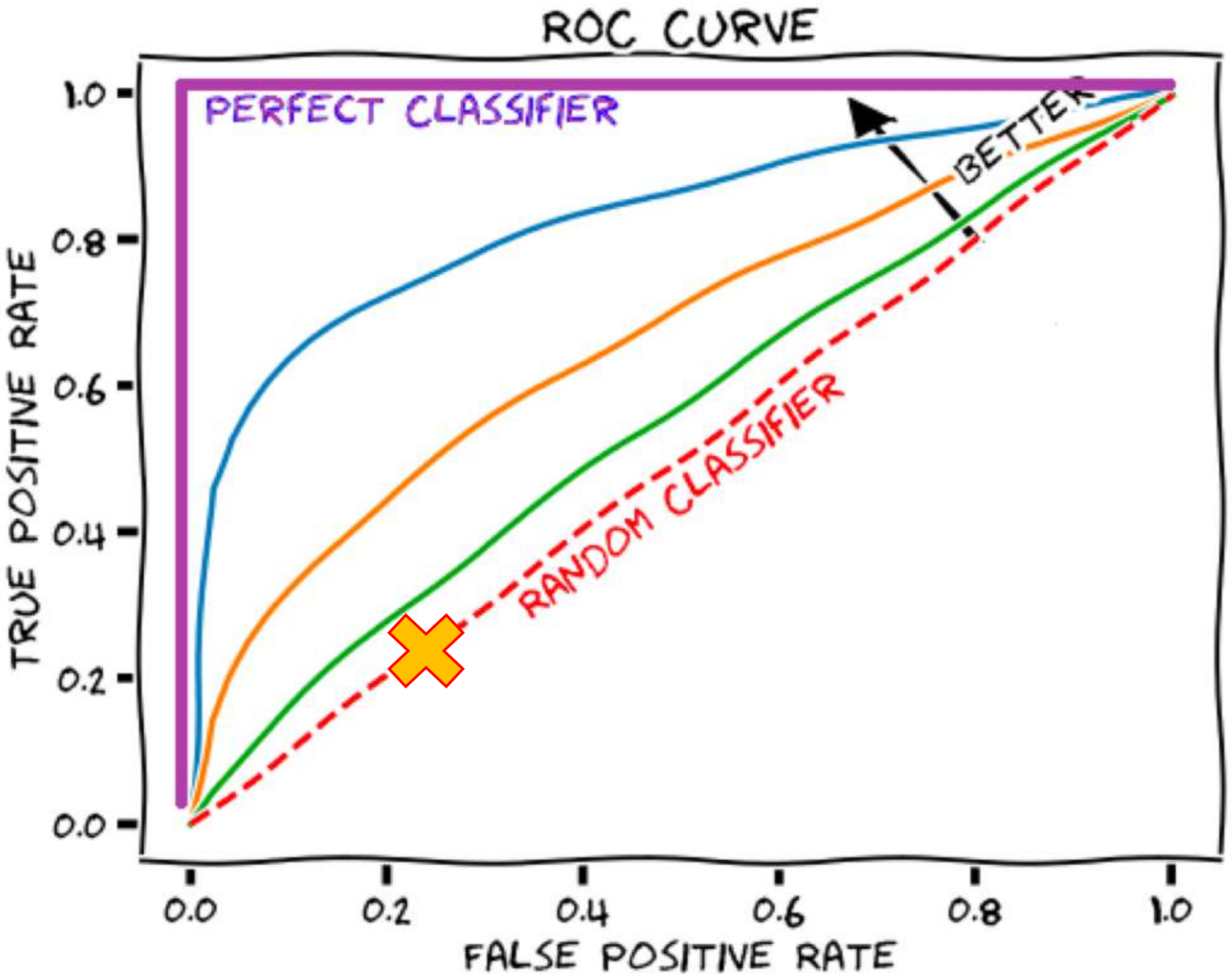

Any random guess will result into a point along the diagonal line (**no-discrimination**)

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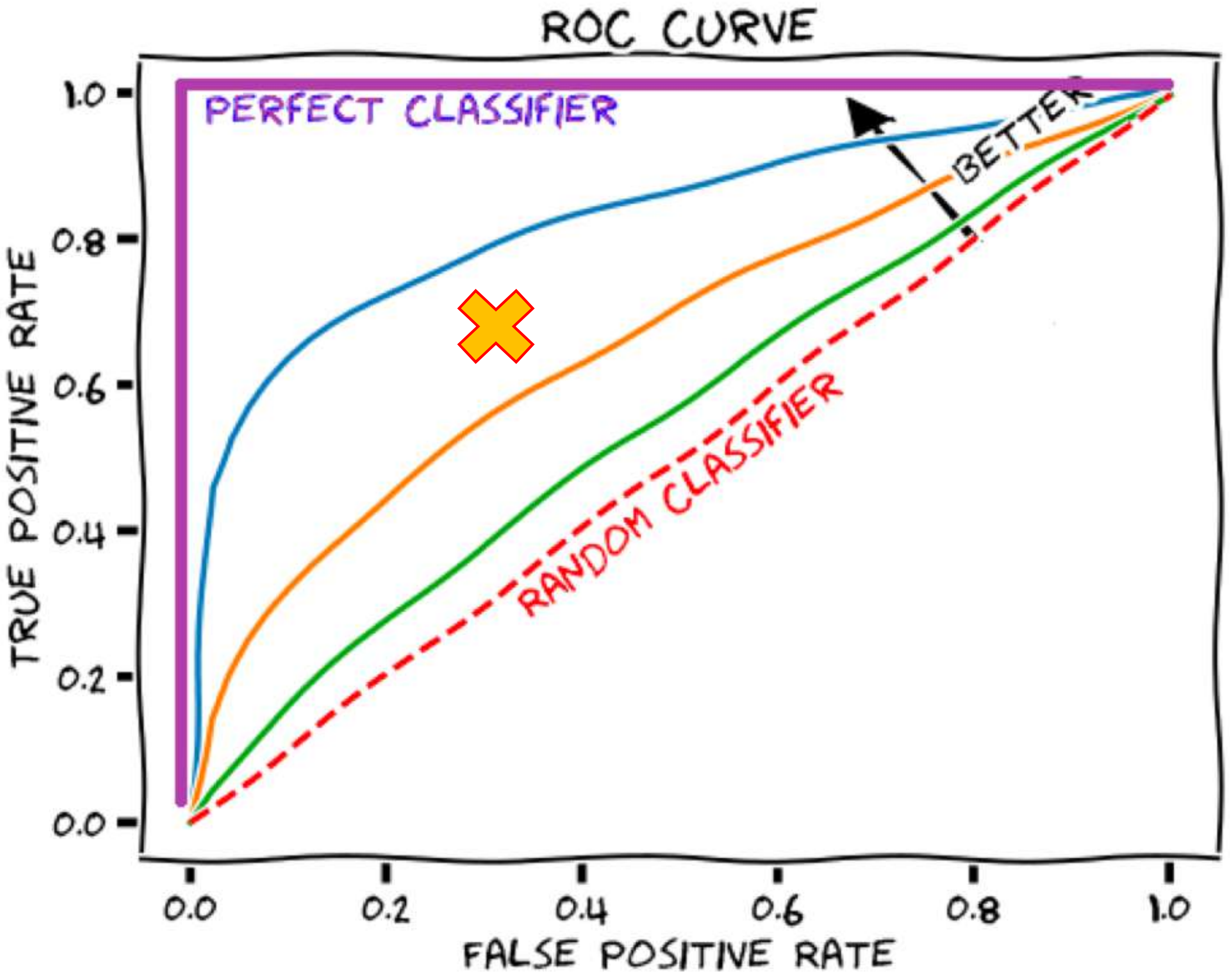

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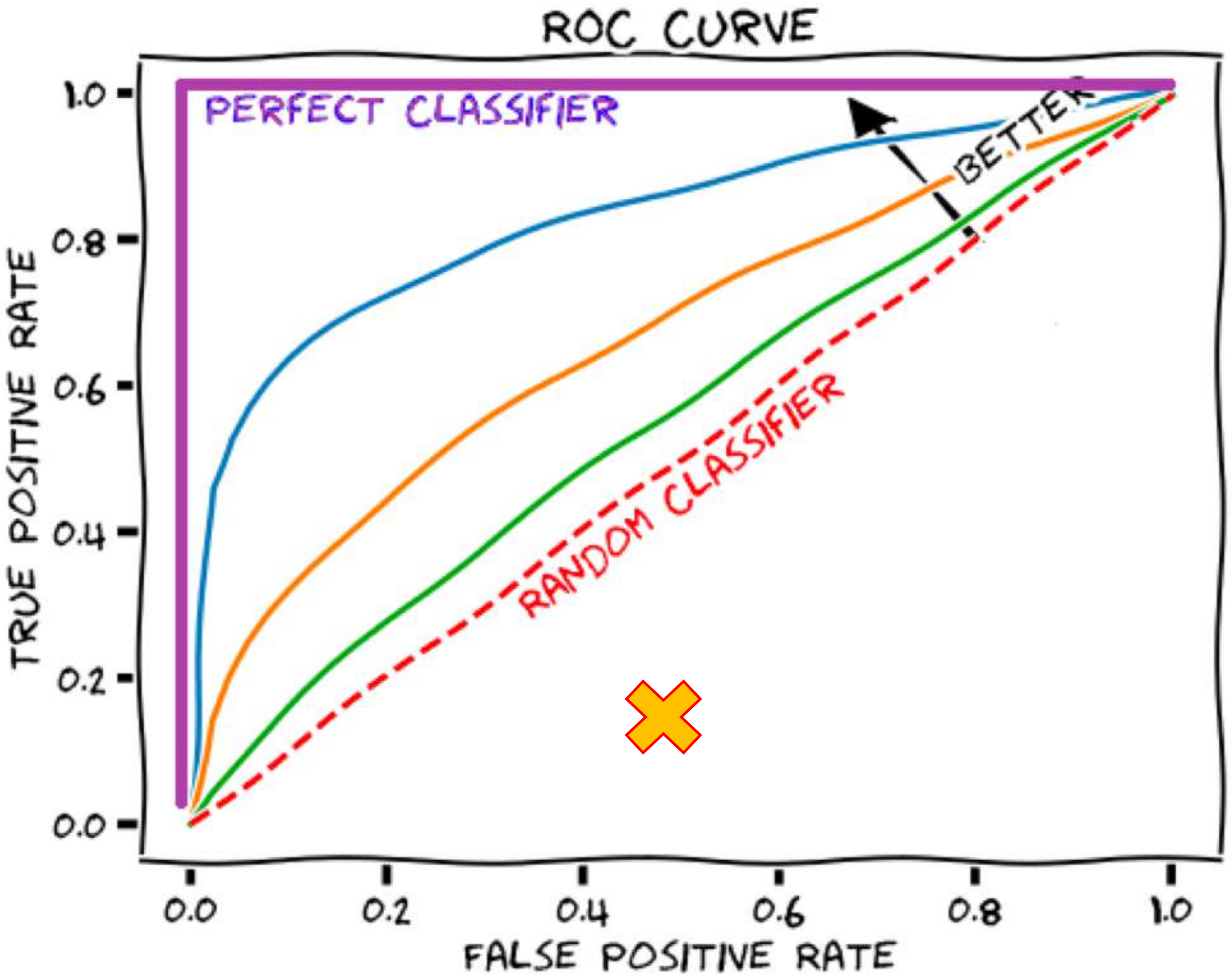

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Points above the diagonal are good classification results (**better than random**)

points below the diagonal are bad classification results (**worse than random**)

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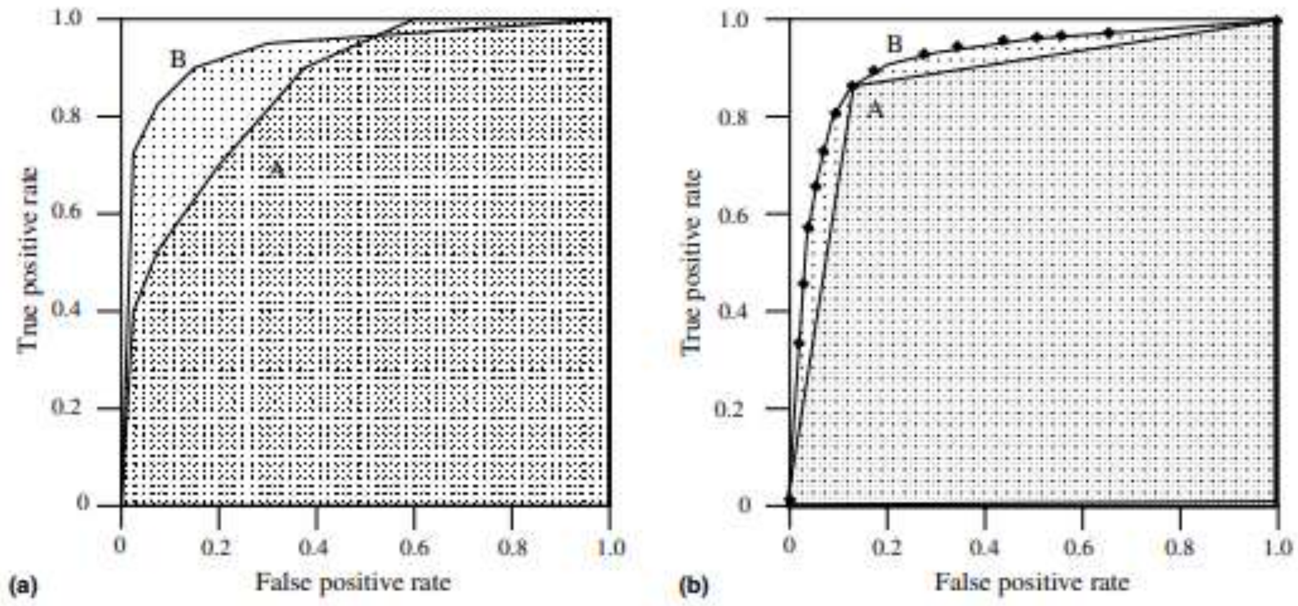
- The random classifier lies along the diagonal line and has ROC AUC = 0.5
- Any realistic and useful classifier should have ROC AUC > 0.5

ROC AUC: Area Under the ROC Curve



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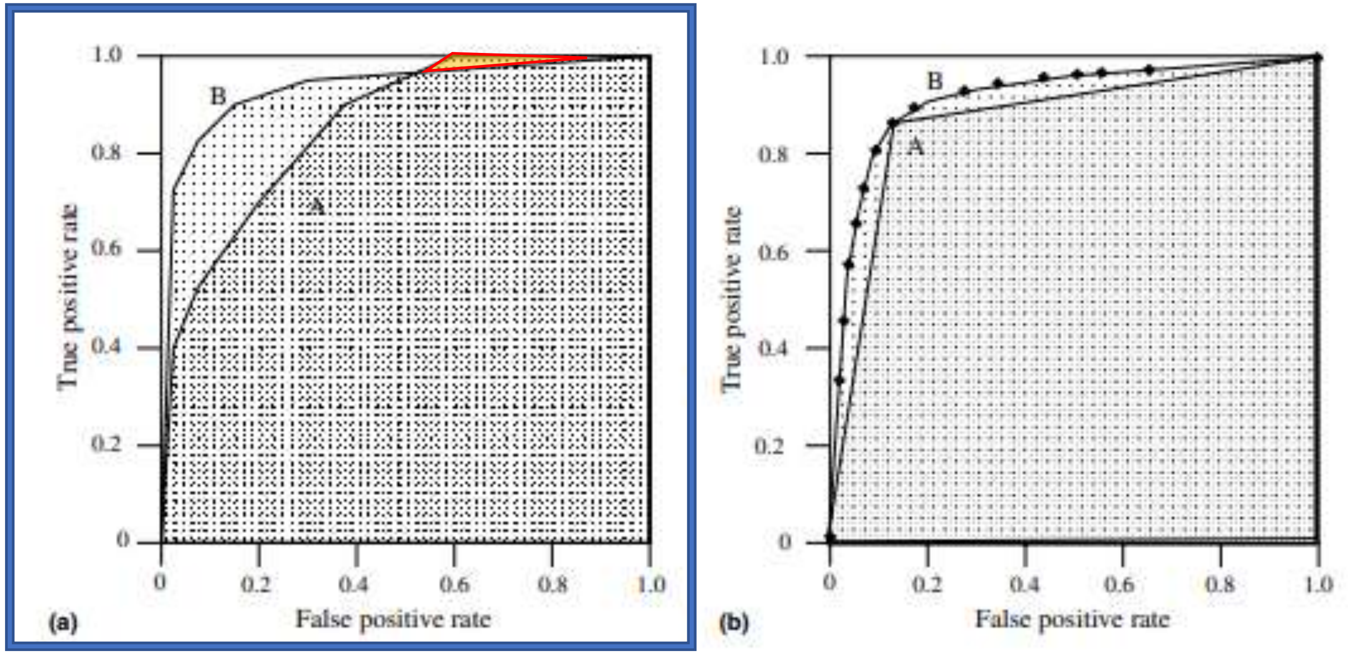
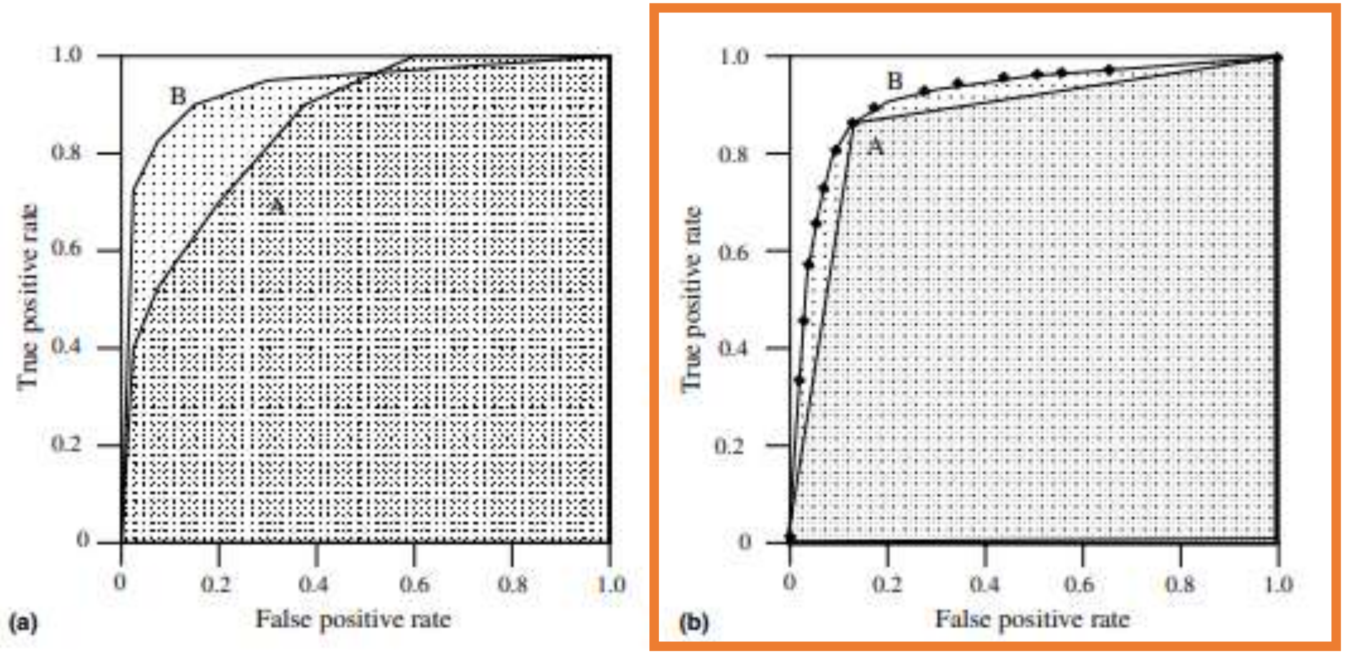


Classifier B has a greater ROC AUC than classifier A, although the latter may outperform the former at some specific threshold
(e.g., at FPR = 0.6 A is performing better than B)

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

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- 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