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
  - Decision Trees (and ensemble of those)

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We need a robust evaluation framework to assess models performance

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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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- There is no strict rule on what should be minimized in all the situations as this depends on the business needs and the context of the problem
- We might want to minimize either FPs or FNs

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- In order to capture **all** cancer cases, we might end up classifying as cancerous patients who are actually **not** having cancer

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 FPs is more important than minimizing FNs

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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    - 97% accuracy would indicate a very good performing model

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

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  - TP = 5 → Recall = 5/5 = 100%

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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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- <u>Example:</u> 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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$$\boxed{\text{MCC} = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}}$$

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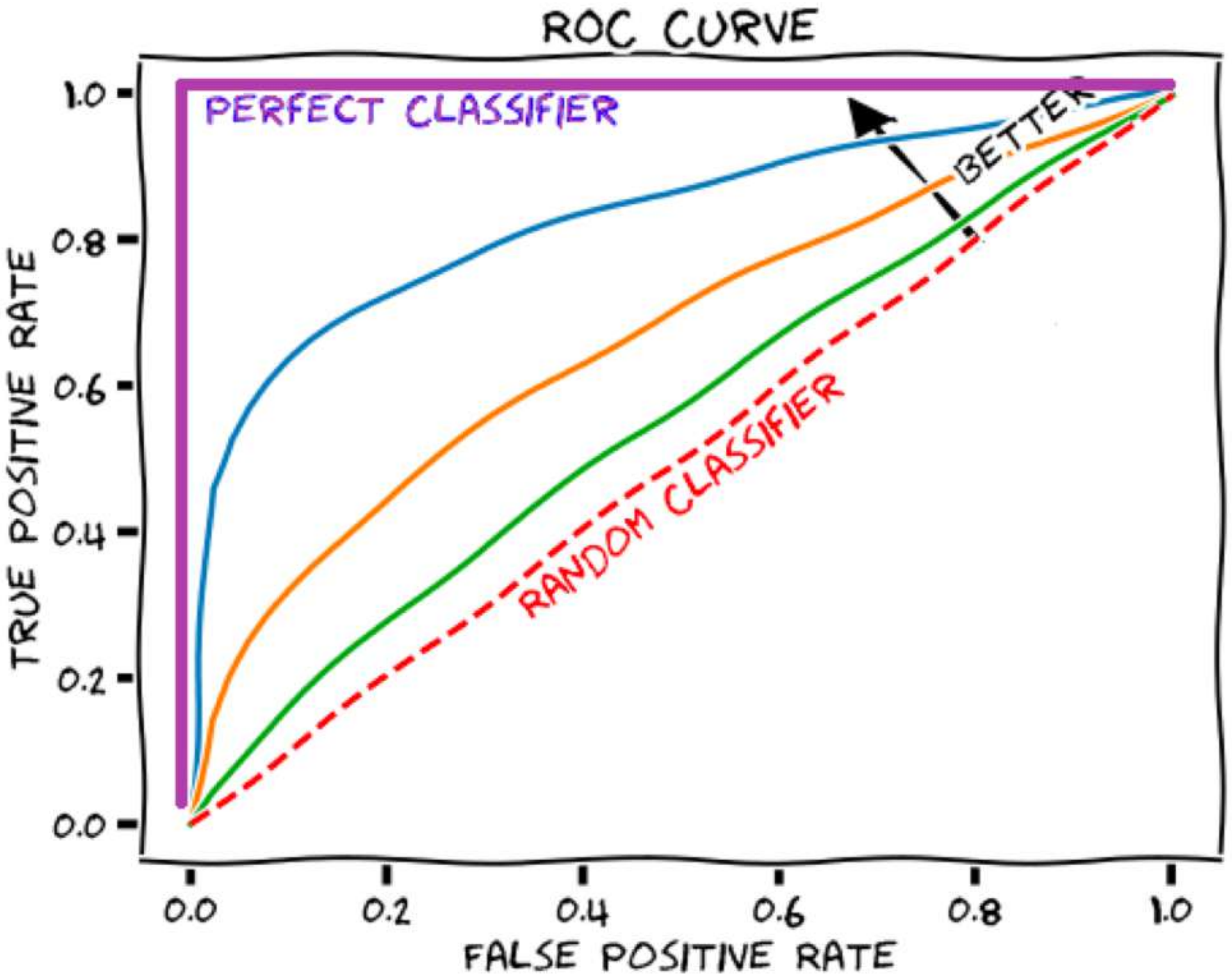
- It is created by plotting the true positive rate (TPR) against the false positive rate (FPR) at various threshold settings
- TPR is equivalent to Recall (or Sensitivity)
- FPR is also known as Fall-Out (or 1-Specificity)

ROC Curve: Example



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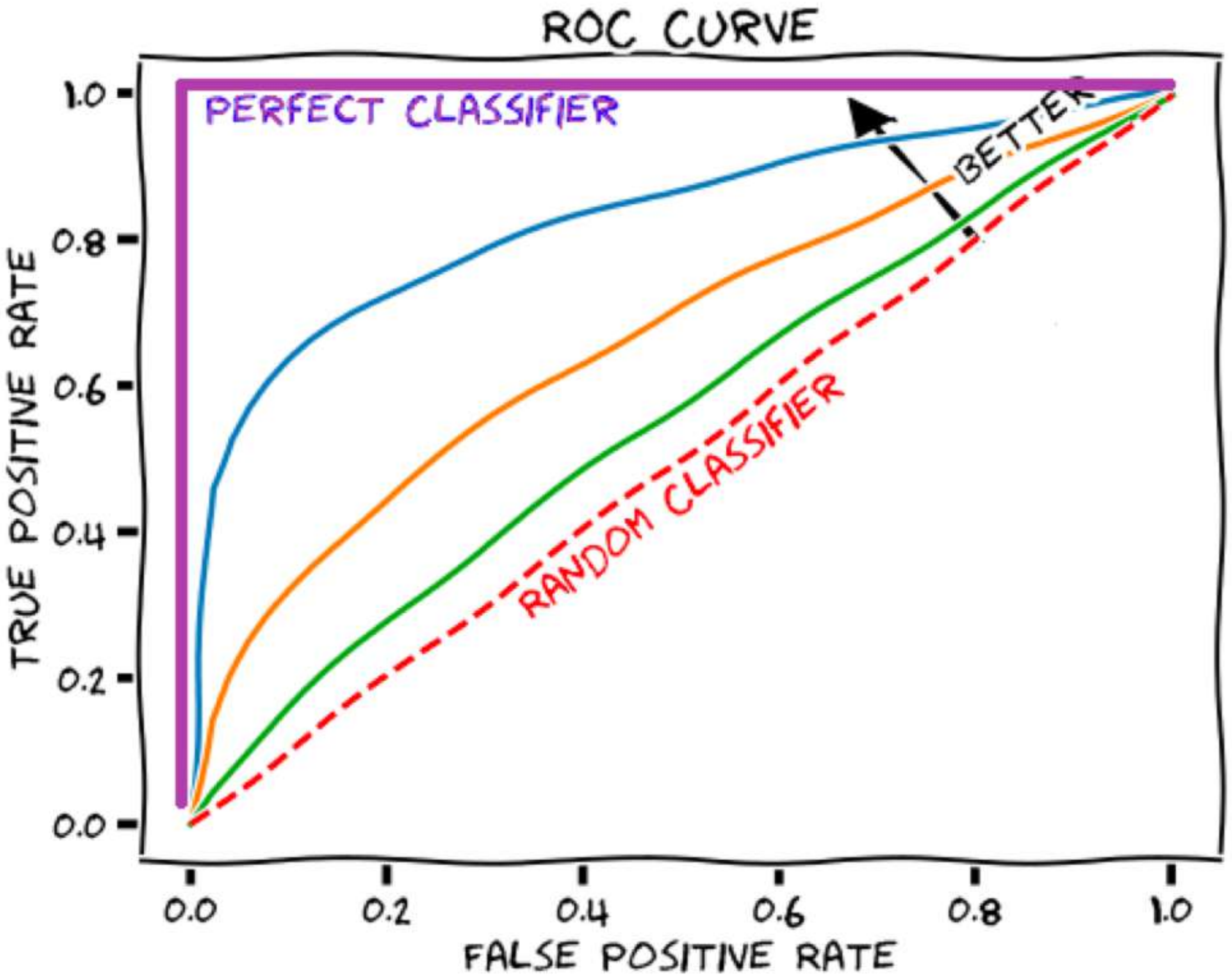

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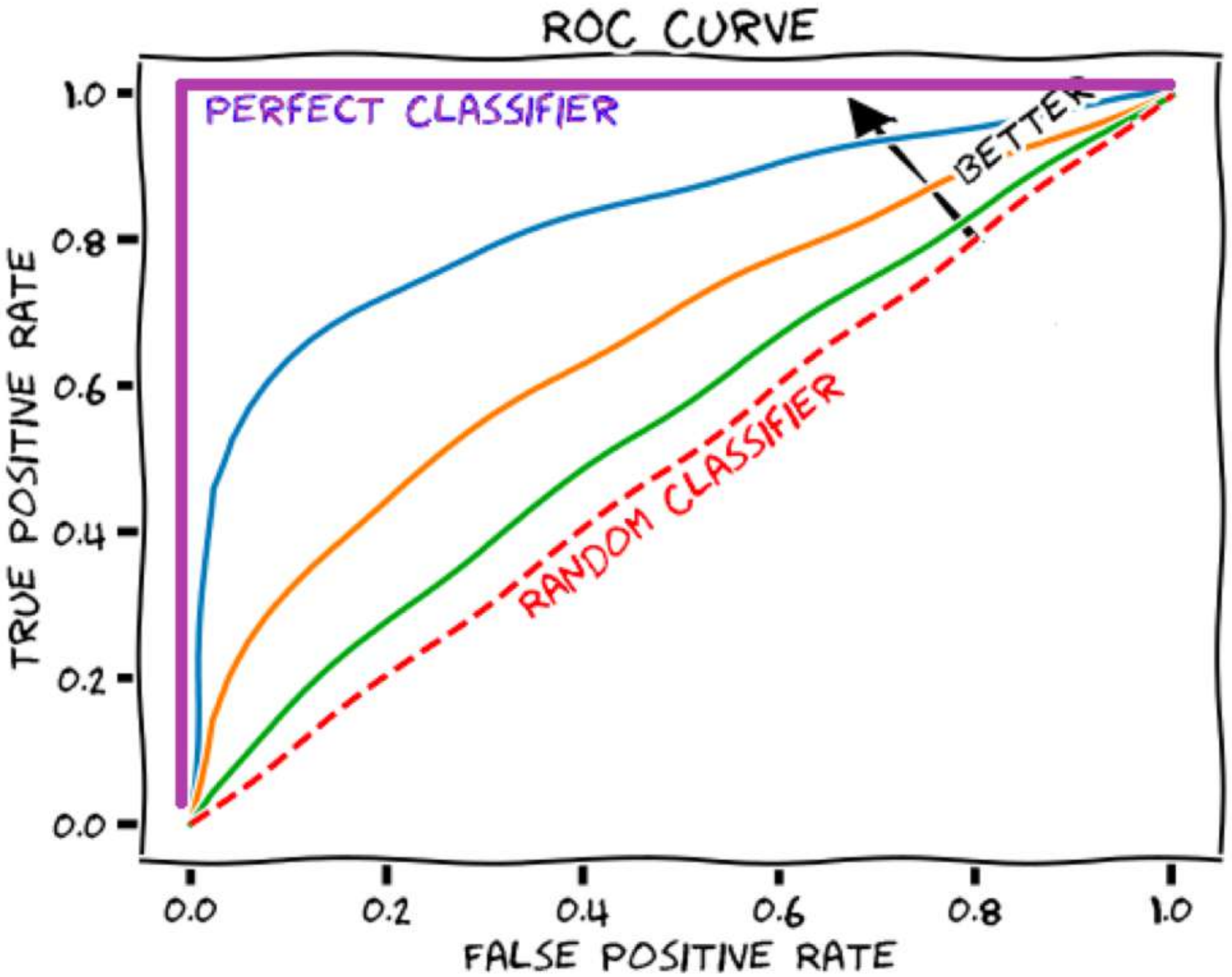

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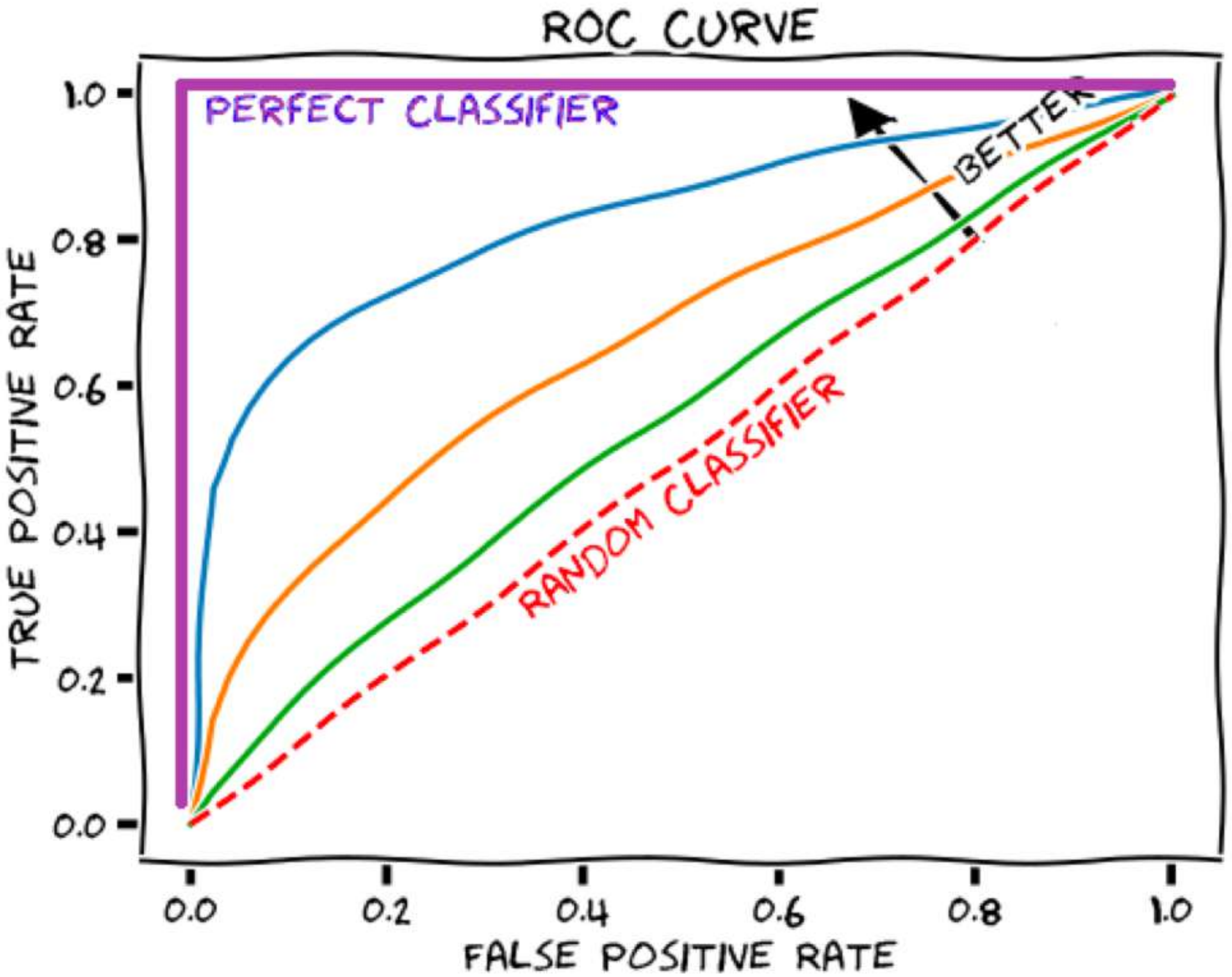
No True Positives either

ROC Curve: Example



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

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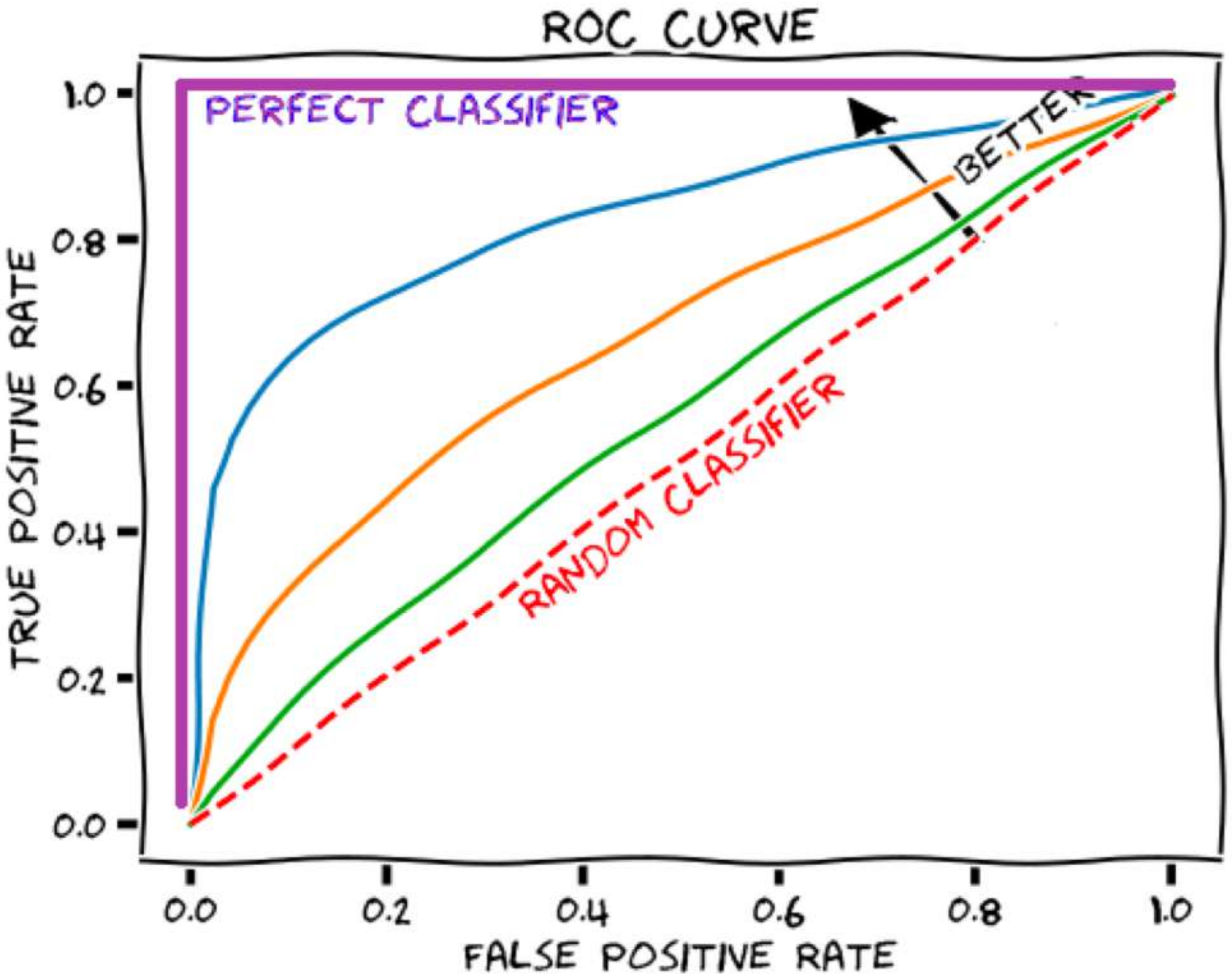

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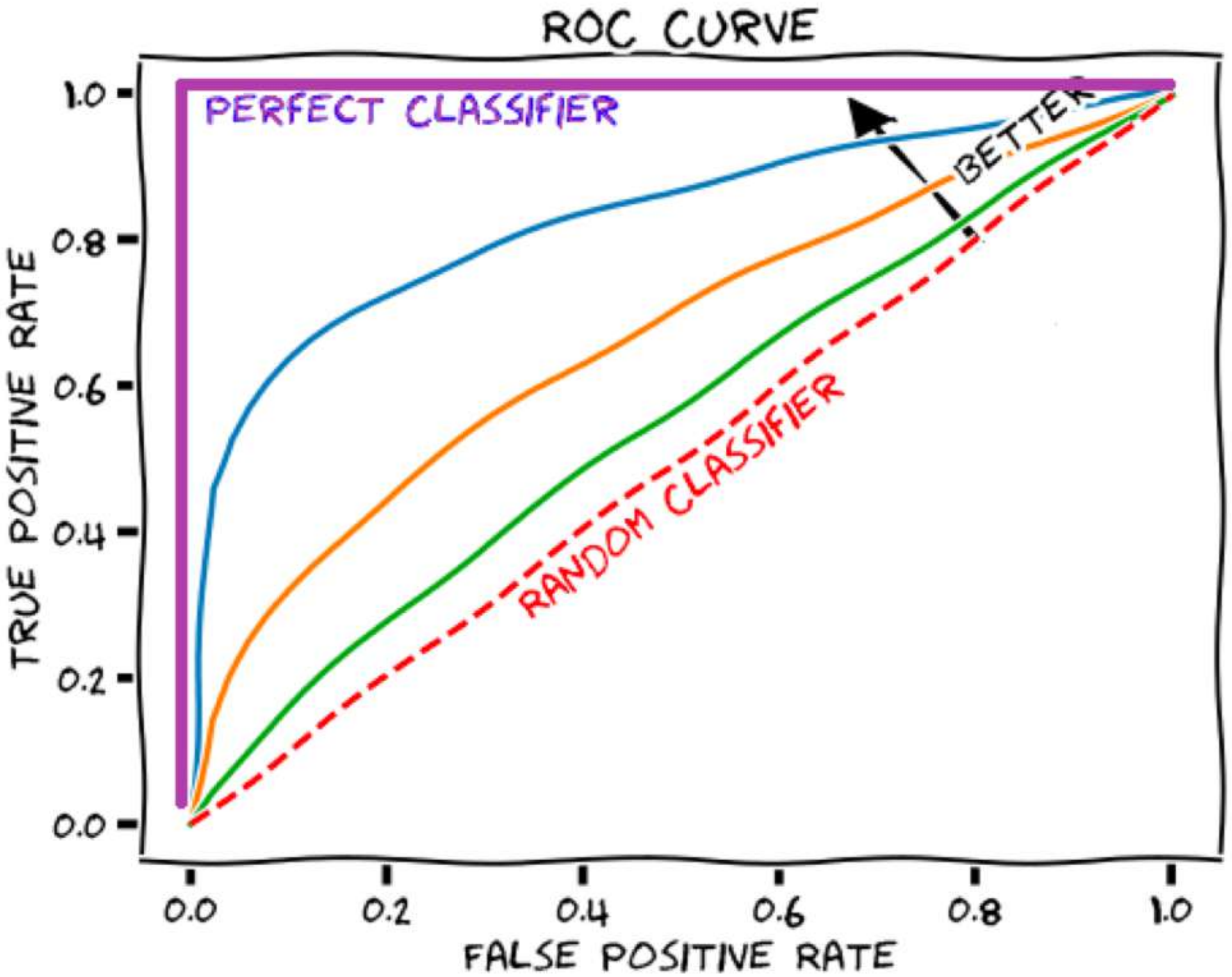

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High False Positives

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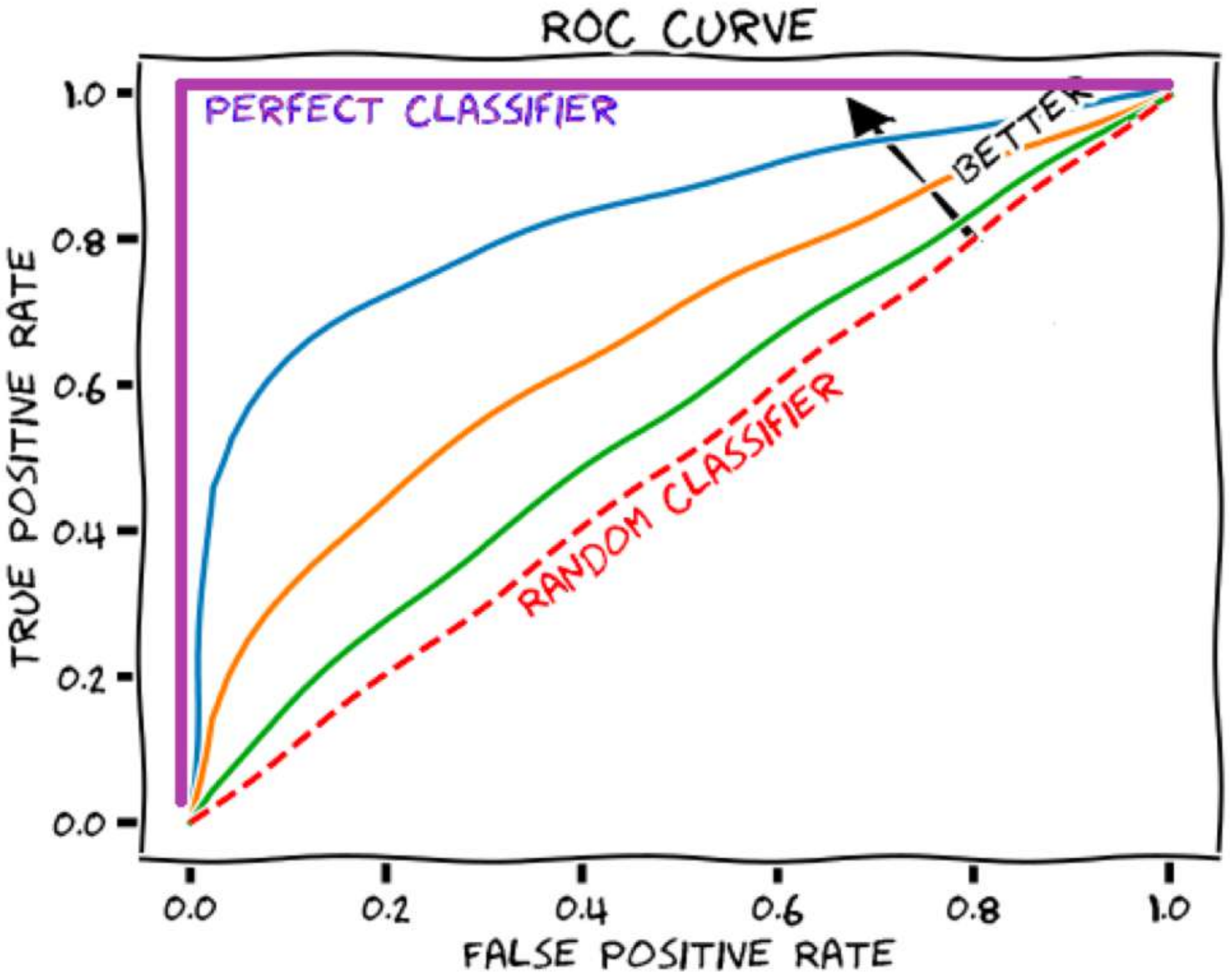

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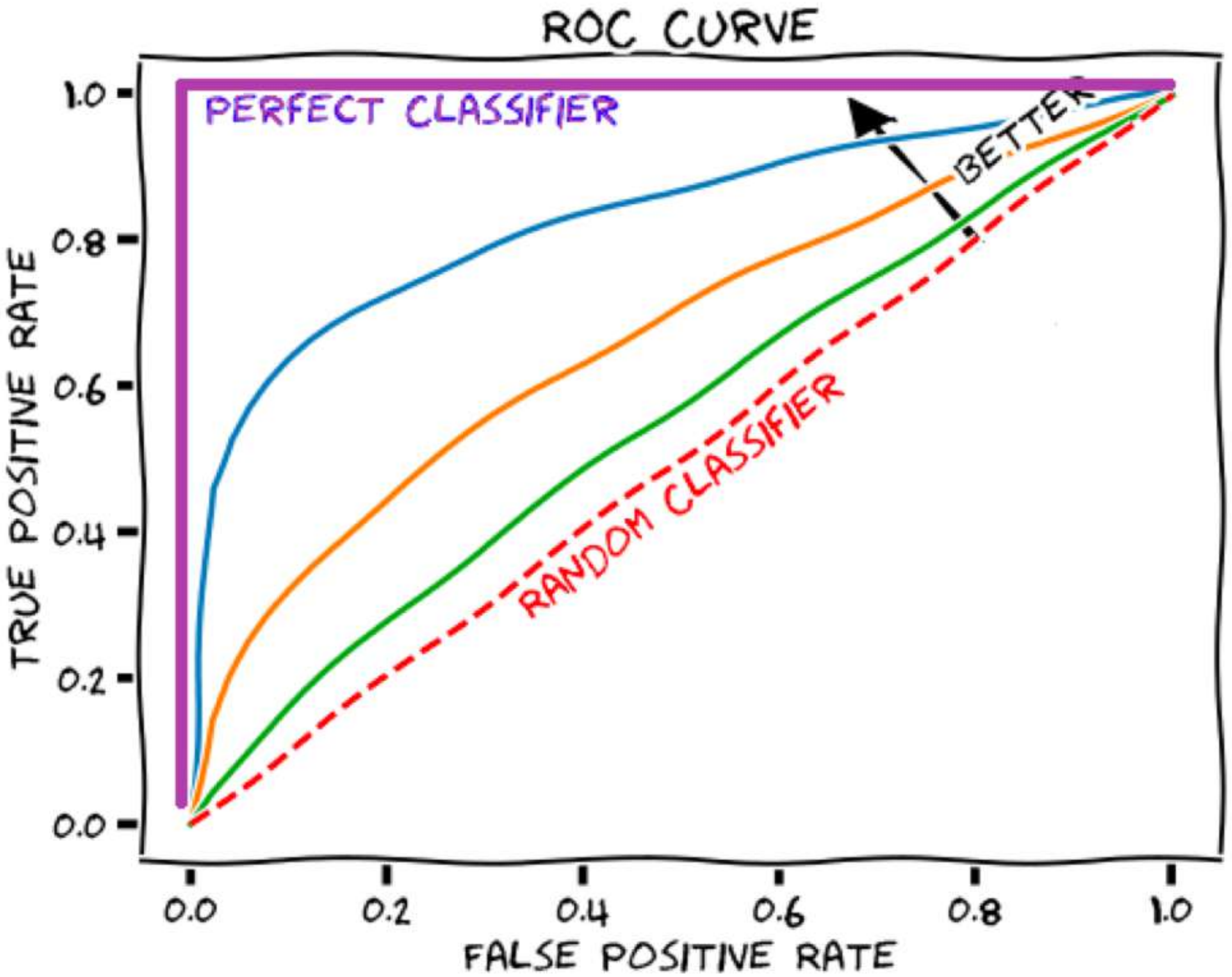

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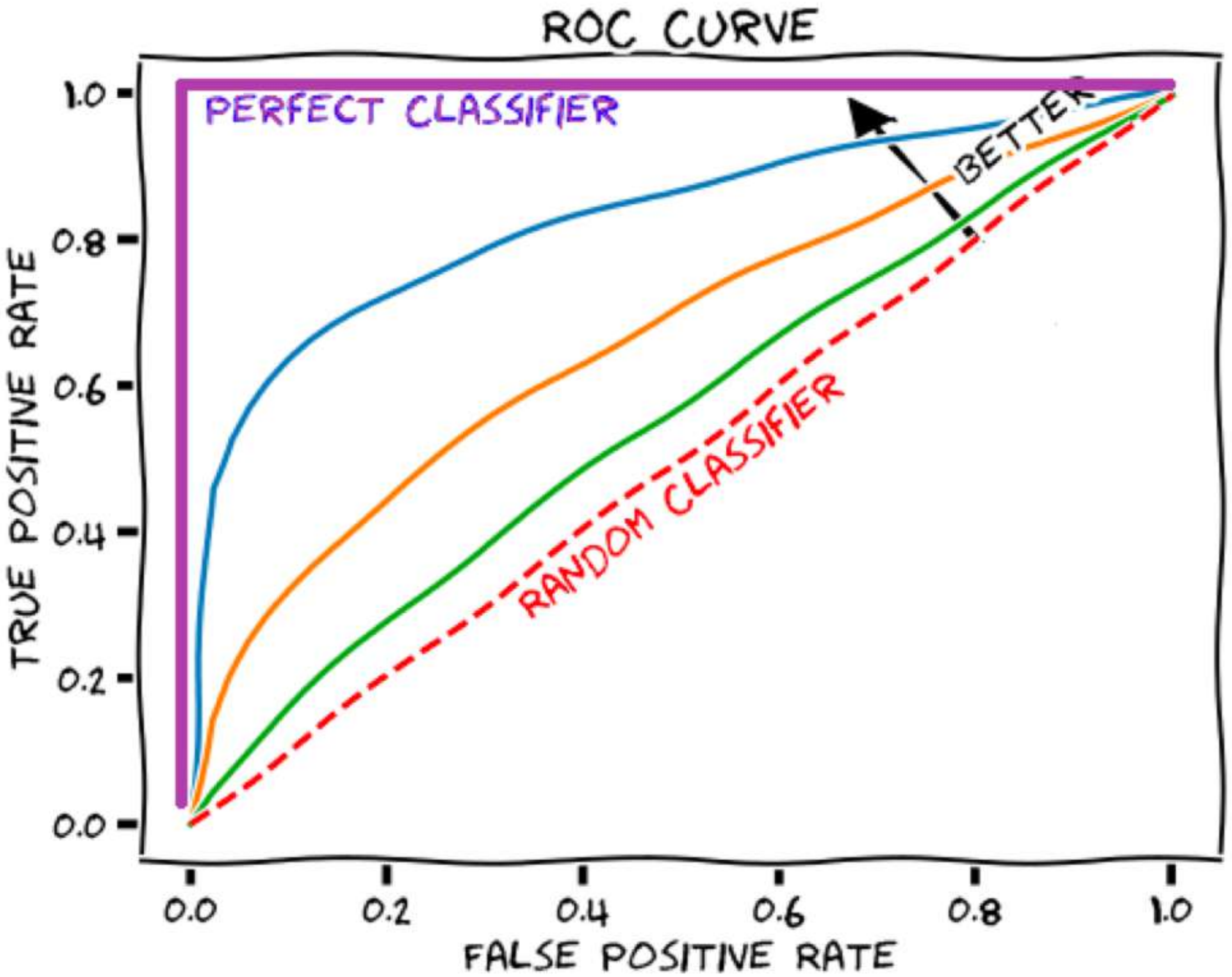

(0, 1) represents the **best** classifier possible

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100% Specificity

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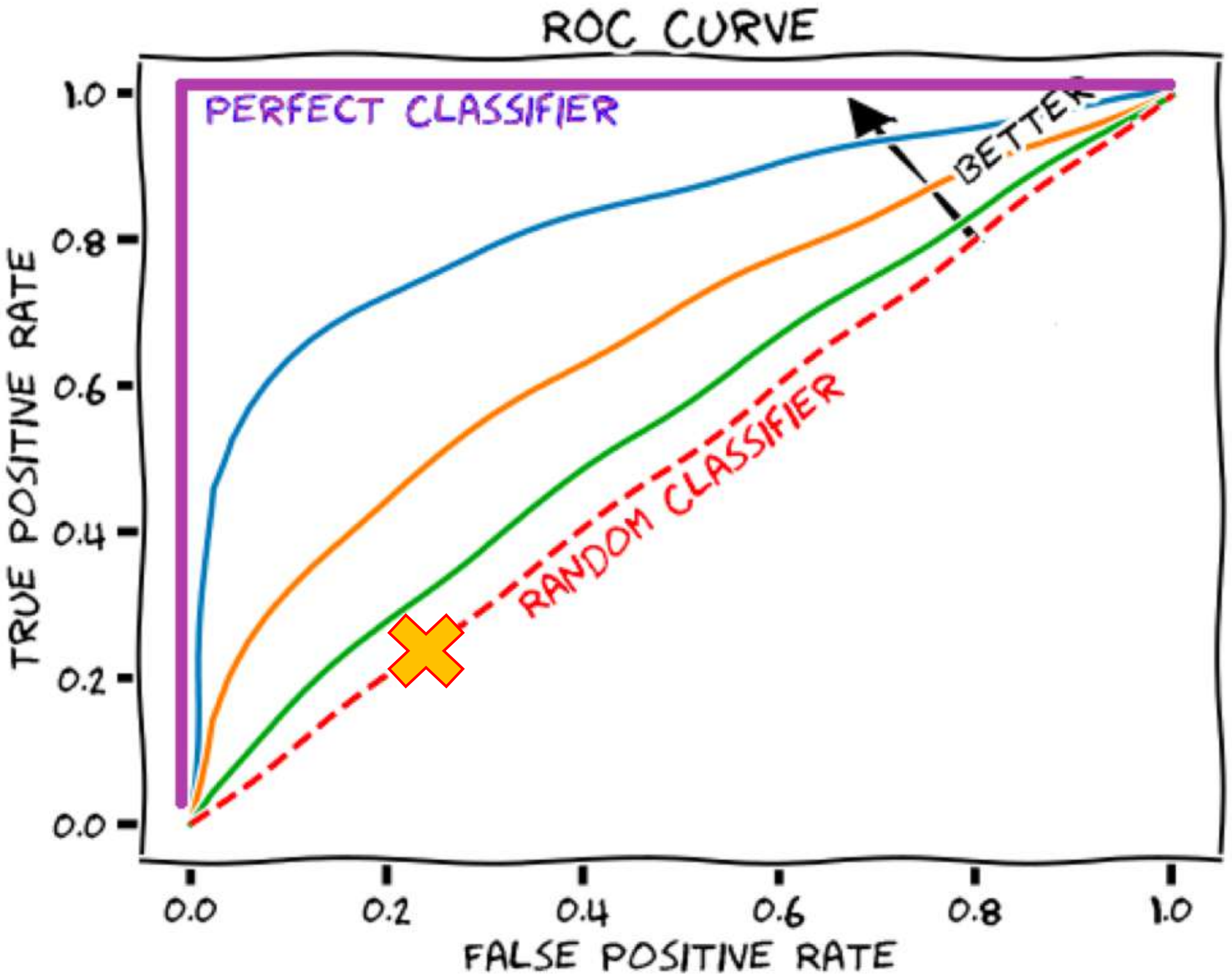

Any random guess will result into a point along the diagonal line (no-discrimination)

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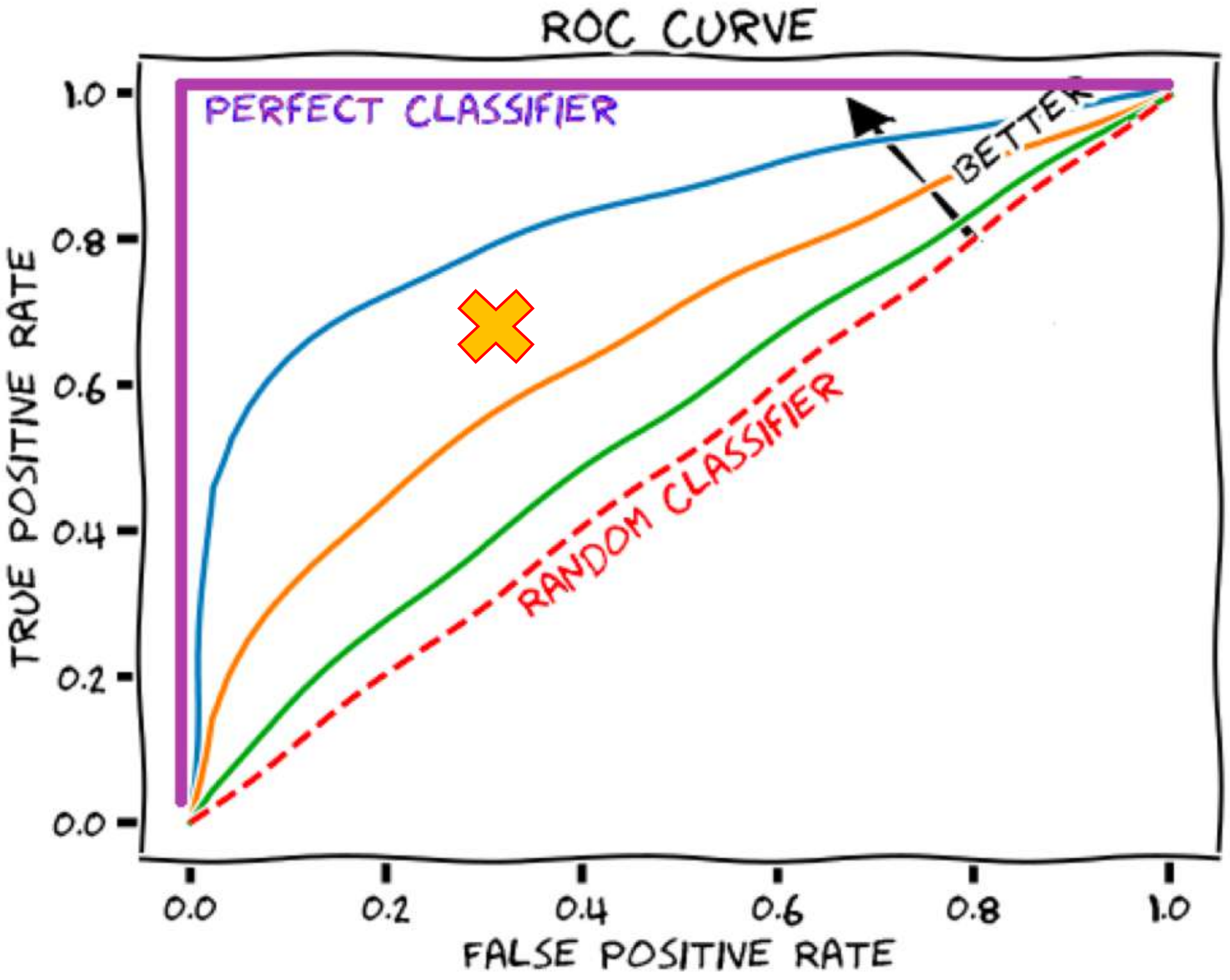

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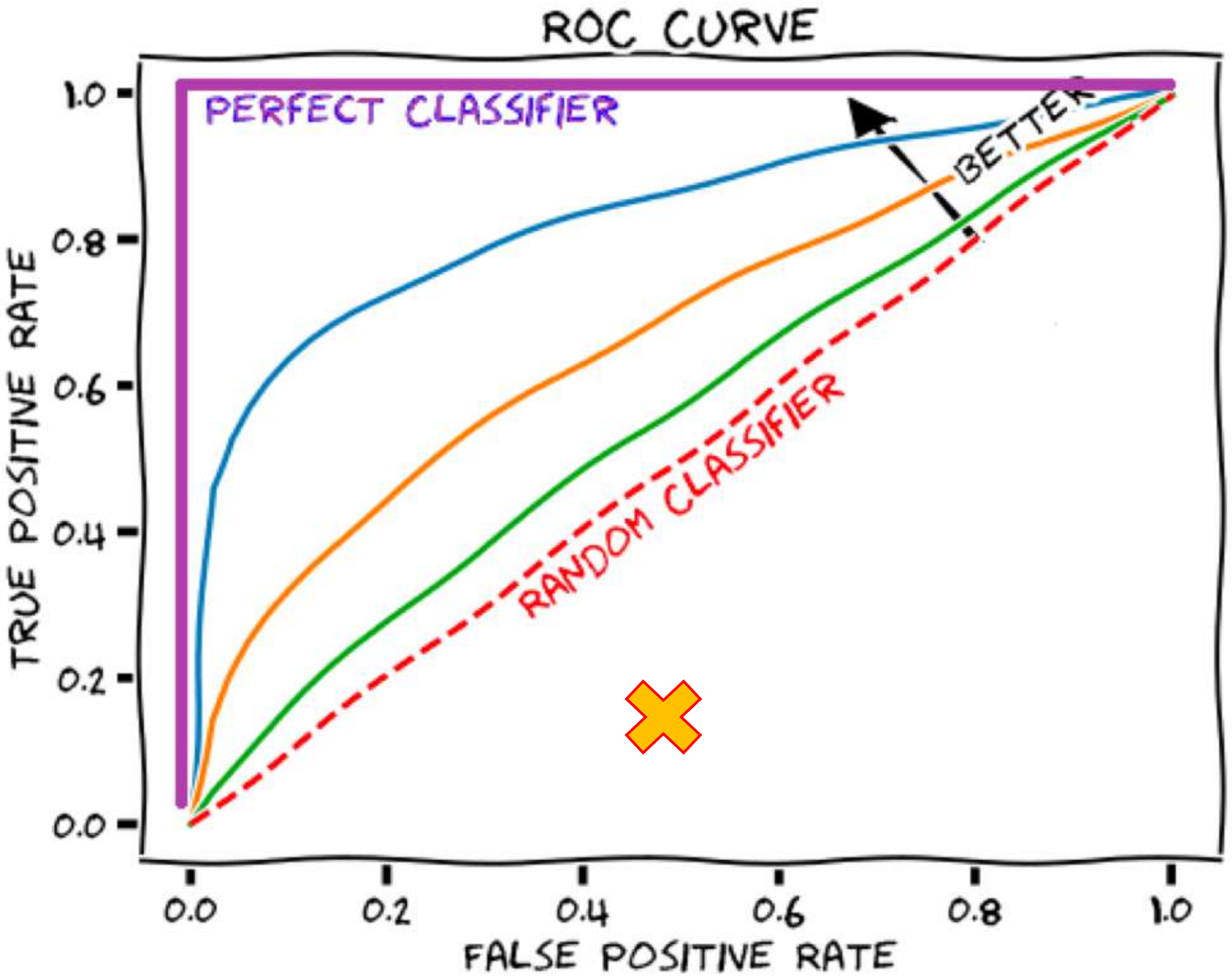

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Points above the diagonal are good classification results (better than random)

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)

ROC AUC: Area Under the ROC Curve

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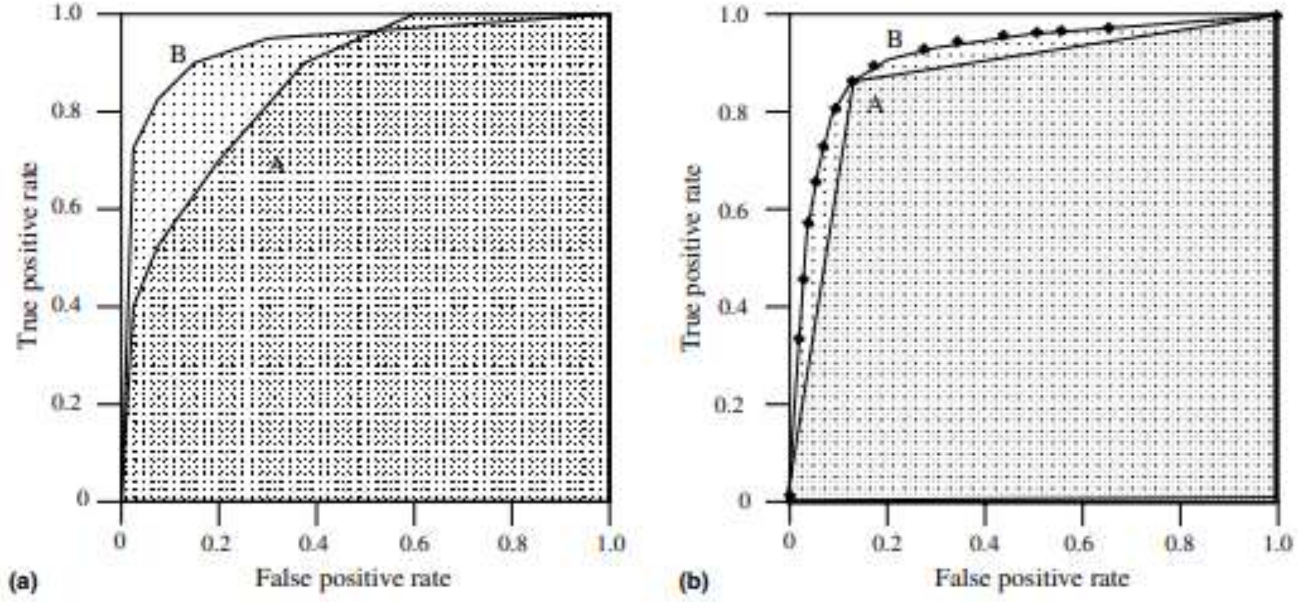
- The AUC of a ROC curve is a portion of the unit-square surface
- As such, it always ranges between 0 and 1
- The random classifier lies along the diagonal line and has ROC AUC = 0.5
- Any realistic and useful classifier should have ROC AUC > 0.5

ROC AUC: Area Under the ROC Curve



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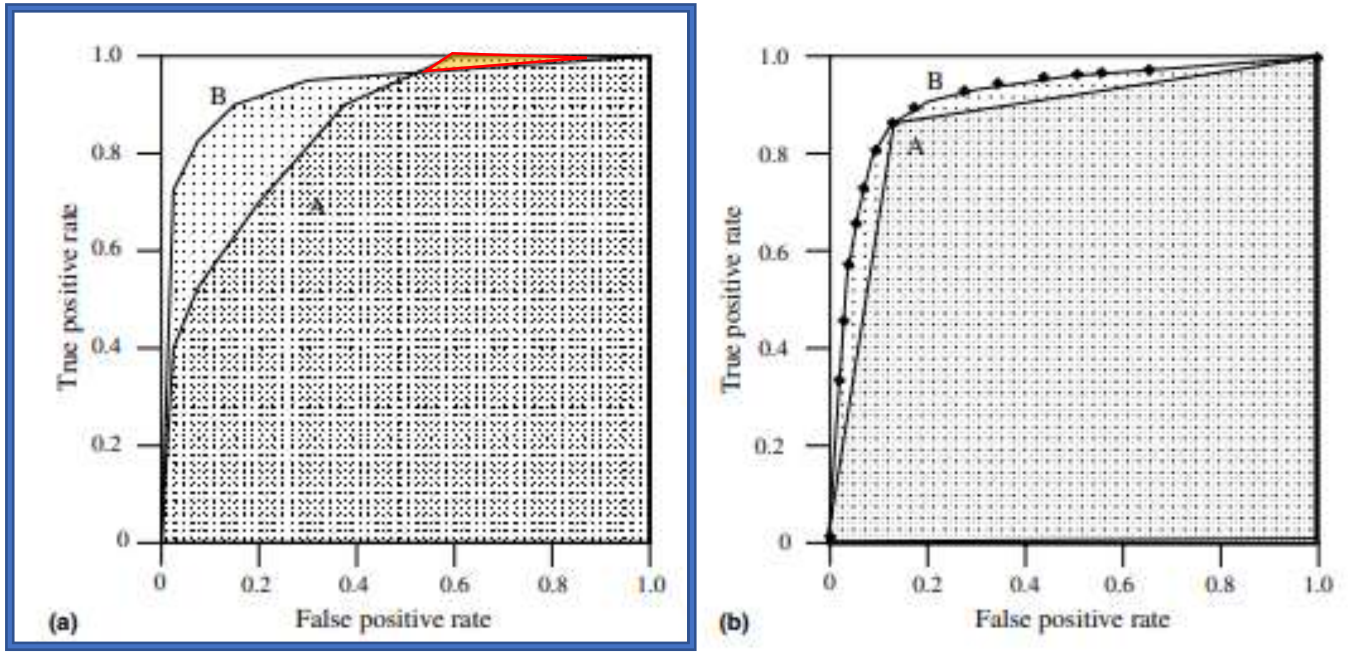
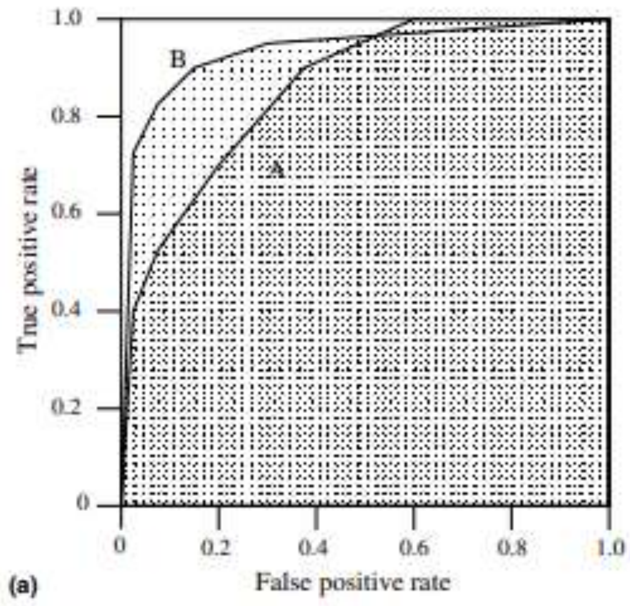
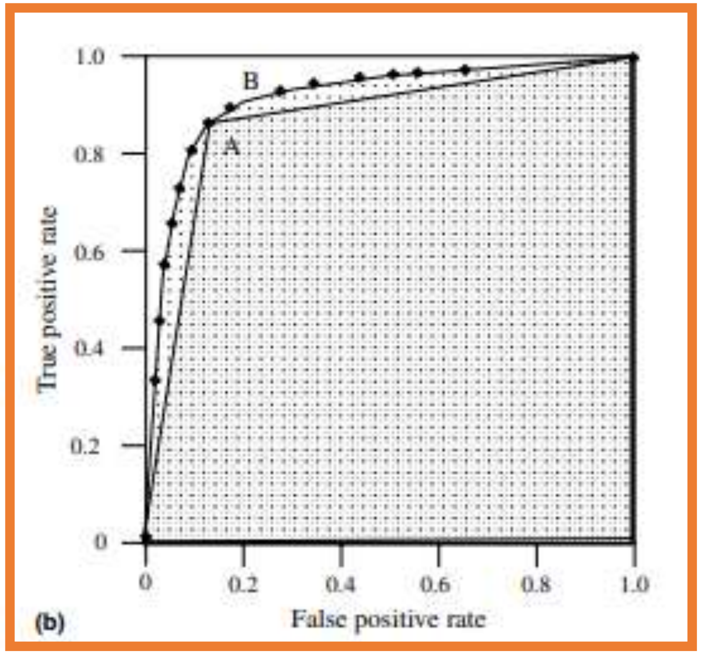


Classifier B has a greater ROC AUC than classifier A, although the latter may outperform the former at some specific threshold
(e.g., at FPR = 0.6 A is performing better than B)

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

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classification-threshold-invariant

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

Evaluation Metrics: Last Remarks

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  - 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