

# **Classification**

**DS 4400 | Machine Learning and Data Mining I**

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# Today's Outline

- Classification
- Metrics
- k-Nearest Neighbors

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- **Classification**
- Metrics
- k-Nearest Neighbors

# Classification

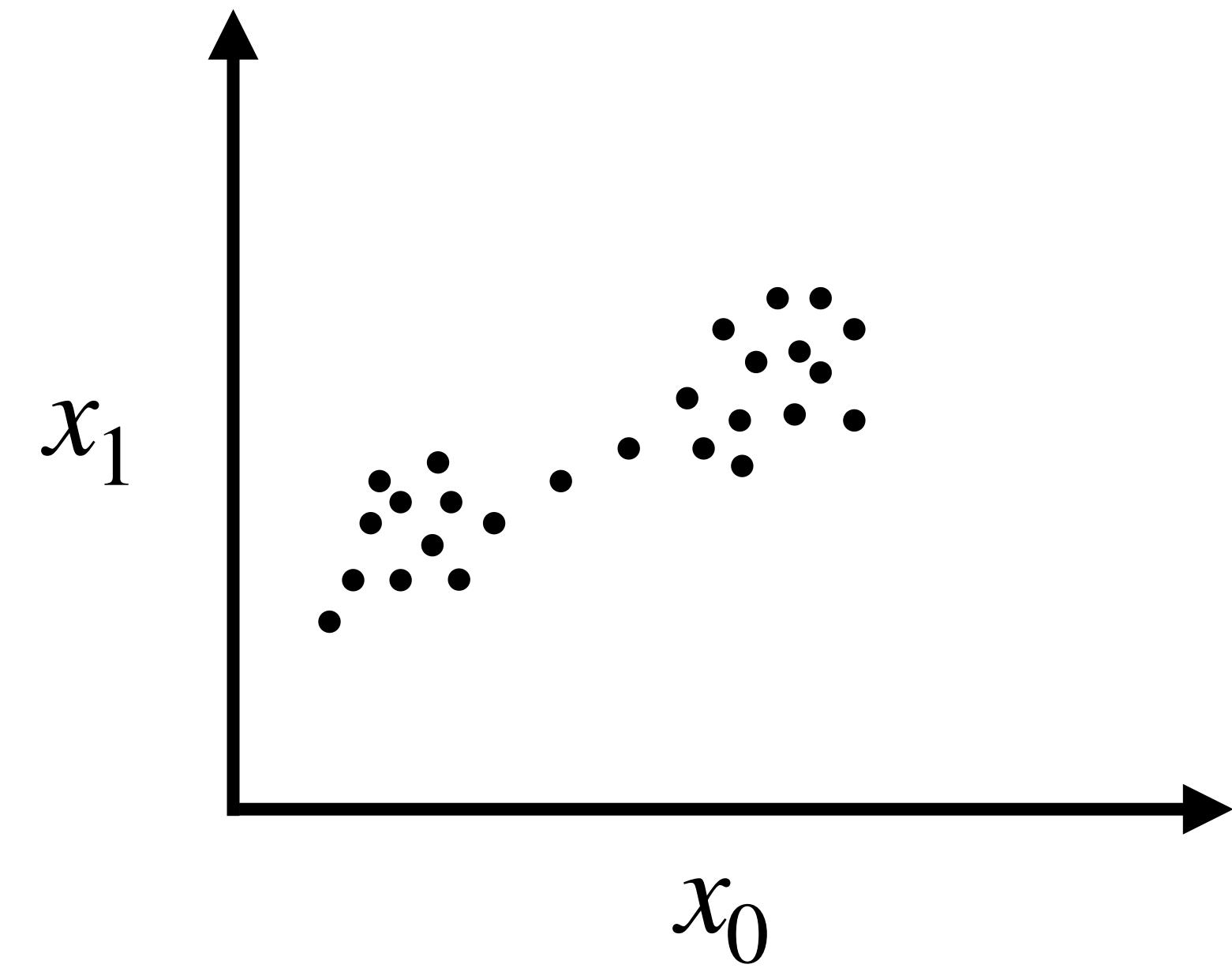
## Introduction

- Classification is a supervised learning task where the goal is to predict a discrete class label  $y$  for a given input  $x$
- For binary classification,  $y \in \{0, 1\}$
- For multi-class classification,  $y \in \{1, 2, \dots, k\}$  where  $k > 2$

# Classification

## Decision Boundary

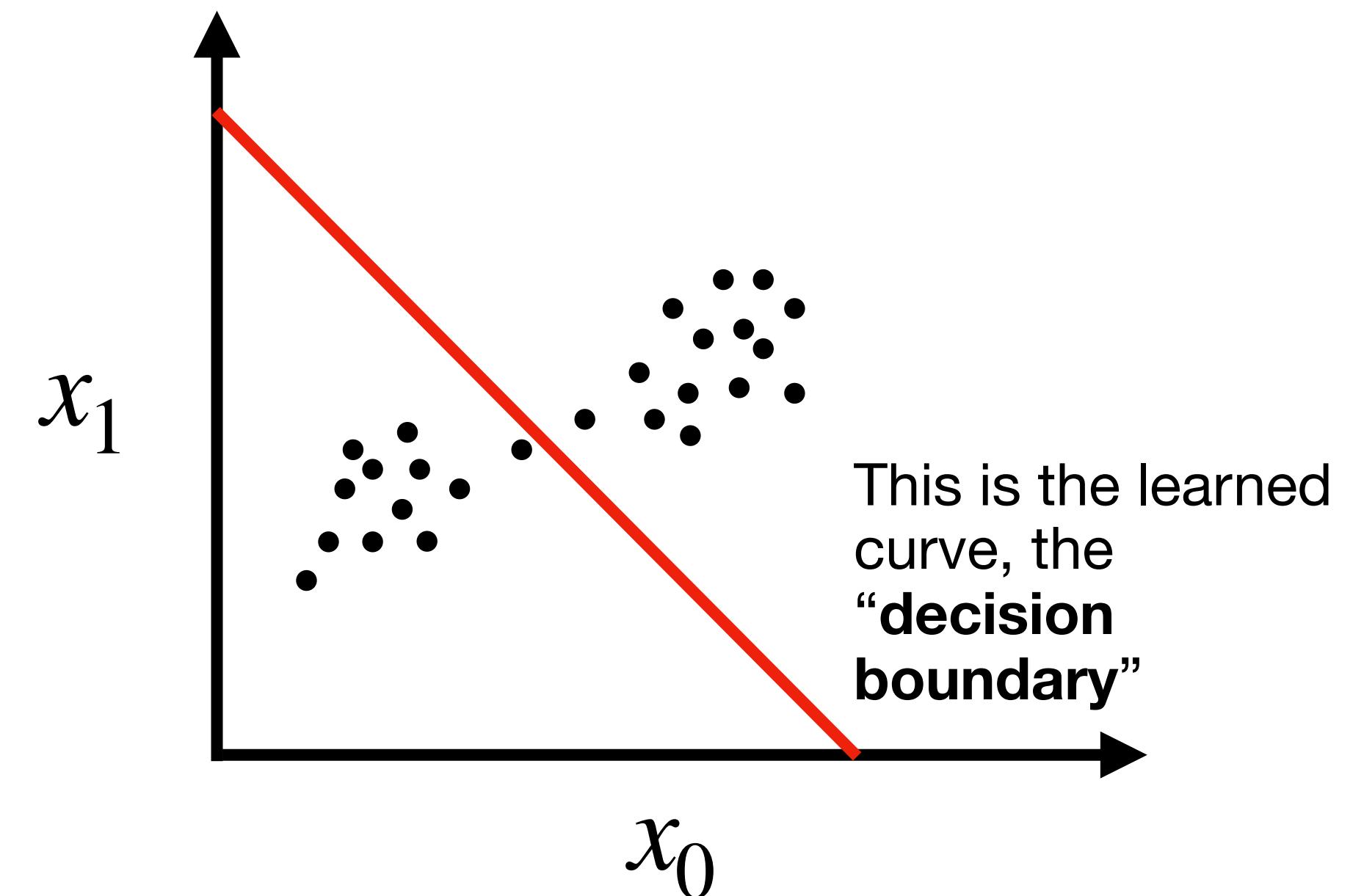
- A classifier partitions space into multiple sections, each section corresponding to a class.



# Classification

## Decision Boundary

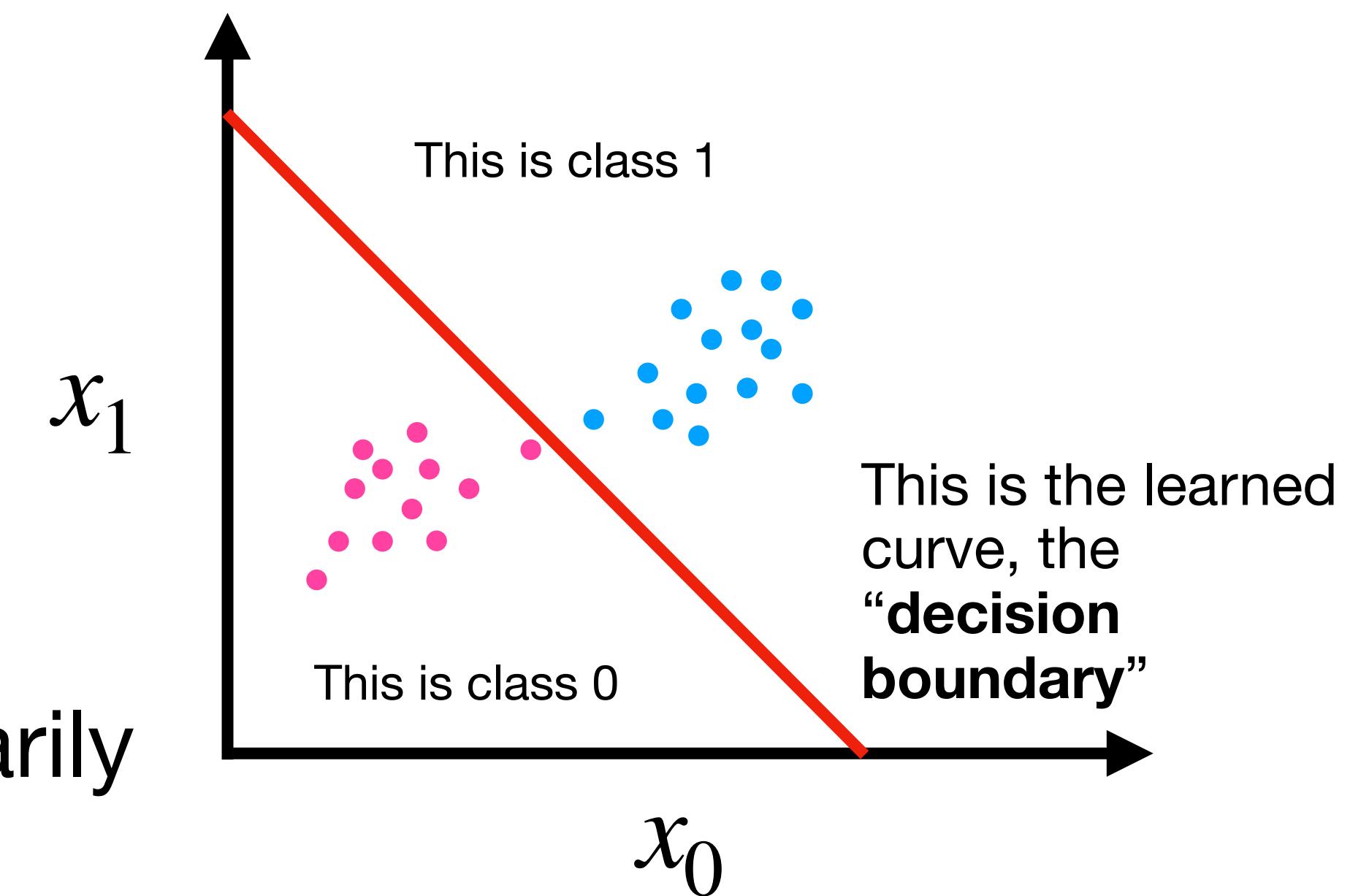
- A classifier partitions space into multiple sections, each section corresponding to a class.



# Classification

## Decision Boundary

- A classifier partitions space into multiple sections, each section corresponding to a class.
- Different algorithms produce different boundary shapes
  - Linear classifiers produce hyperplanes
  - Non-linear classifiers can produce arbitrarily complex boundaries.



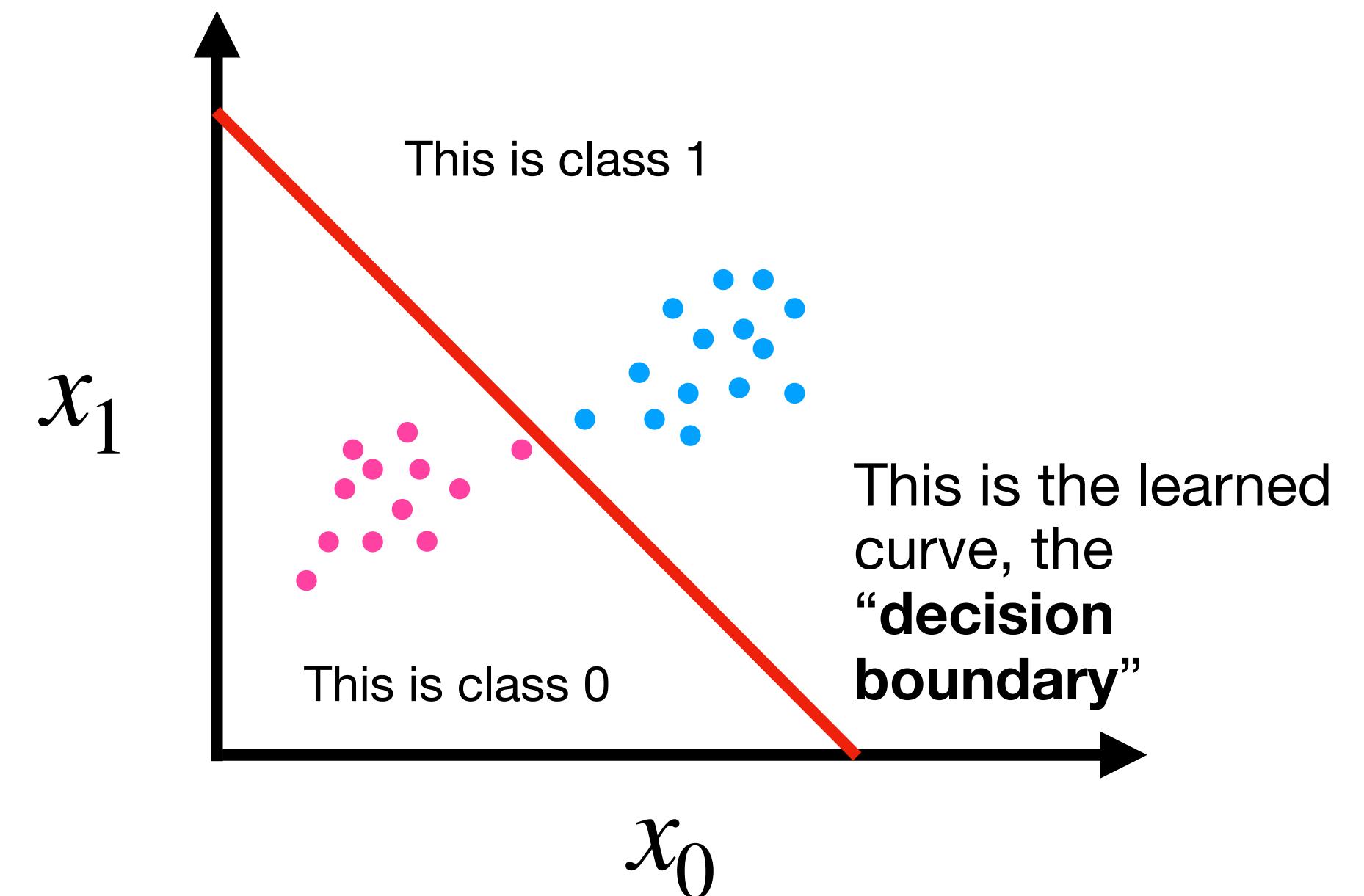
# Classification

## Decision Boundary

- But practically speaking, your classifier will output a probability value between 0 and 1

- Example:

- $\mathbb{P}(\text{cat} \mid \text{image}_1) = 0.61$
  - $\mathbb{P}(\text{cat} \mid \text{image}_2) = 0.52$

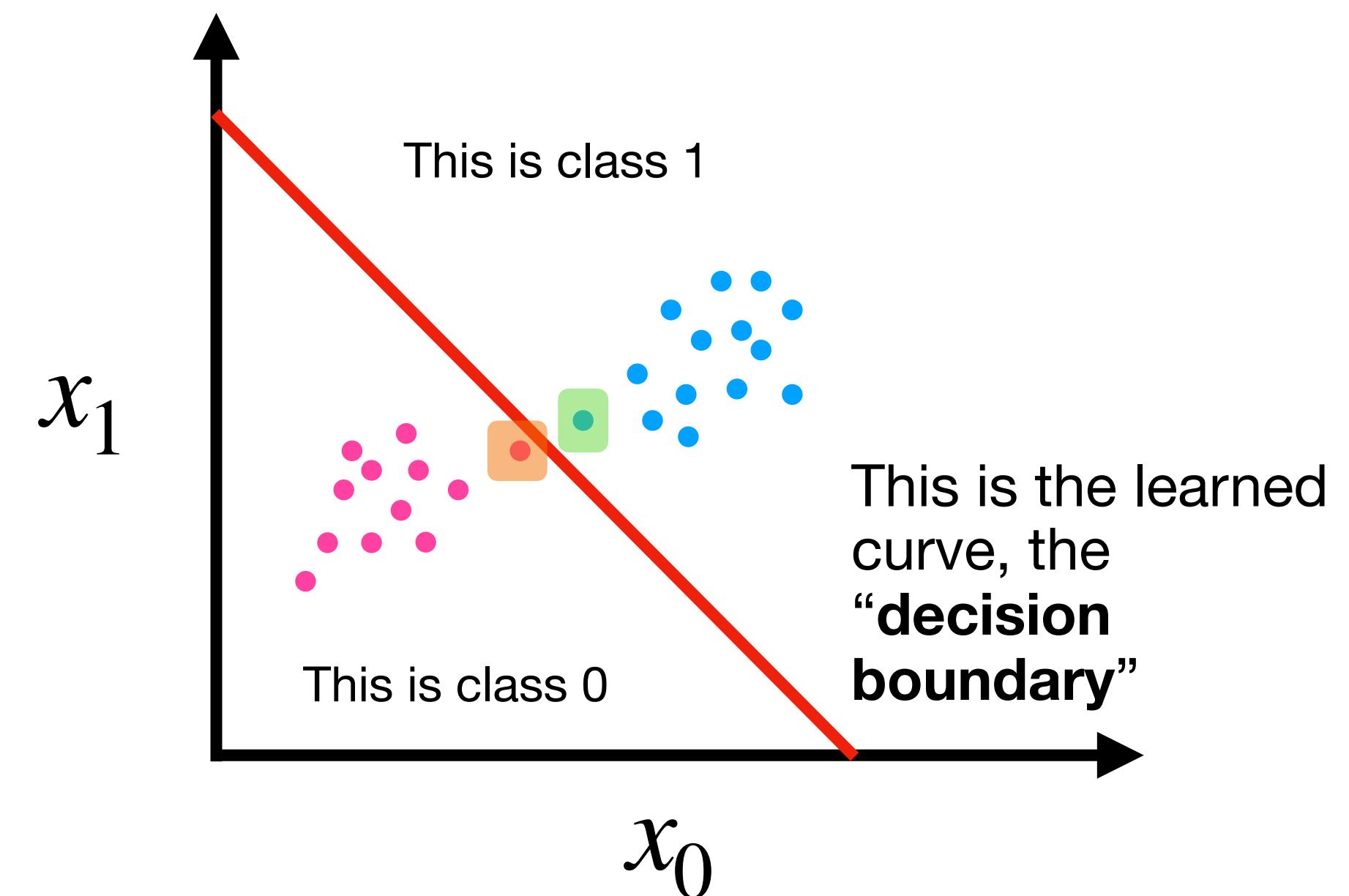


# Classification

## Decision Boundary

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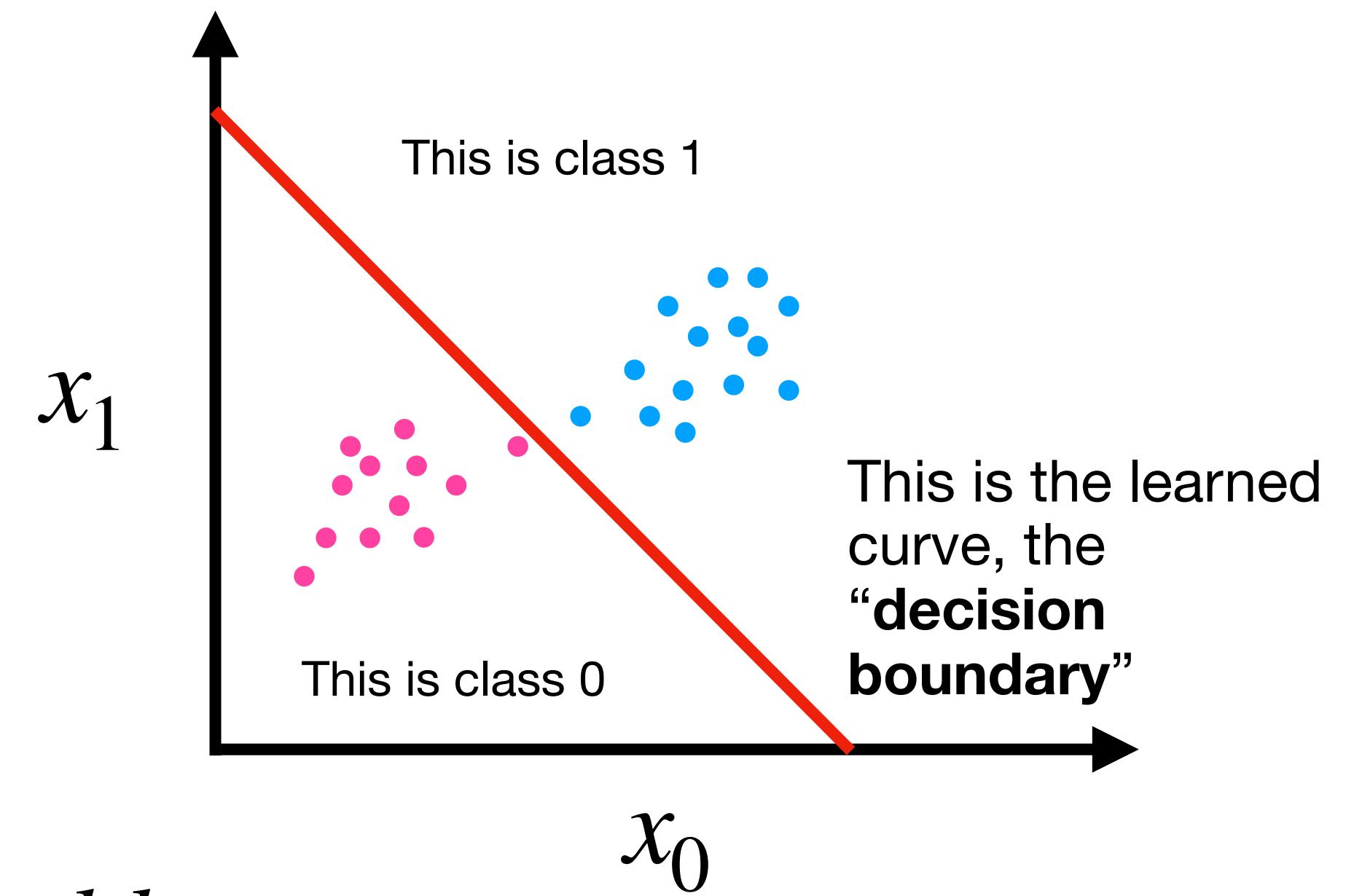
- $\mathbb{P}(\text{cat} \mid \text{image}_1) = 0.61$
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# Classification

## Decision Boundary

- But practically speaking, your classifier will output a probability value between 0 and 1
- Example:
  - $\mathbb{P}(\text{cat} \mid \text{image}_1) = 0.61$
  - $\mathbb{P}(\text{cat} \mid \text{image}_2) = 0.52$
- Practitioner needs to also set a **threshold**
  - $\text{image}_i$  is a cat if  $\mathbb{P}(\text{cat} \mid \text{image}_i) \geq \text{Threshold}$



# Today's Outline

- Classification
- **Metrics**
- k-Nearest Neighbors

# Metrics

- An obvious metric is **accuracy**

$$Accuracy = \frac{\text{Number of Correct Predictions}}{\text{Total Number of Data Points}}$$

- Say you have a cat classifier with 1000 images. Your classifier gets 797 out of 1000 images correct

$$Accuracy = \frac{797}{1000} = 79\%$$

# Metrics

- But, accuracy does not tell the whole picture
- Especially when data is skewed
  - For example, if your training data is of size 1000 images
    - 900 of them are of dogs
    - 100 of them are cats
  - **Question:** Why would accuracy not work in this case?

# Metrics

## Confusion Matrix

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
<b>Actual Positive</b>	True Positive (TP)	False Negative (FN)
<b>Actual Negative</b>	False Positive (FP)	True Negative (TN)

# Metrics

## Confusion Matrix

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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# Metrics

## Confusion Matrix

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# Metrics

## Accuracy

	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
Actual Negative	False Positive (FP)	True Negative (TN)

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

The proportion of correct predictions.

Simple and intuitive, but misleading for imbalanced data.

A classifier that always predicts the majority class achieves high accuracy on imbalanced datasets while being useless.

# Metrics

## Precision and Recall

$$\text{Precision} = \frac{TP}{TP + FP}$$

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
<b>Actual Positive</b>	True Positive (TP)	False Negative (FN)
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# Metrics

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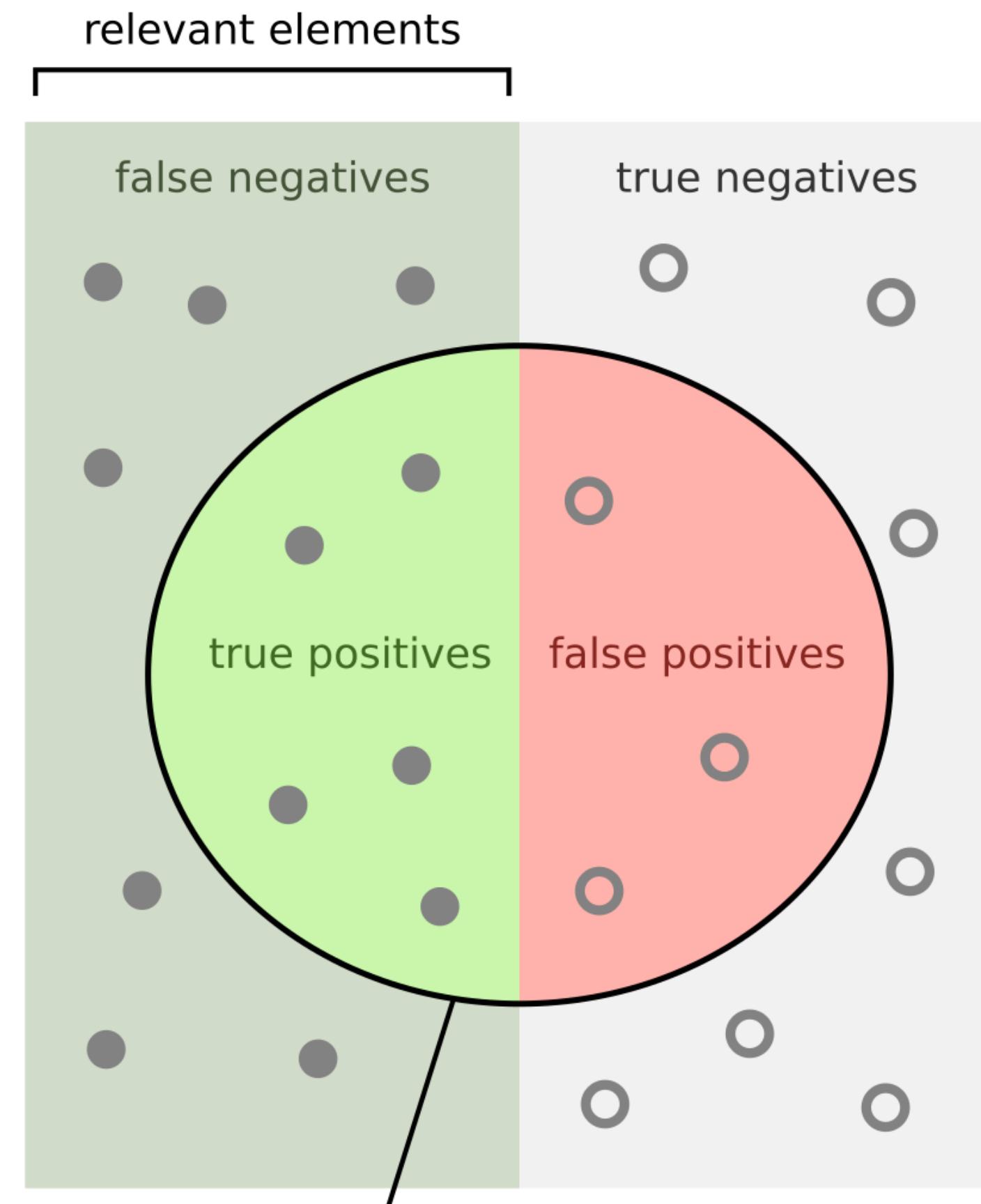
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# Metrics

## Precision and Recall

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$



How many retrieved items are relevant?

$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$



How many relevant items are retrieved?

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$



	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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# Metrics

## Precision and Recall

$$\text{Precision} = \frac{TP}{TP + FP}$$

Of all instances predicted as positive, what fraction actually are positive? Precision measures the **reliability of positive predictions**. High precision means **few false alarms**.

$$\text{Recall} = \frac{TP}{TP + FN}$$

**When to care about precision?**  
When false positives are costly.

Examples include spam filtering (users hate losing important emails), recommendation systems (irrelevant recommendations erode trust), and legal contexts (wrongful accusations).

	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
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# Metrics

## Precision and Recall

$$\text{Precision} = \frac{TP}{TP + FP}$$

Of all actual positive instances, **what fraction did we correctly identify?** Recall measures coverage of positive instances. High recall means **few missed positives**.

**When to care about recall?**

When false negatives are costly.

$$\text{Recall} = \frac{TP}{TP + FN}$$

Examples include disease screening (missing a diagnosis can be fatal), security threats (missing an attack is catastrophic), and search engines (users want all relevant results).

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
<b>Actual Positive</b>	True Positive (TP)	False Negative (FN)
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# Metrics

## Precision vs Recall Tradeoff - F1 Score

$$\text{Precision} = \frac{TP}{TP + FP}$$

Precision and recall are **inherently in tension**.

$$\text{Recall} = \frac{TP}{TP + FN}$$

Decreasing the threshold has the opposite effect.

The optimal balance depends on the application's cost structure.

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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# Metrics

## Precision vs Recall Tradeoff - F1 Score

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$F1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall} = \frac{2TP}{2TP + FP + FN}$$

The harmonic mean of precision and recall

F1 score is high only when **both** precision and recall are high

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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$$\text{Recall} = \frac{TP}{TP + FN}$$

$$\text{Specificity} = \frac{TN}{TN + FP}$$

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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$$F1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall} = \frac{2TP}{2TP + FP + FN}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$\text{Specificity} = \frac{TN}{TN + FP}$$

$$\text{False Positive Rate} = \frac{FP}{TN + FP}$$

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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$$\text{Specificity} = \frac{TN}{TN + FP}$$

$$\text{False Positive Rate} = \frac{FP}{TN + FP}$$

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Same denominator

# Metrics

## Precision vs Recall Tradeoff - F1 Score

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$F1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall} = \frac{2TP}{2TP + FP + FN}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$\text{Specificity} = \frac{TN}{TN + FP}$$

$$\text{False Positive Rate} = \frac{FP}{TN + FP}$$

Same denominator

FPR = 1 - Specificity

	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
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## Precision vs Recall Tradeoff - F1 Score

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$$\boxed{\text{Recall} = \frac{TP}{TP + FN}}$$

$$\text{Specificity} = \frac{TN}{TN + FP}$$

$$\text{False Positive Rate} = \frac{FP}{TN + FP}$$

	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
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**Recall is the True Positive Rate**

# Metrics

## Why so many metrics?

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

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

Assume your training data looks like this:

1000 rows  
10 rows are spam emails  
990 are legitimate emails

Scenario 1:

Classifier always outputs legit  
**What is the accuracy?**

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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Assume your training data looks like this:

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Scenario 1:

Classifier always outputs legit  
**What is the accuracy?**

$$Acc = \frac{0 + 990}{0 + 990 + 0 + 10} = 99\%$$

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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Scenario 2:

Classifier predicts **one** spam email as spam, and rest as legitimate  
**What is the precision?**

# Metrics

## Why so many metrics?

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Scenario 2:

Classifier predicts **one** spam email as spam, and rest as legitimate  
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$$Precision = \frac{1}{1 + 0} = 100\%$$

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Scenario 2:

Classifier predicts **one** spam email as spam, and rest as legitimate  
**What is the precision?**

$$Precision = \frac{1}{1 + 0} = 100\%$$

Scenario 3:

Classifier always outputs spam  
**What is the recall?**

# Metrics

## Why so many metrics?

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

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Classifier always outputs legit  
**What is the accuracy?**

$$Acc = \frac{0 + 990}{0 + 990 + 0 + 10} = 99\%$$

Scenario 2:

Classifier predicts **one** spam email as spam, and rest as legitimate  
**What is the precision?**

$$Precision = \frac{1}{1 + 0} = 100\%$$

Scenario 3:

Classifier always outputs spam  
**What is the recall?**

$$Recall = \frac{10}{10 + 0} = 100\%$$

# Metrics

## Precision vs Recall Tradeoff - F1 Score

**Question:**

How is this a tradeoff?  
How would you increase/decrease the true positives?

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
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# Metrics

## Precision vs Recall Tradeoff - F1 Score

**Question:**

How is this a tradeoff?  
How would you increase/decrease the true positives?

**Answer: By changing the threshold**

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## Precision vs Recall Tradeoff - F1 Score

$$\text{Precision} = \frac{TP}{TP + FP}$$

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### Answer: By changing the threshold

	Predicted Positive	Predicted Negative
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- Cat in image if  $\mathbb{P}(\text{cat} \mid \text{image}_i) \geq 0$
- Precision goes down, Recall goes up

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## Precision vs Recall Tradeoff - F1 Score

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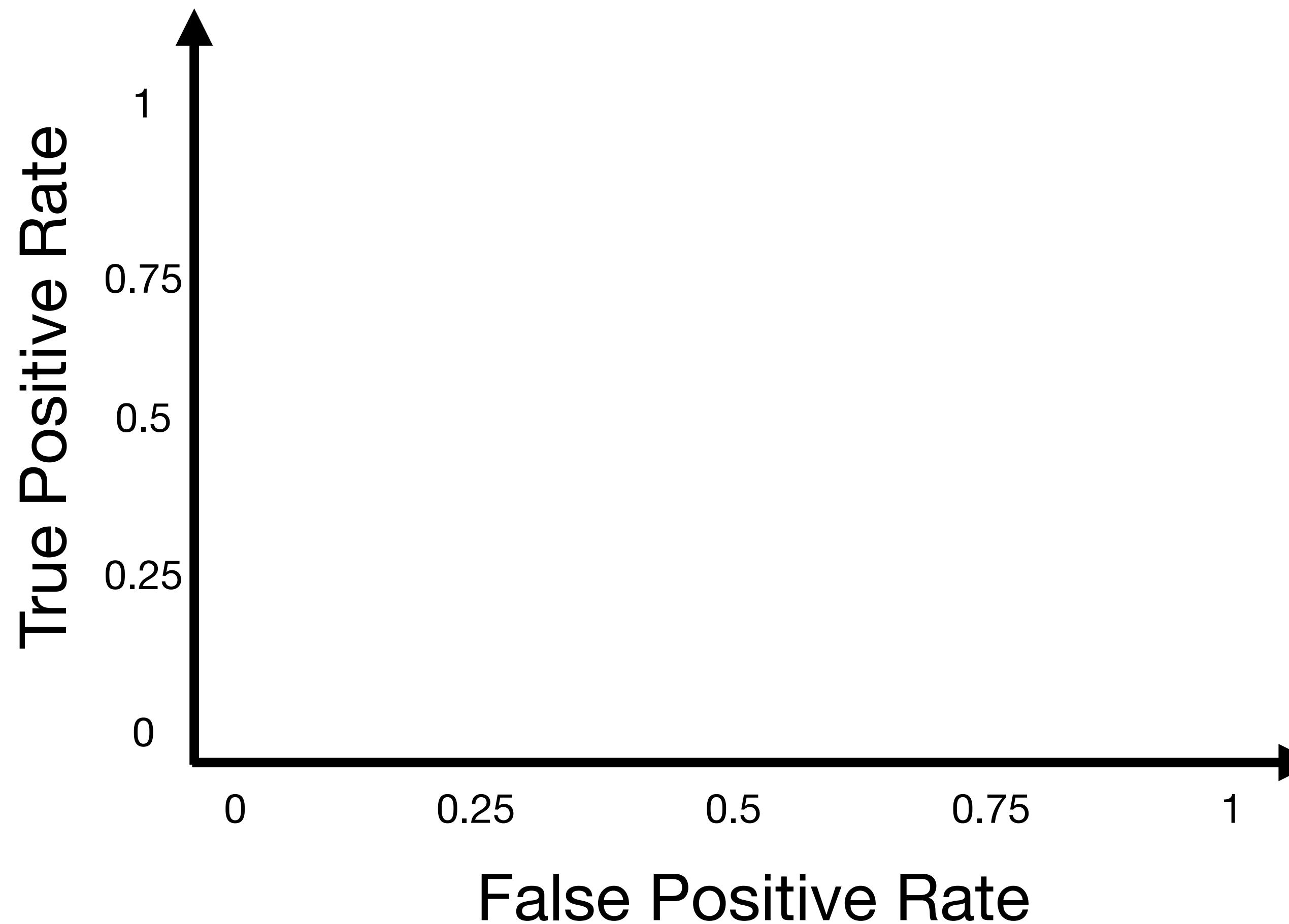
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# Metrics

## AUC-ROC Curve

$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{TN + FP}$$

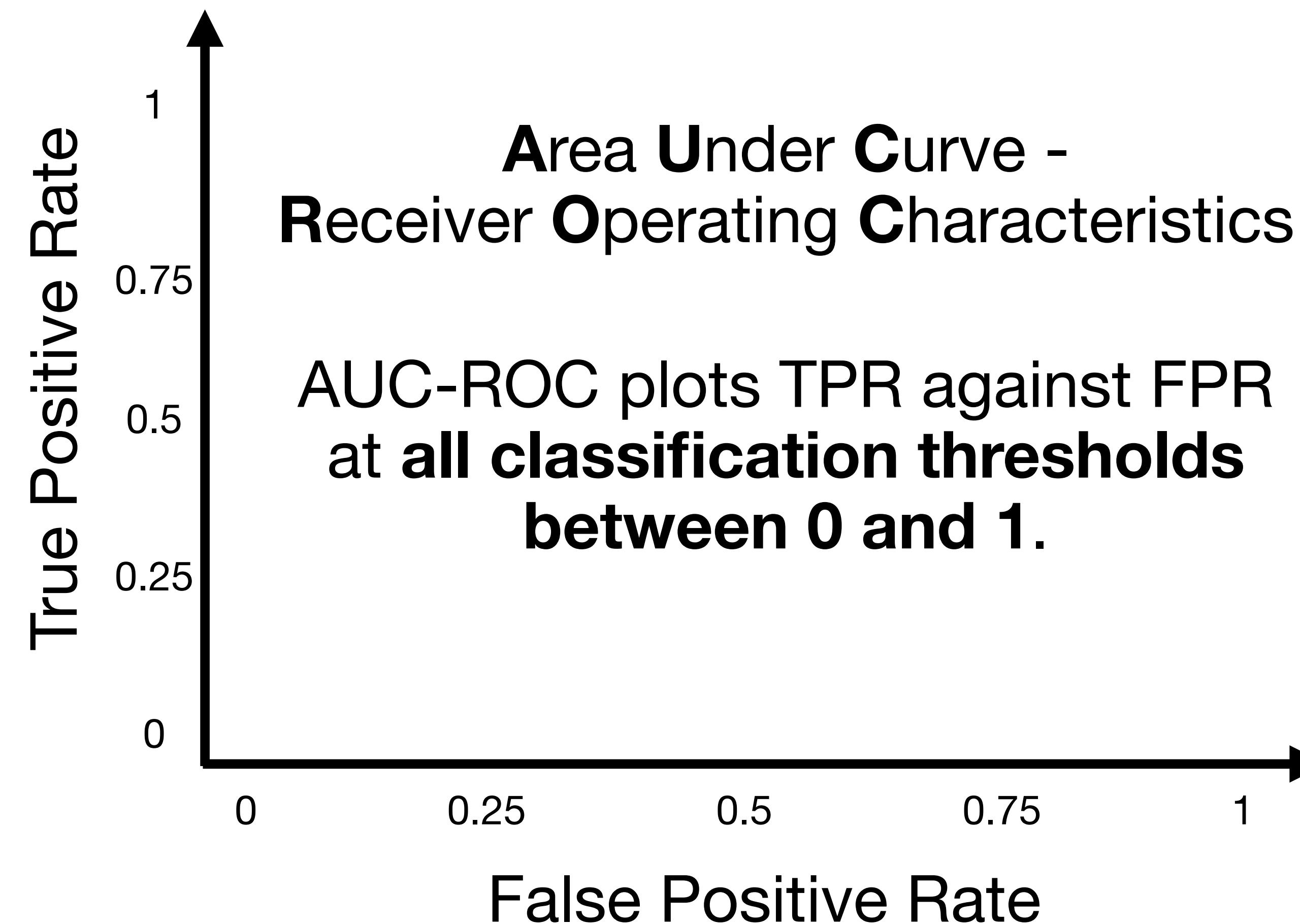


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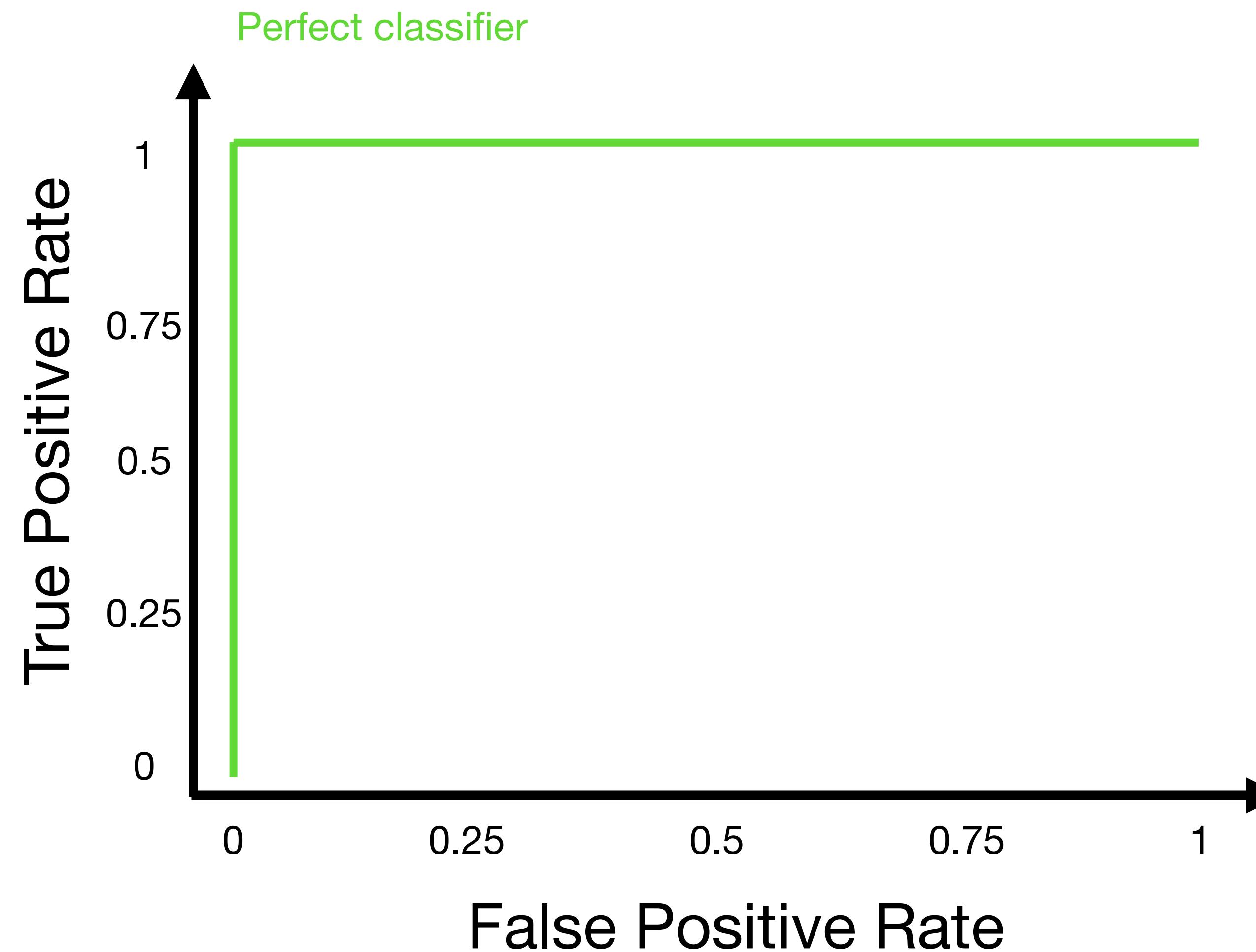


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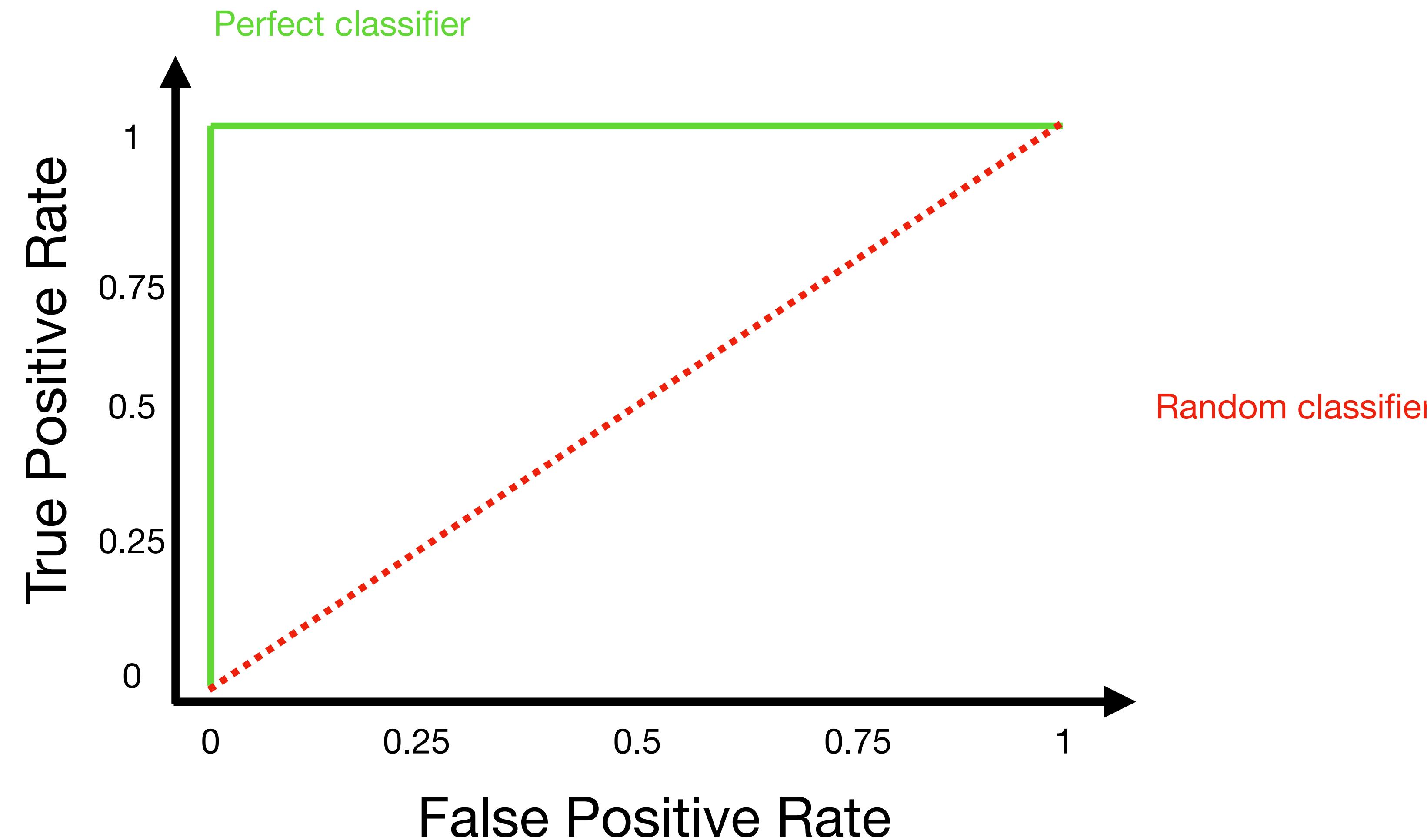


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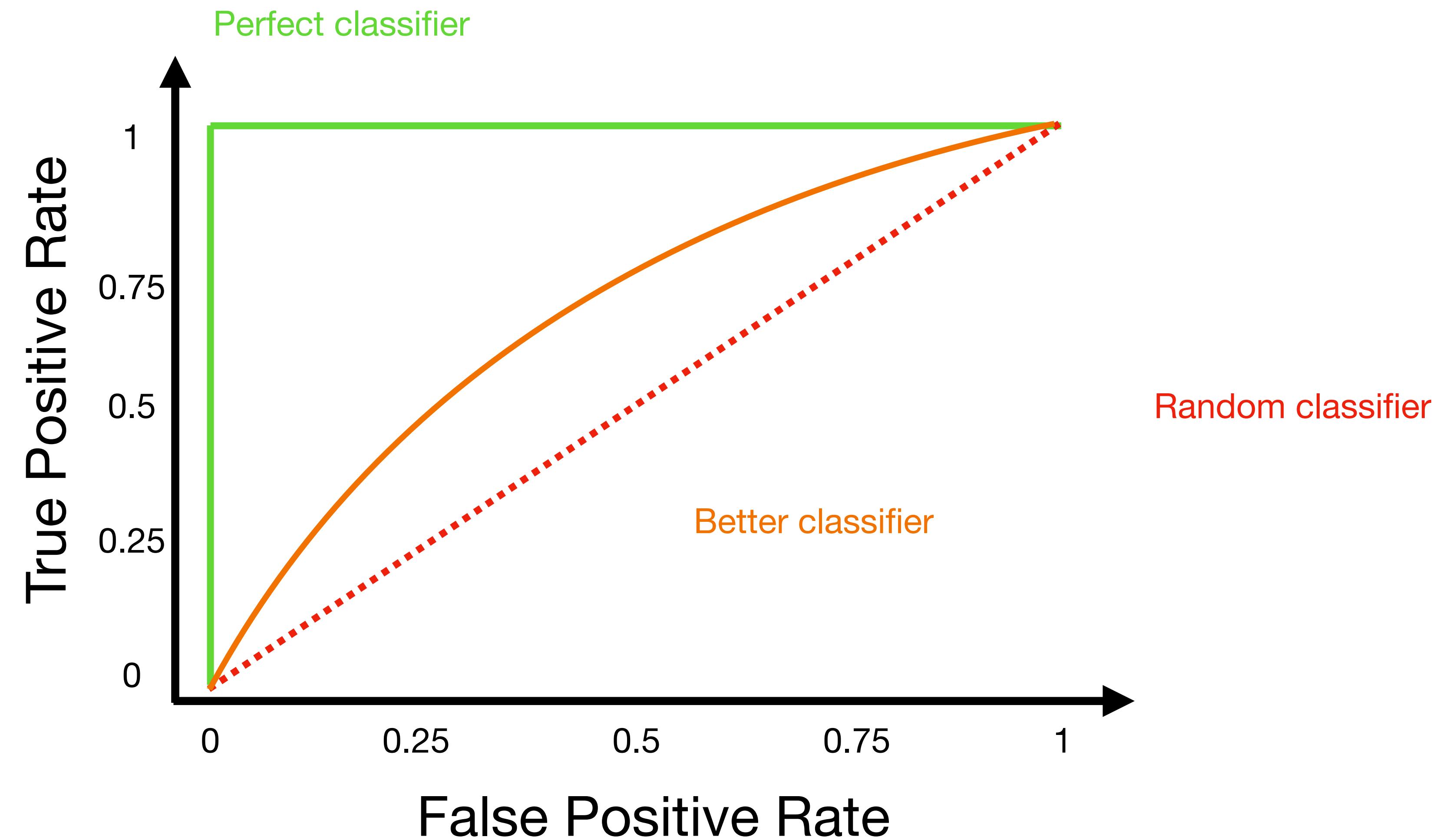


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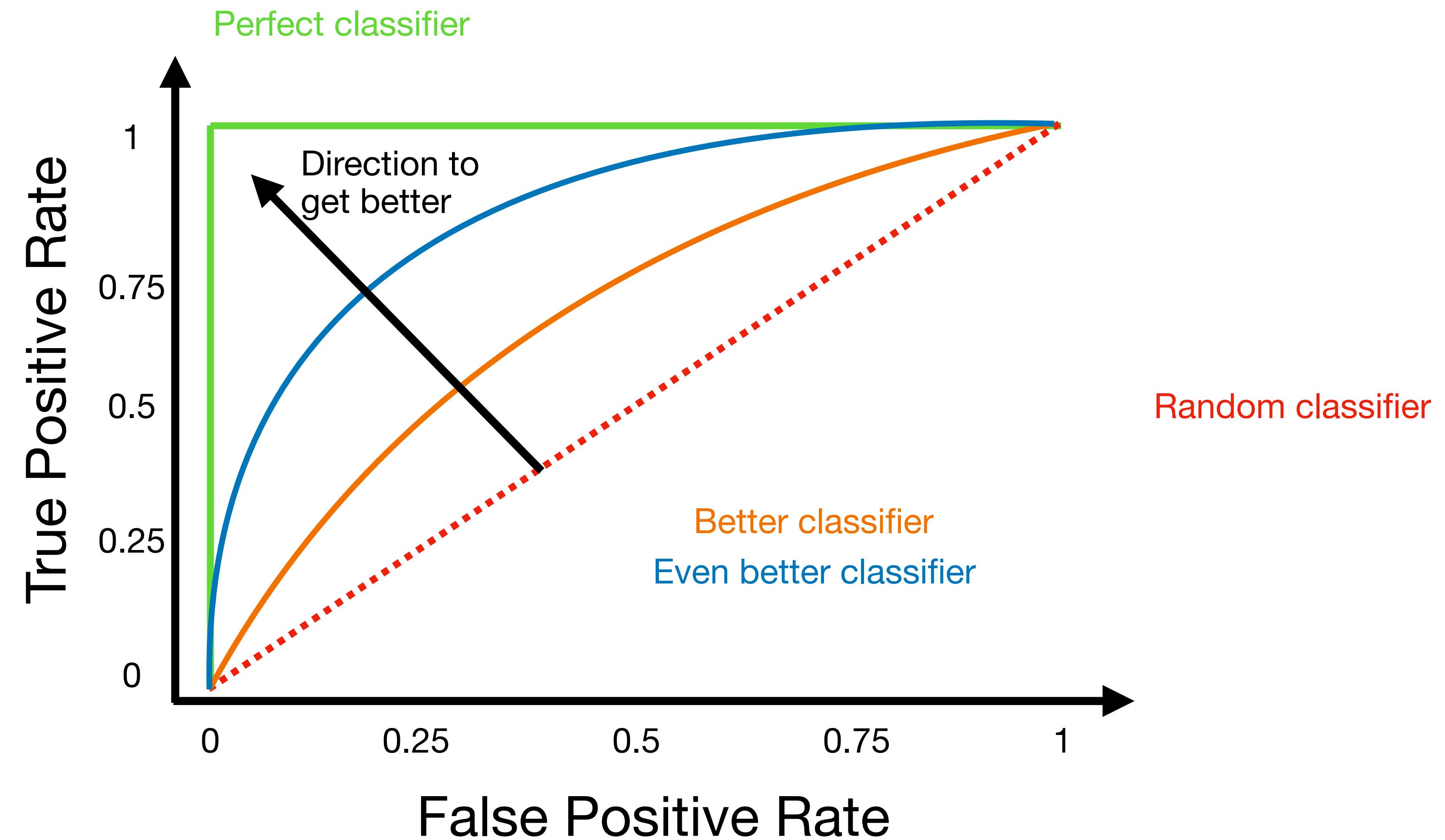


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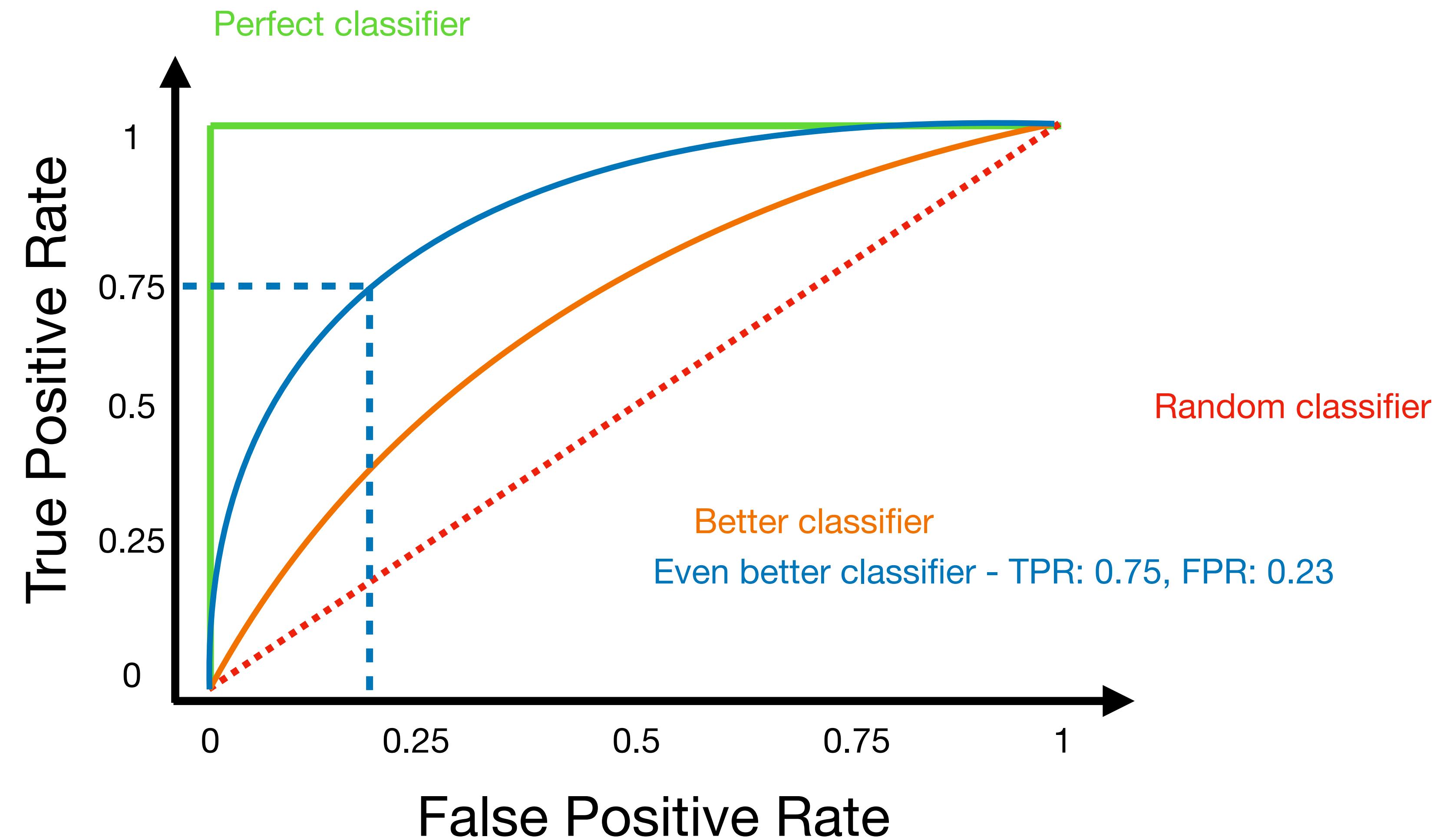


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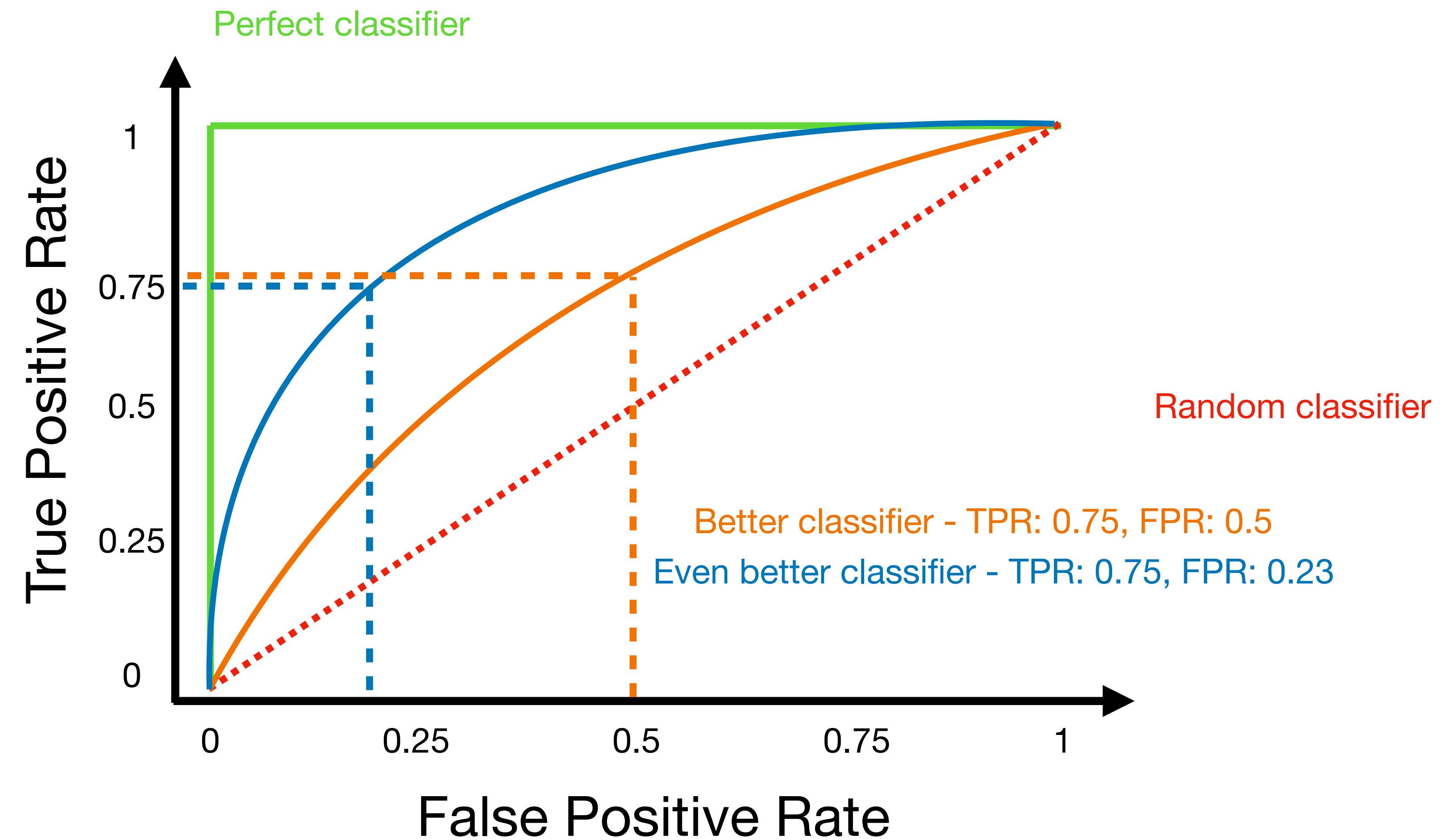


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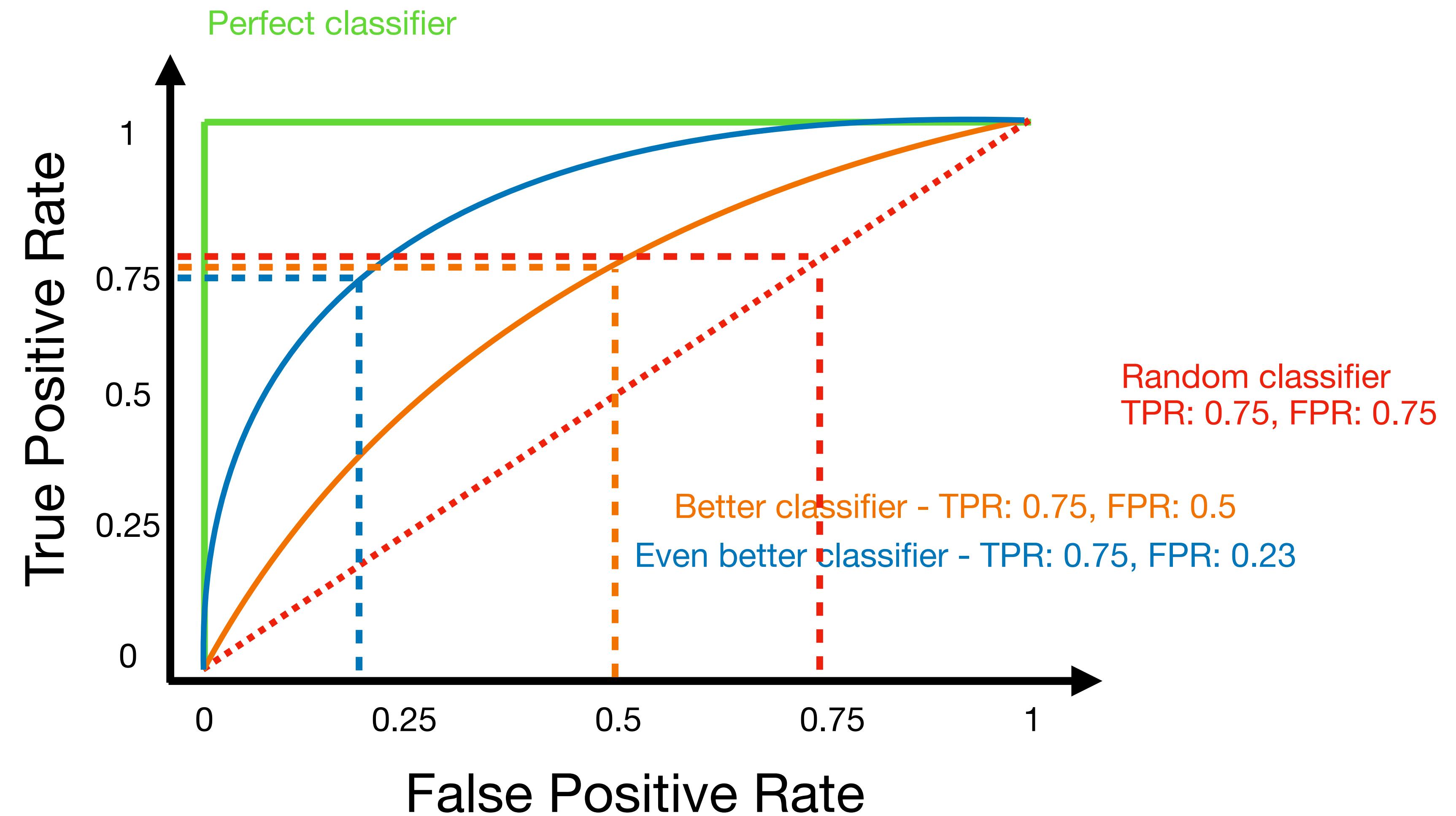


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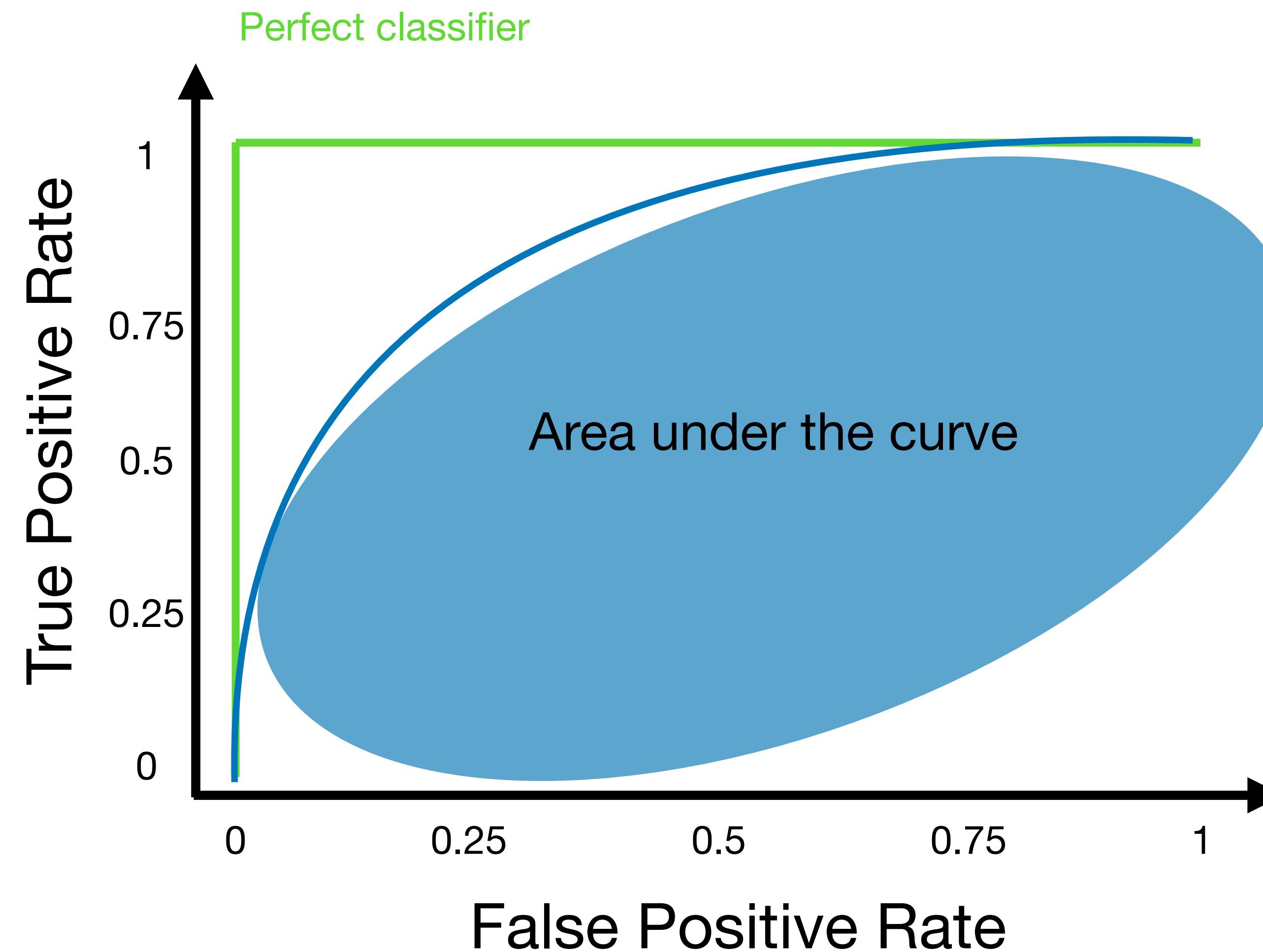


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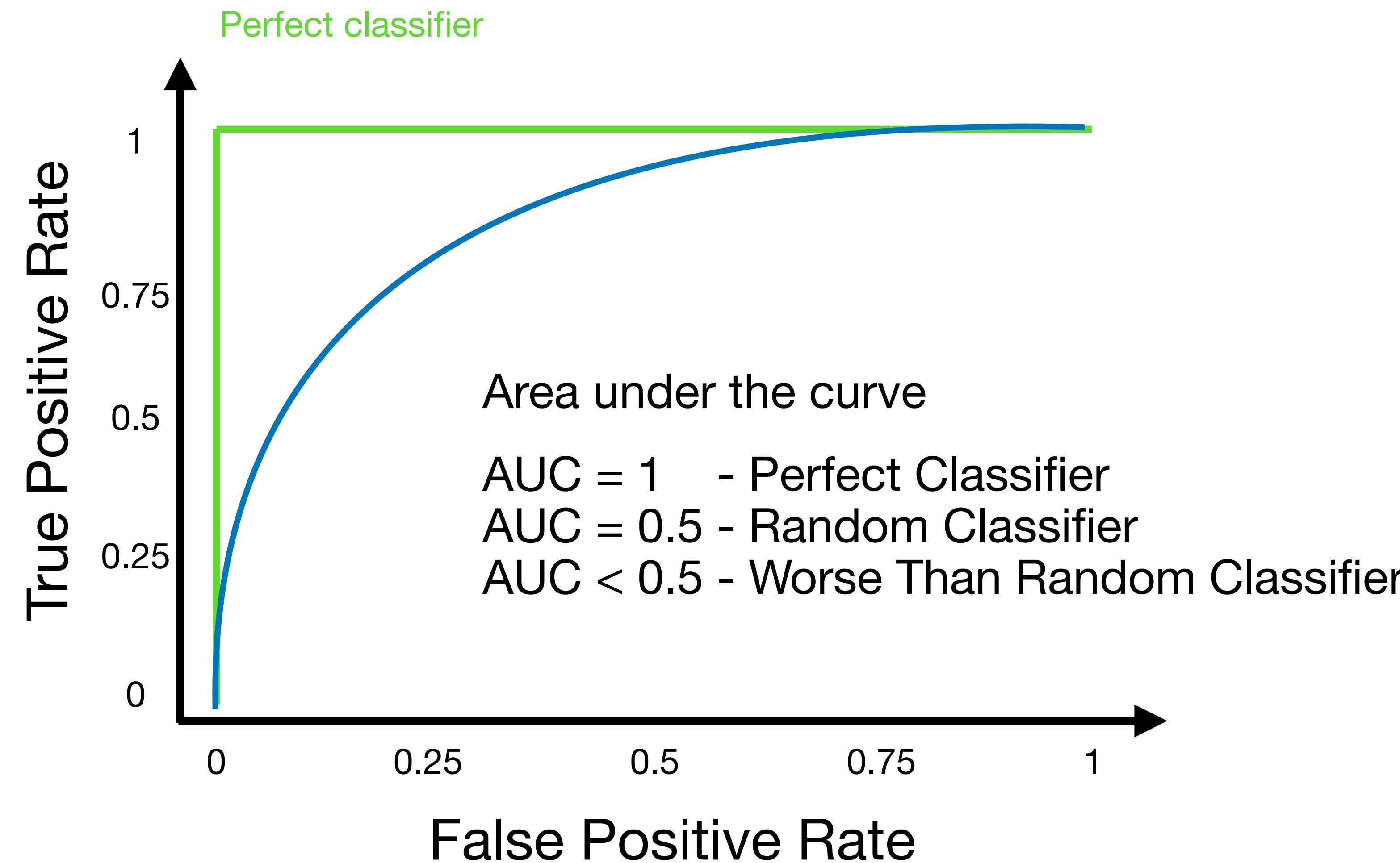


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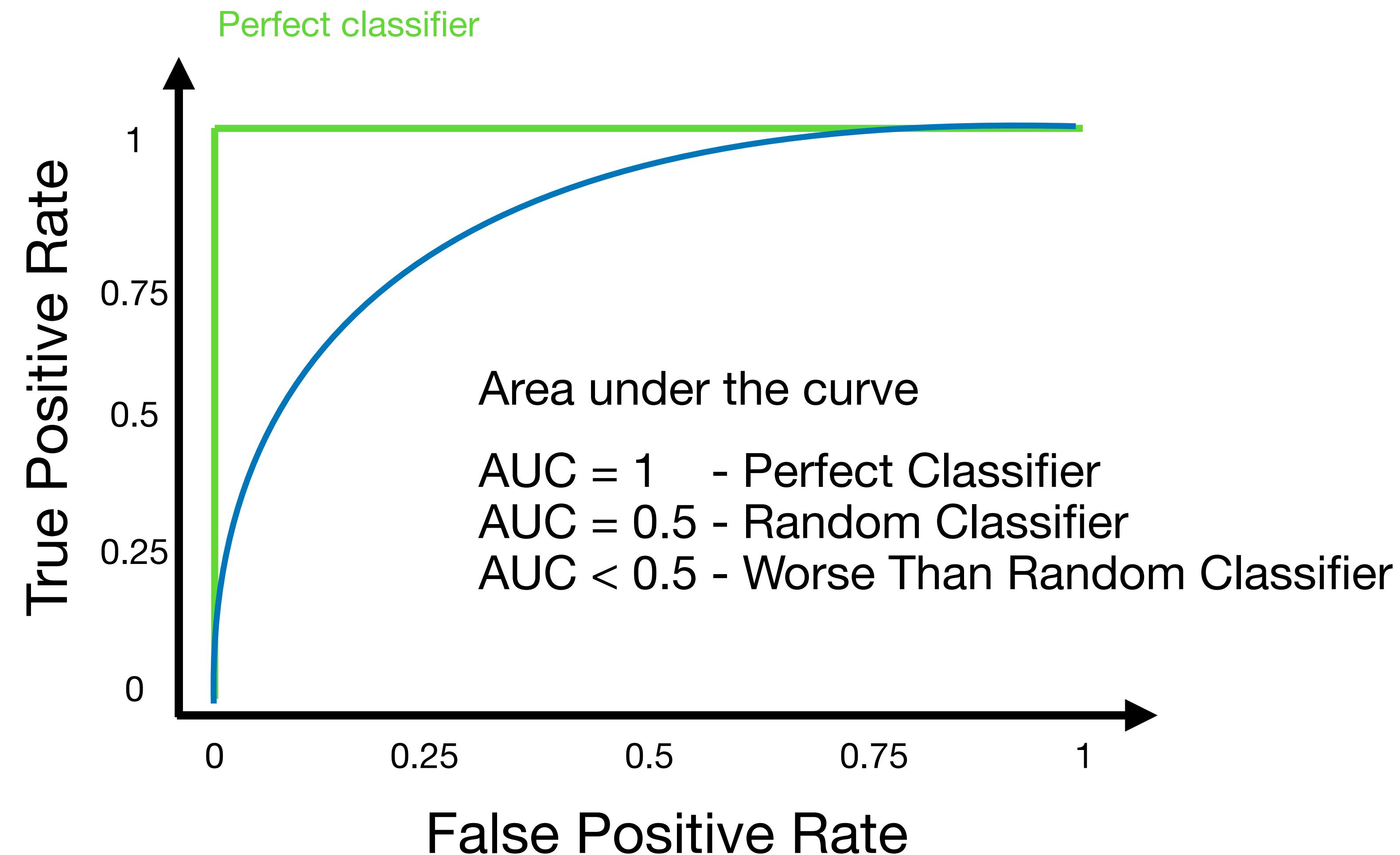
# Metrics

## AUC-ROC Curve

**Intuition:**  
AUC equals the probability that a randomly chosen positive instance is **ranked higher** than a randomly chosen negative instance by the classifier's scores.

$$TPR = \frac{TP}{TP + FN}$$

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# Metrics

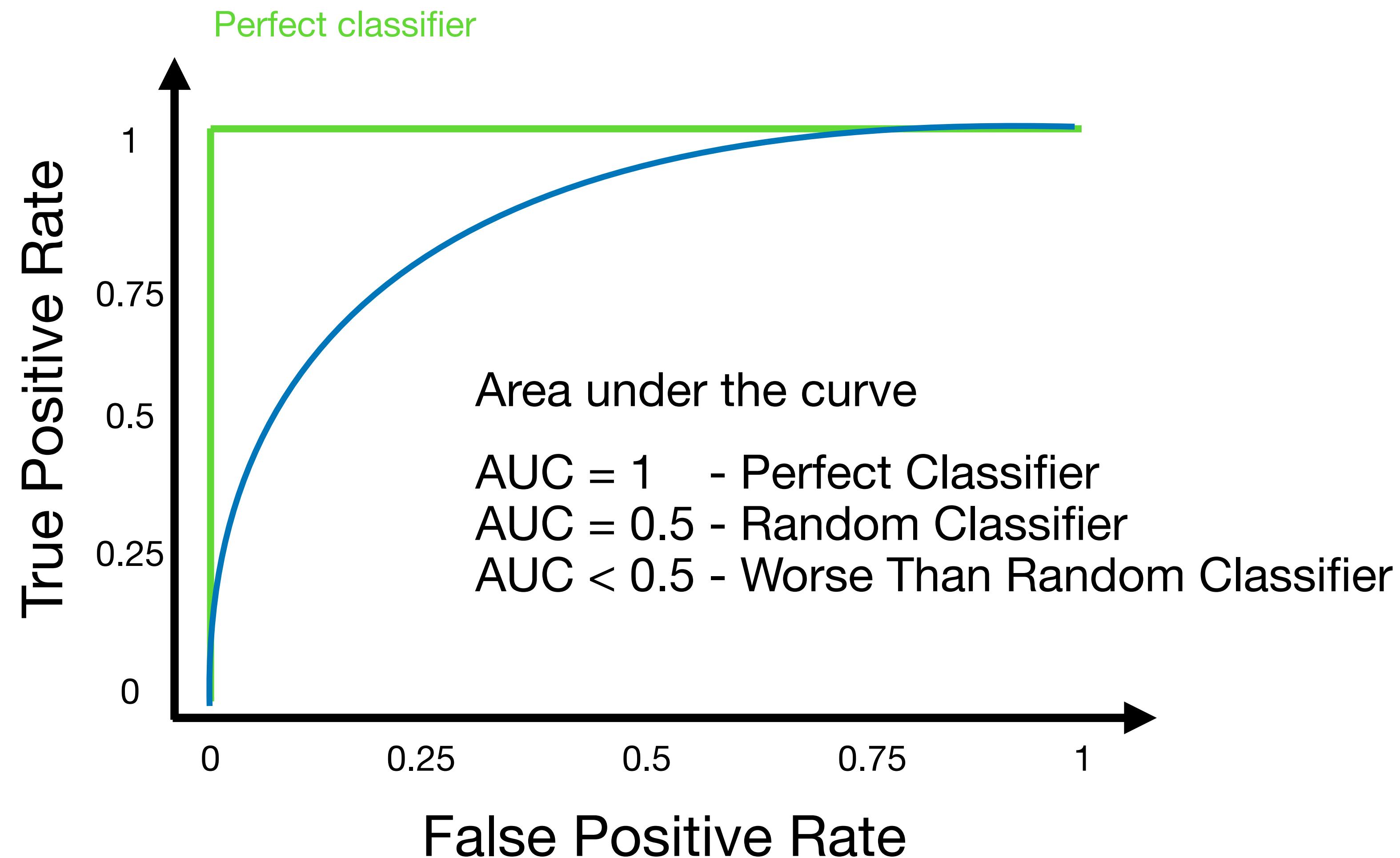
## AUC-ROC Curve

**Intuition:**  
AUC equals the probability that a randomly chosen positive instance is **ranked higher** than a randomly chosen negative instance by the classifier's scores.

**Limitation:**  
ROC curves can be overly optimistic for **highly imbalanced datasets** because the **FPR denominator** is dominated by the large TN count.

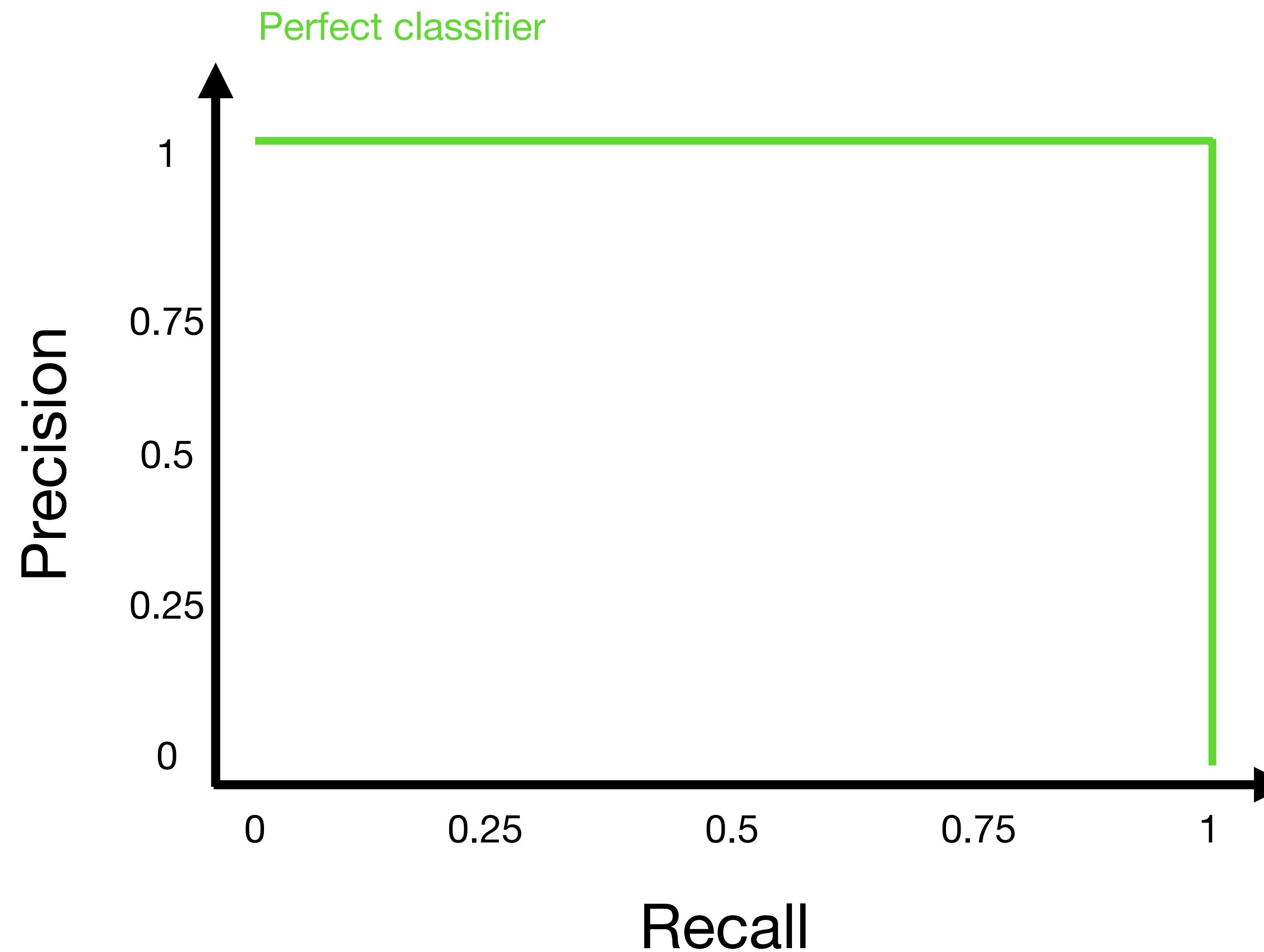
$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{TN + FP}$$



# Metrics

## Area Under Precision-Recall Curve (AUP)



Perfect classifier:

Precision stays at 1.0 across all recall values.  
 $AUC-PR = 1.0$ .

Every positive prediction is correct, and all actual positives are found.

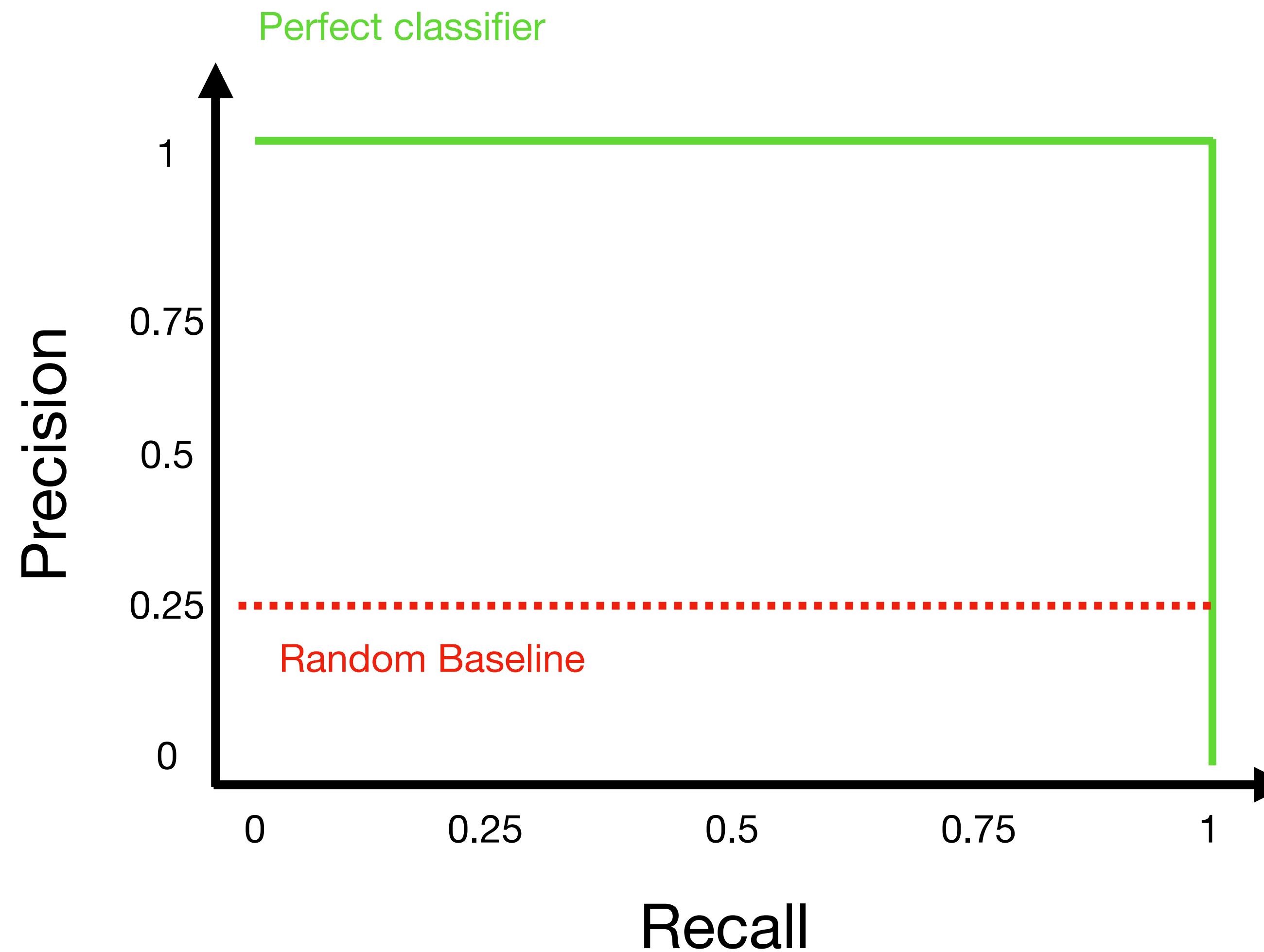
# Metrics

## Area Under Precision-Recall Curve (AUP)

**Random classifier:**

Horizontal line at the proportion of positives (25% here).

AUC-PR equals the class proportion. No predictive power.



**Perfect classifier:**

Precision stays at 1.0 across all recall values. AUC-PR = 1.0.

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# Metrics

## Area Under Precision-Recall Curve (AUP)

### Random classifier:

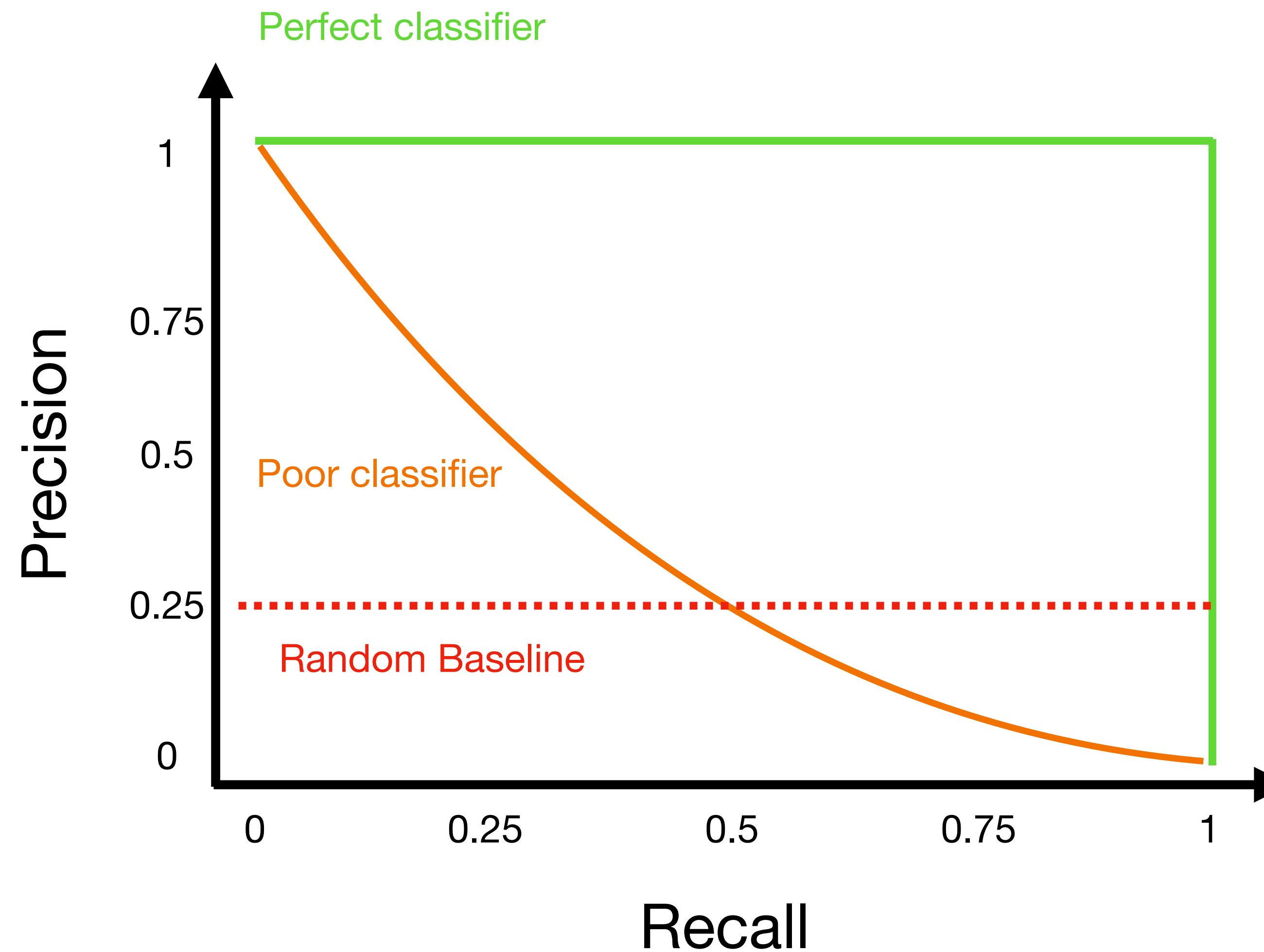
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AUC-PR equals the class proportion. No predictive power.

### Poor classifier:

Precision drops steadily as recall increases.

Still better than random, but significant tradeoff between precision and recall.



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Precision stays at 1.0 across all recall values. AUC-PR = 1.0.

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# Metrics

## Area Under Precision-Recall Curve (AUP)

**Random classifier:**

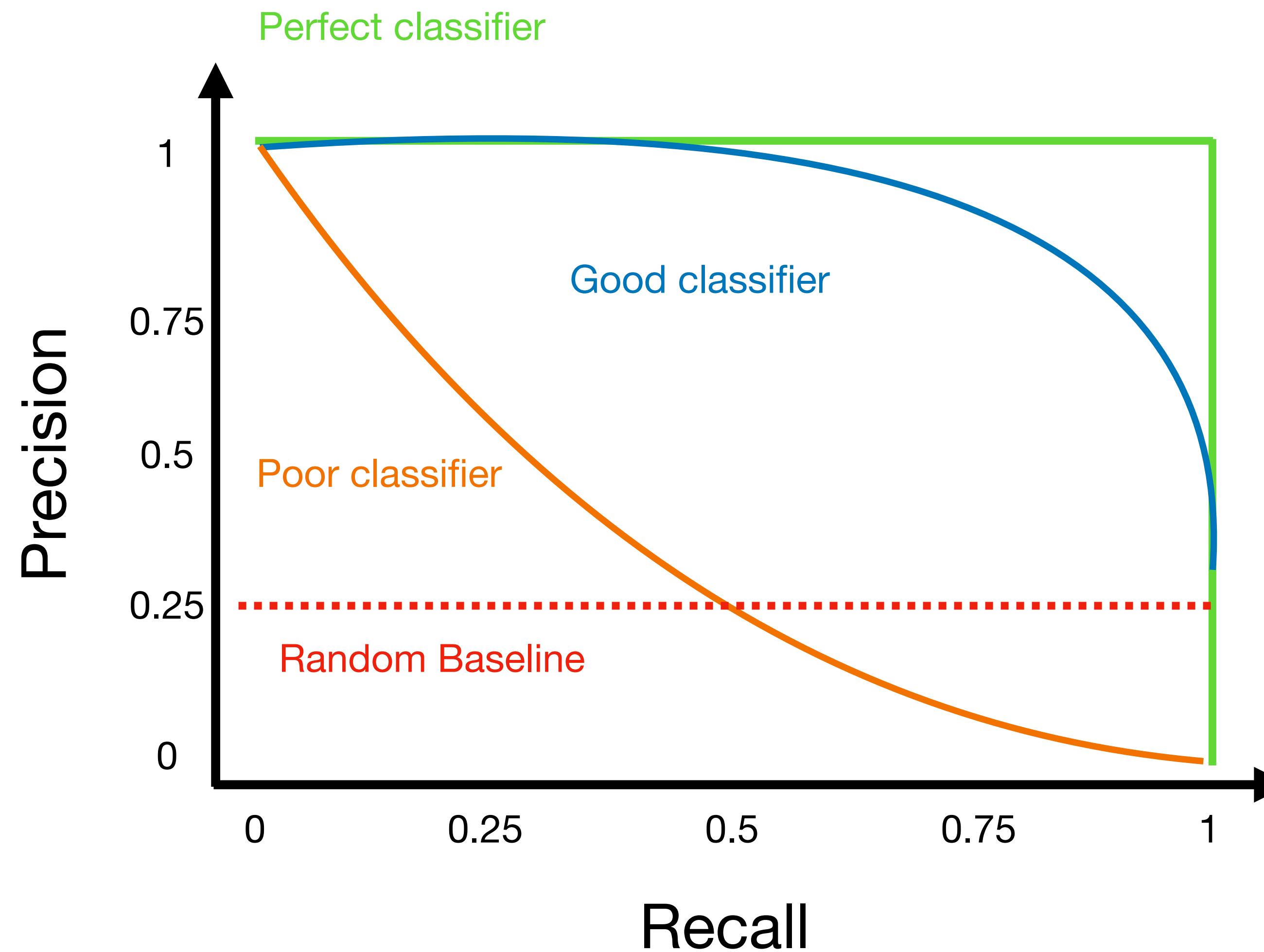
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Still better than random, but significant tradeoff between precision and recall.



**Perfect classifier:**

Precision stays at 1.0 across all recall values. AUC-PR = 1.0.

Every positive prediction is correct, and all actual positives are found.

**Good classifier:**

High precision maintained until high recall.

The curve hugs the top-right corner.

# Today's Outline

- Classification
- Metrics
- **k-Nearest Neighbors**

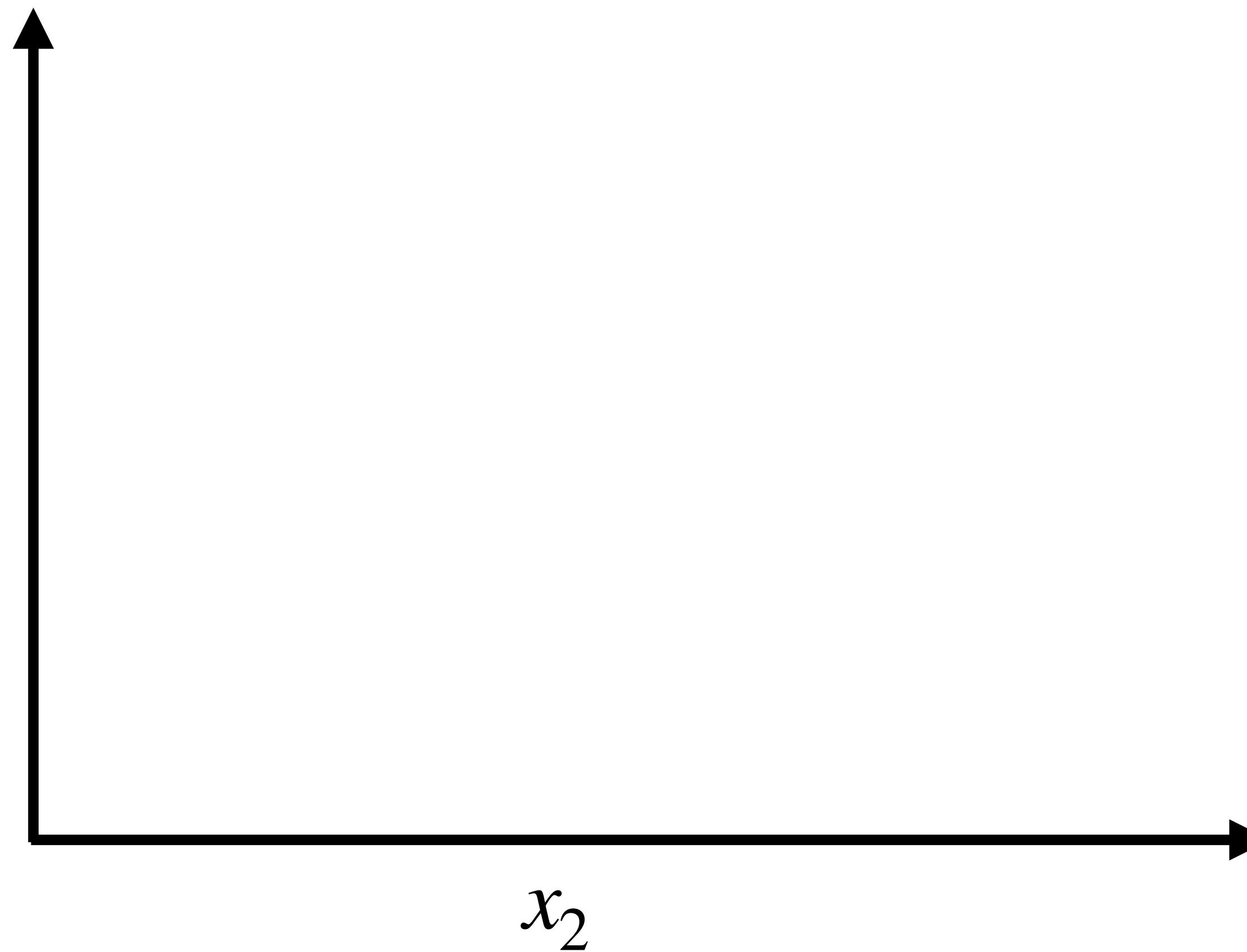
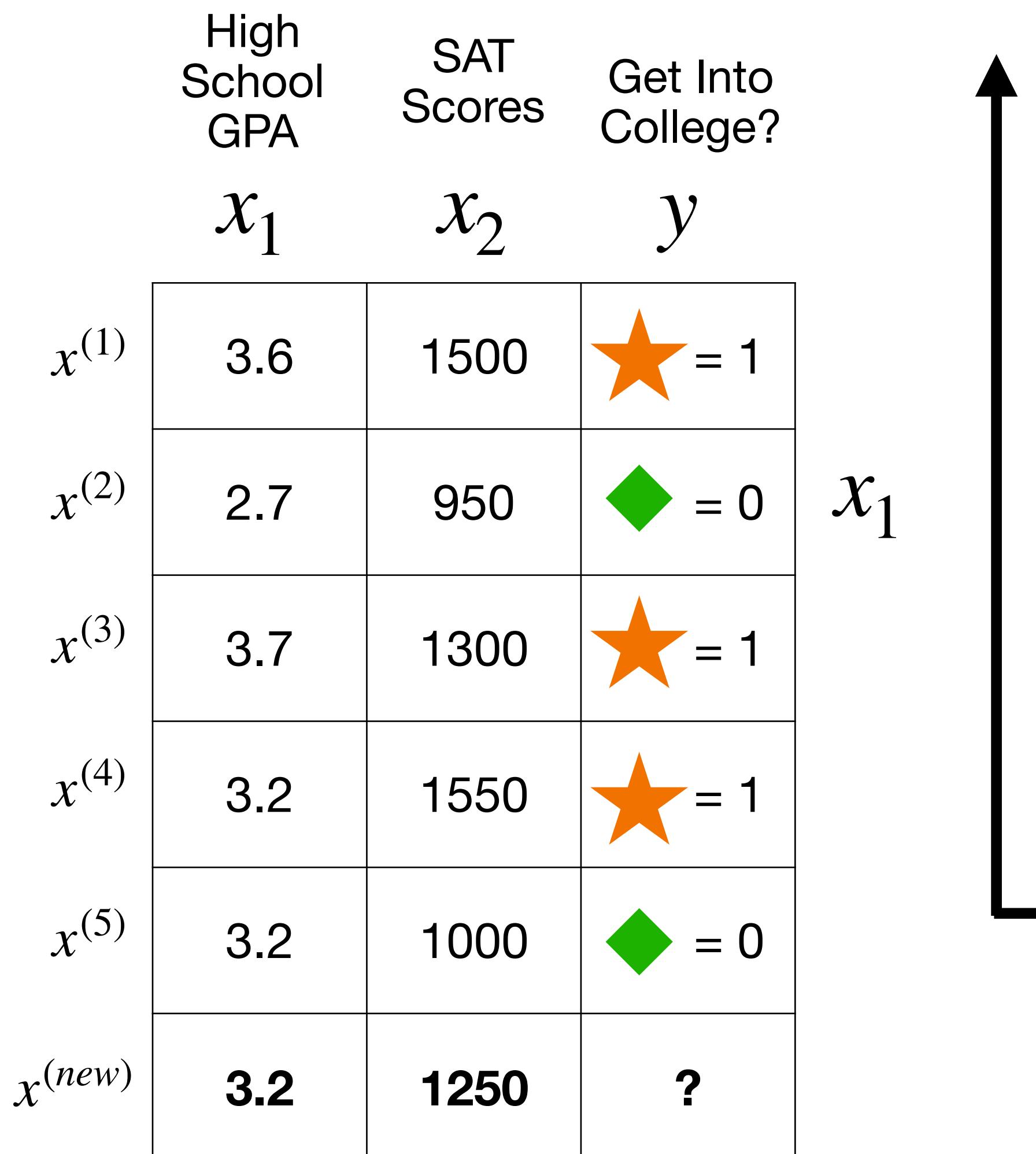
# k-Nearest Neighbors

- KNN is a **non-parametric**, instance-based (lazy) learning algorithm.
- It makes no assumptions about the underlying data distribution and stores all training instances **rather than learning explicit parameters**.

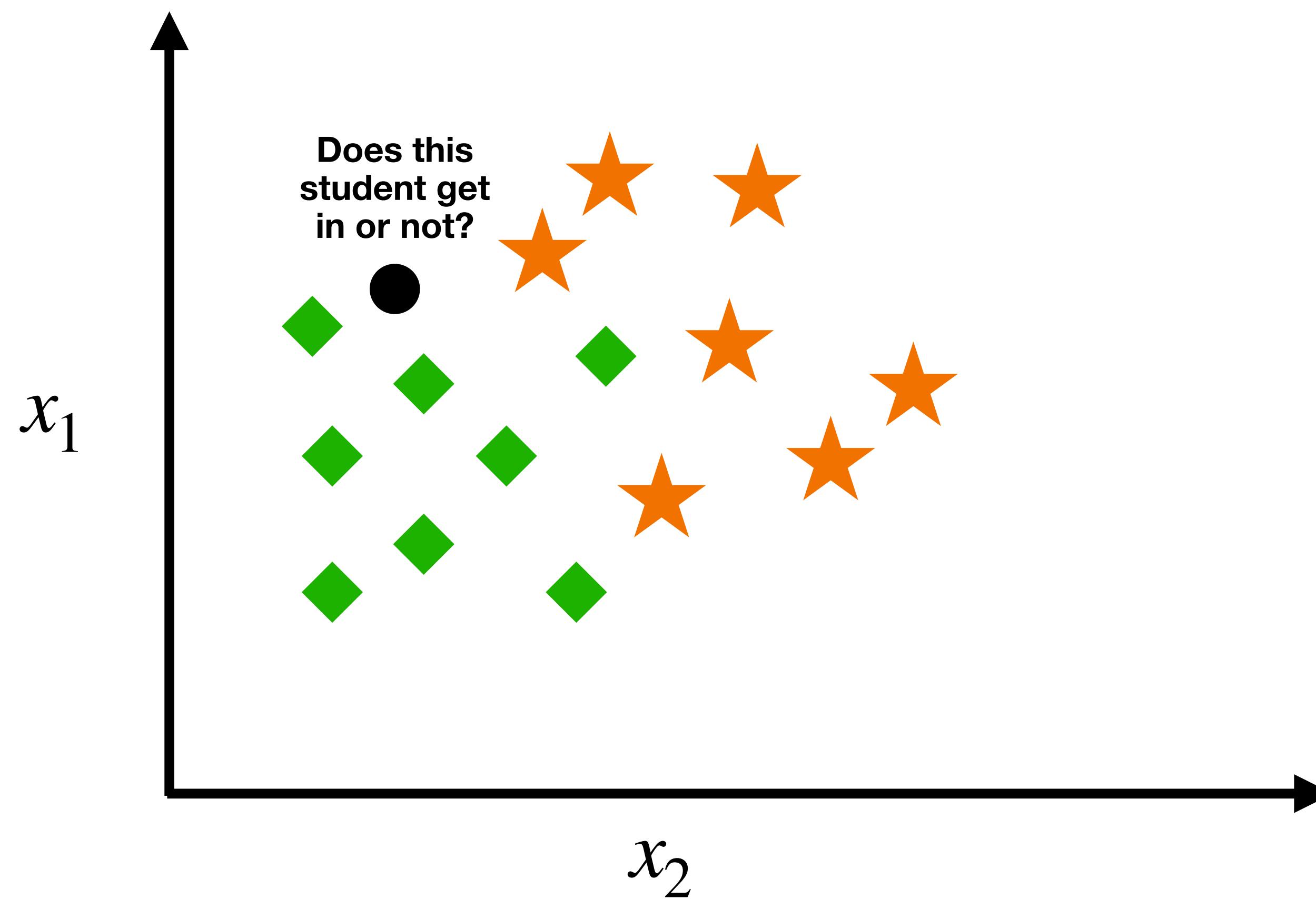
# k-Nearest Neighbors

- KNN is a **non-parametric**, instance-based (lazy) learning algorithm.
- It makes no assumptions about the underlying data distribution and stores all training instances **rather than learning explicit parameters**.
- **Key Idea:**
  - Similar instances have similar labels.
  - To classify a new point, find the **K training instances closest to it** and let them vote

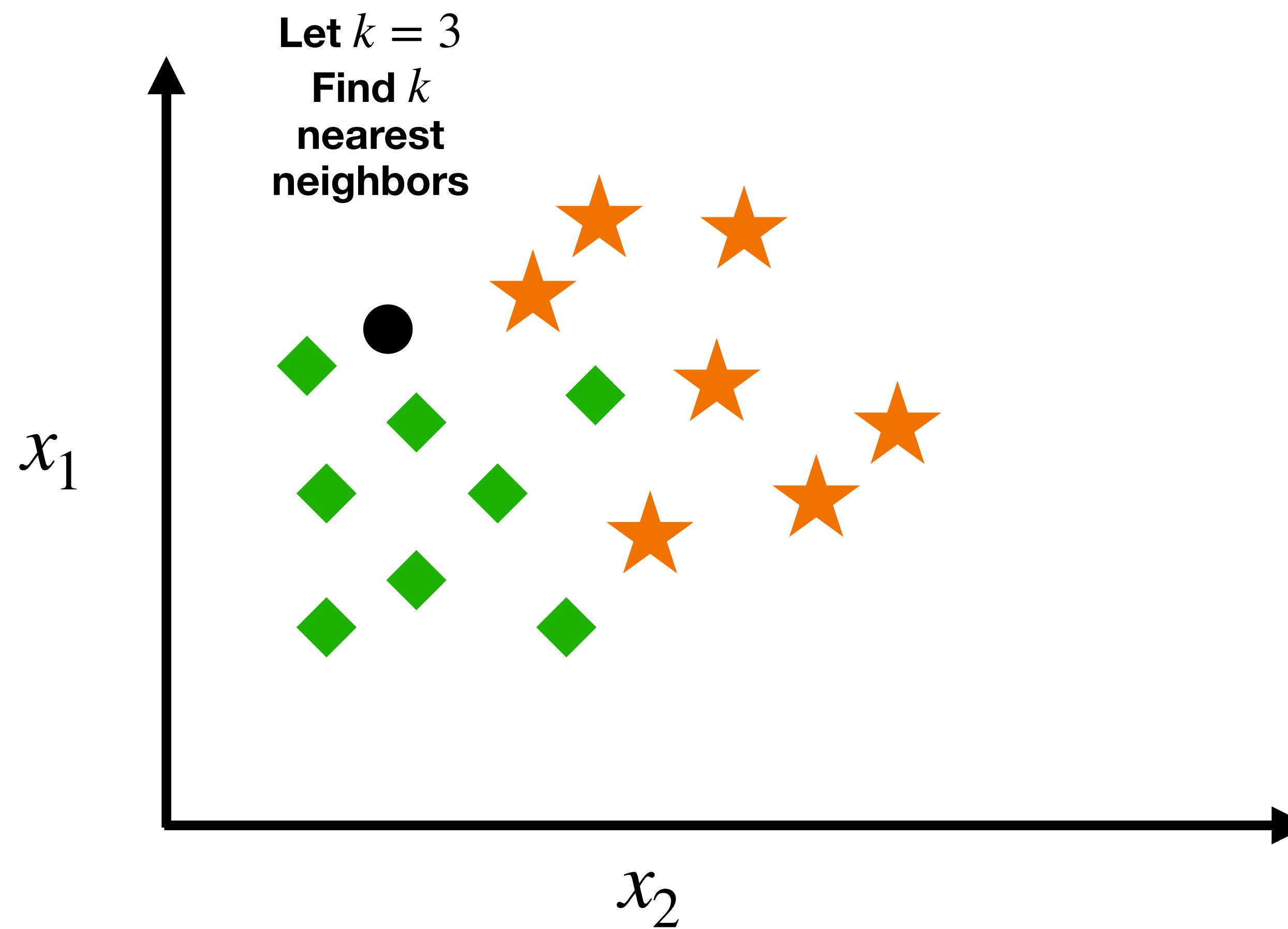
# k-Nearest Neighbors



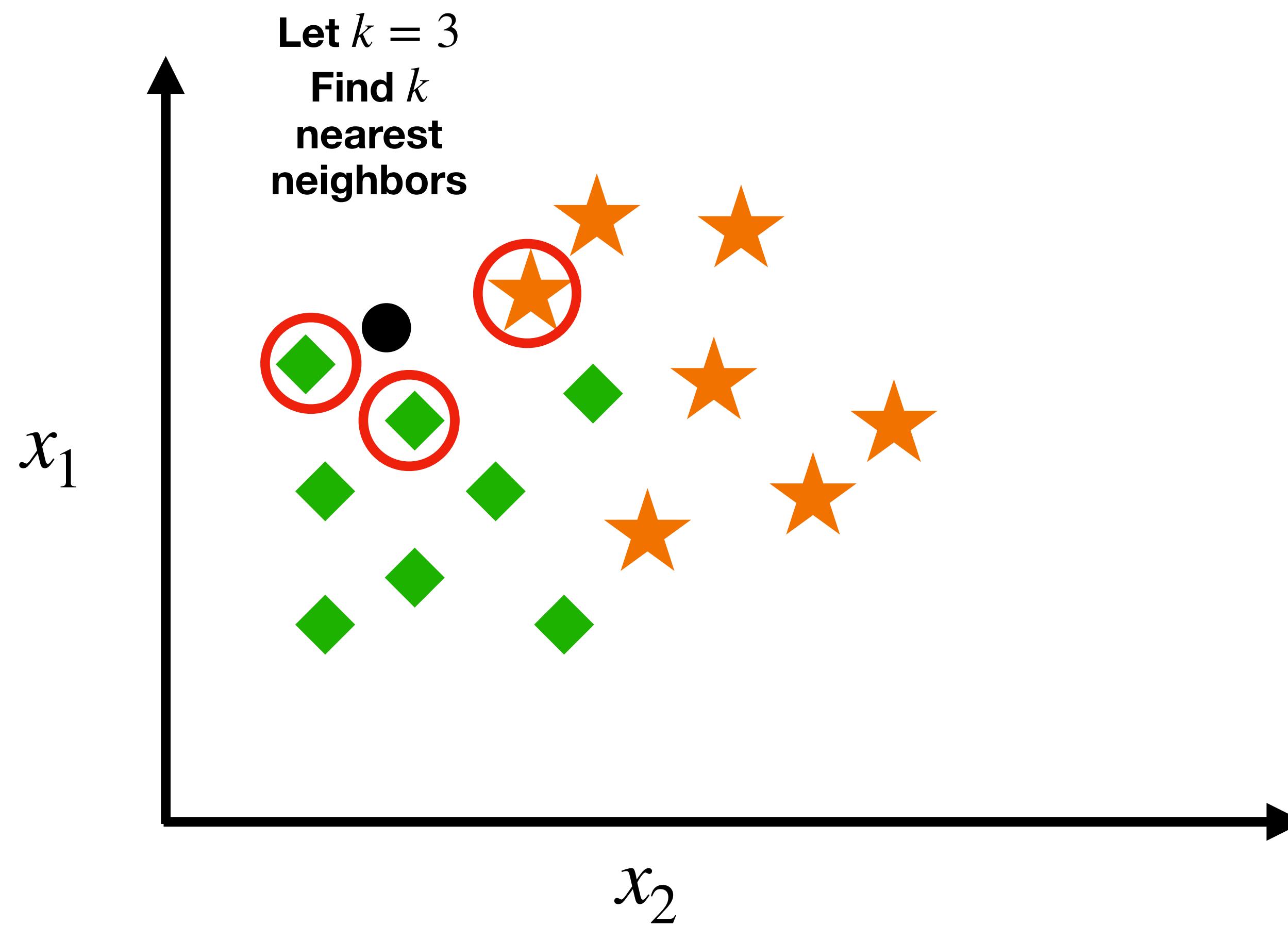
# k-Nearest Neighbors



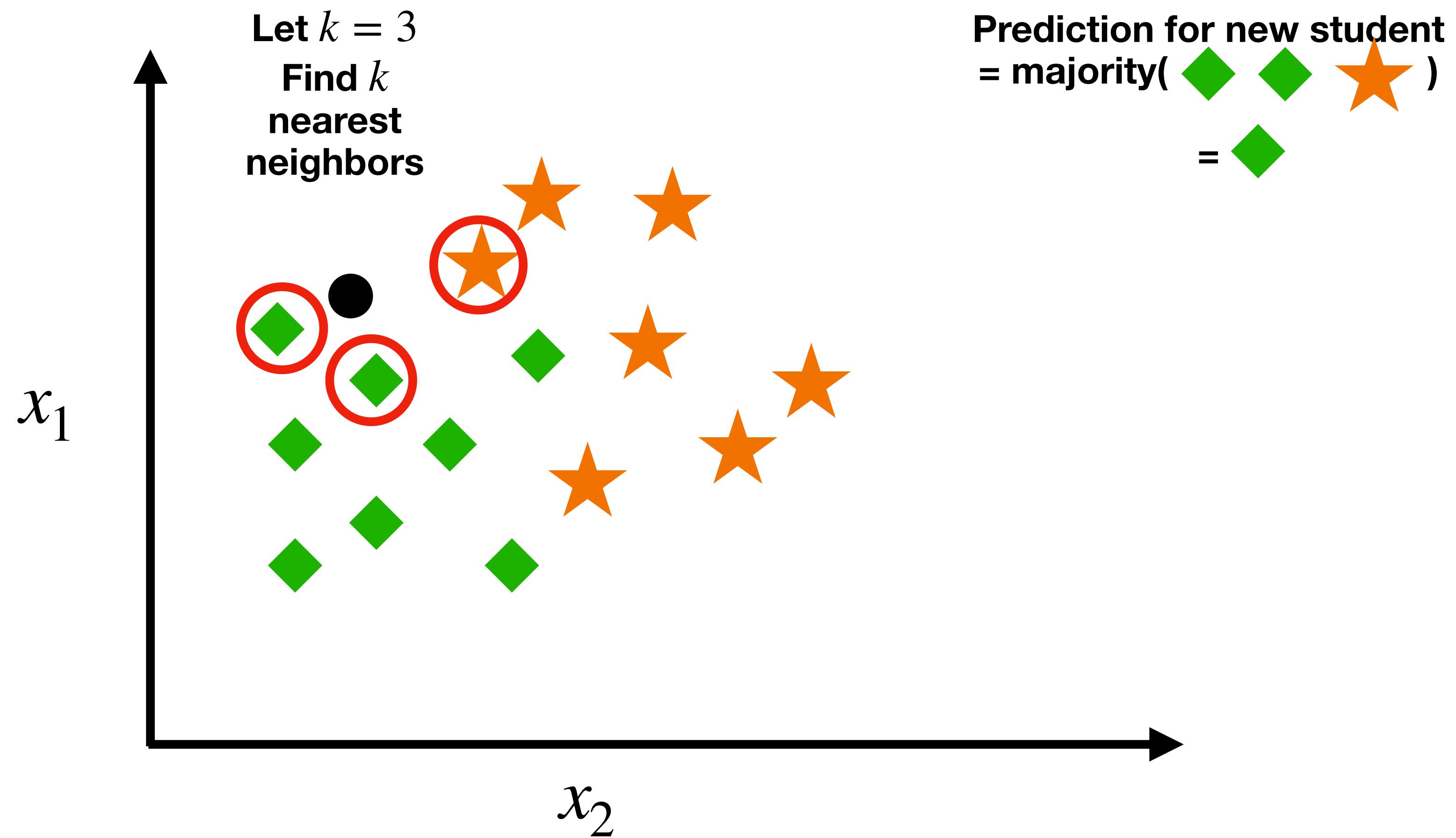
# k-Nearest Neighbors



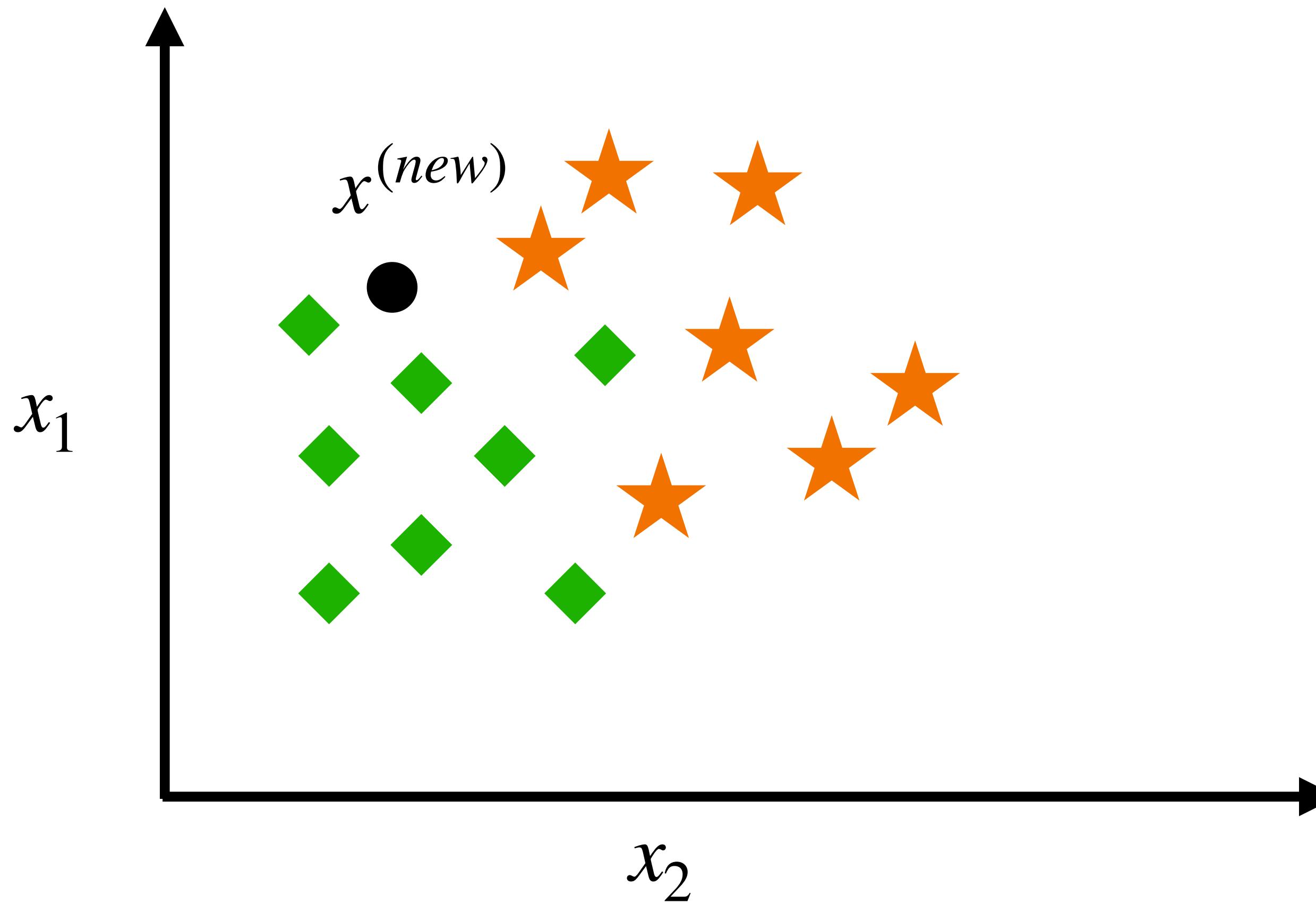
# k-Nearest Neighbors



# k-Nearest Neighbors



# k-Nearest Neighbors



## Algorithm:

### Training Phase:

Store all training instances  $(x_{train}, y_{train})$   
No computation required. We are not learning any parameters

### Prediction/Testing Phase:

1. Compute distance from new point  $x^{(new)}$  to every other point in the training data
2. Select the top  $k$ -nearest neighbors
3. For classification, return majority class amongst top  $k$
4. For regression, return mean or median of the values of the  $k$ -neighbors

# k-Nearest Neighbors

High School GPA	SAT Scores	Get Into College?
$x_1$	$x_2$	$y$
$x^{(1)}$	3.6	1500  $= 1$
$x^{(2)}$	2.7	950  $= 0$
$x^{(3)}$	3.7	1300  $= 1$
$x^{(4)}$	3.2	1550  $= 1$
$x^{(5)}$	3.2	1000  $= 0$
$x^{(new)}$	3.2	1250 ?

## Algorithm:

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Store all training instances  $(x_{train}, y_{train})$   
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### Prediction/Testing Phase:

1. Compute **distance** from new point  $x^{(new)}$  to every other point in the training data
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# k-Nearest Neighbors

The choice of the distance metric fundamentally affects which points are being considered “neighbors”

**Euclidean Distance ( $L_2$  Norm):**

$$d(x^{(new)}, x^{(i)}) = \sqrt{\sum_{j=0}^n (x_j^{(new)} - x_j^{(i)})^2}$$

**Manhattan Distance ( $L_1$  Norm):**

$$d(x^{(new)}, x^{(i)}) = \sum_{j=0}^n |x_j^{(new)} - x_j^{(i)}|$$

**Cosine Similarity:**

$$sim(x^{(new)}, x^{(i)}) = \frac{x^{(new)} \cdot x^{(i)}}{\|x^{(new)}\| \|x^{(i)}\|}$$

$$(distance = 1 - sim(x^{(new)}, x^{(i)}))$$

**Algorithm:**

Training Phase:

Store all training instances ( $x_{train}, y_{train}$ )

No computation required. We are not learning any parameters

Prediction/Testing Phase:

1. Compute **distance** from new point  $x^{(new)}$  to every other point in the training data
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# k-Nearest Neighbors

Most common choice, but sensitive to **feature scales**

**Euclidean Distance ( $L_2$  Norm):**

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Store all training instances ( $x_{train}, y_{train}$ )

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# k-Nearest Neighbors

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**Cosine Similarity:**

$$sim(x^{(new)}, x^{(i)}) = \frac{x^{(new)} \cdot x^{(i)}}{\|x^{(new)}\| \|x^{(i)}\|}$$

$$(distance = 1 - sim(x^{(new)}, x^{(i)}))$$

Sum of **absolute** differences.

More **robust to outliers** than Euclidean.  
Appropriate when features represent fundamentally different quantities.

**Algorithm:**

Training Phase:

Store all training instances ( $x_{train}, y_{train}$ )  
No computation required. We are not learning any parameters

Prediction/Testing Phase:

1. Compute **distance** from new point  $x^{(new)}$  to every other point in the training data
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# k-Nearest Neighbors

Measures **angle** between vectors, **ignoring magnitude**.

Useful for text data and high-dimensional sparse vectors.

**Euclidean Distance ( $L_2$  Norm):**

$$d(x^{(new)}, x^{(i)}) = \sqrt{\sum_{j=0}^n (x_j^{(new)} - x_j^{(i)})^2}$$

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**Algorithm:**

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# k-Nearest Neighbors

## Hamming Distance:

$$d(x^{(new)}, x^{(i)}) = \sum_{j=0}^n 1 \cdot (x_j^{(new)} \neq x_j^{(i)})$$

Hamming distance is a metric for comparing sequences of equal length - it counts the **number of positions where corresponding elements differ**.

## Example:

$$d([red, small, round], [red, large, round]) = 1$$

$$d([cat, young, male], [dog, old, female]) = 3$$

$$d(ACGT, ACTT) = 1$$

## Use Cases:

Categorical features: When features are categorical (say state a person lives in), Euclidean distance is meaningless.

Hamming distance treats each feature as equal - either it matches or it doesn't.

Measures **angle** between vectors, **ignoring magnitude**.

Useful for text data and high-dimensional sparse vectors.

## Algorithm:

### Training Phase:

Store all training instances  $(x_{train}, y_{train})$

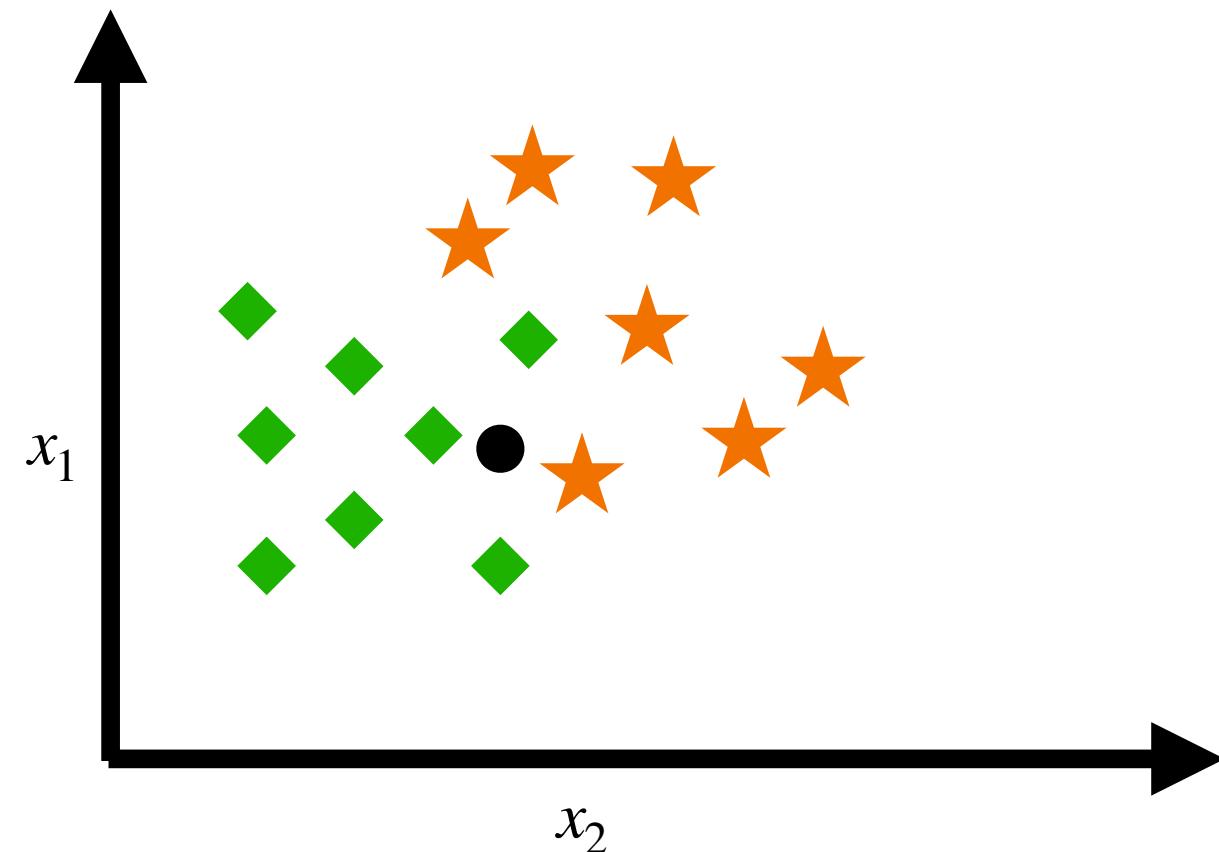
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# k-Nearest Neighbors

## Choosing $k$



- $k$  is the primary hyper-parameter controlling the bias-variance tradeoff

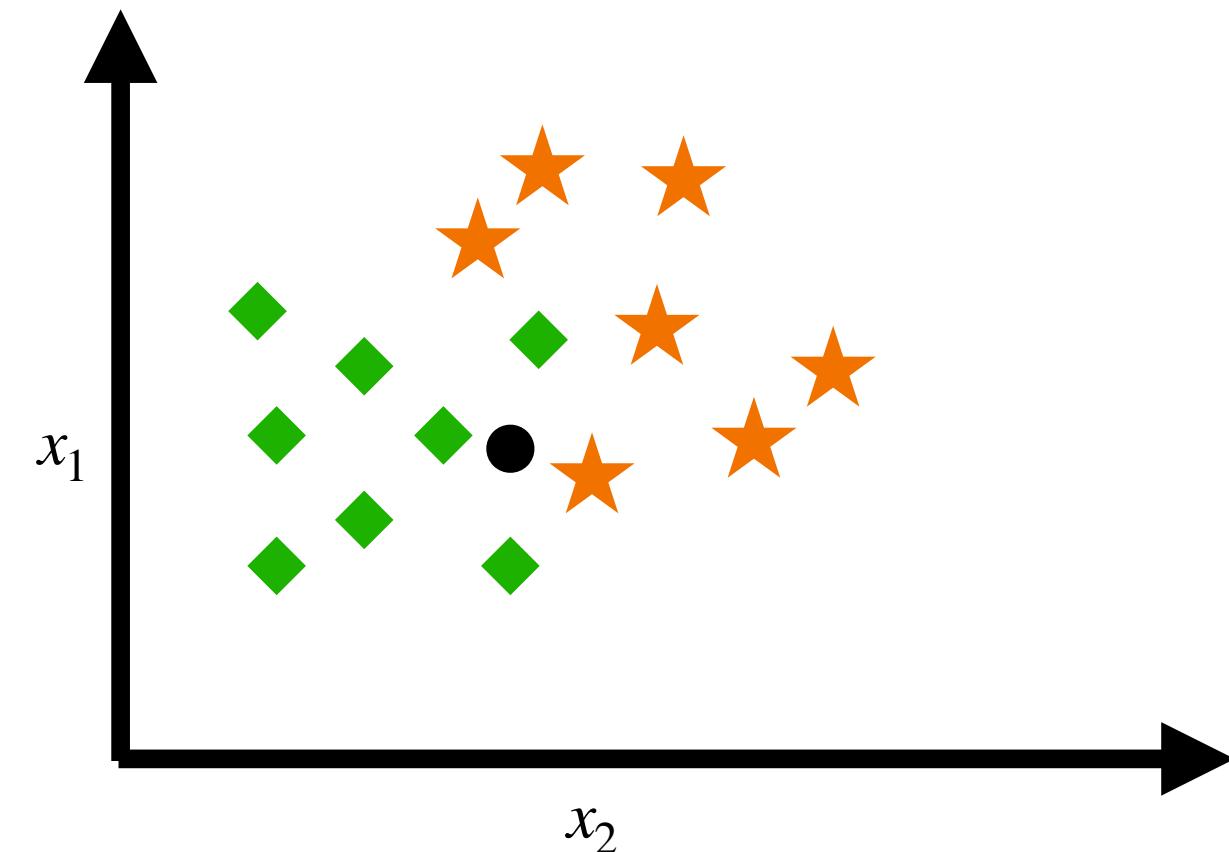
### Small $k$ (e.g. $k = 1$ )

- High variance, low bias
- Decision boundary is highly irregular
- Very sensitive to noise and outliers
- Prone to overfitting, but can capture fine grained structure

### Large $k$ (e.g. $k = m$ )

# k-Nearest Neighbors

## Choosing $k$



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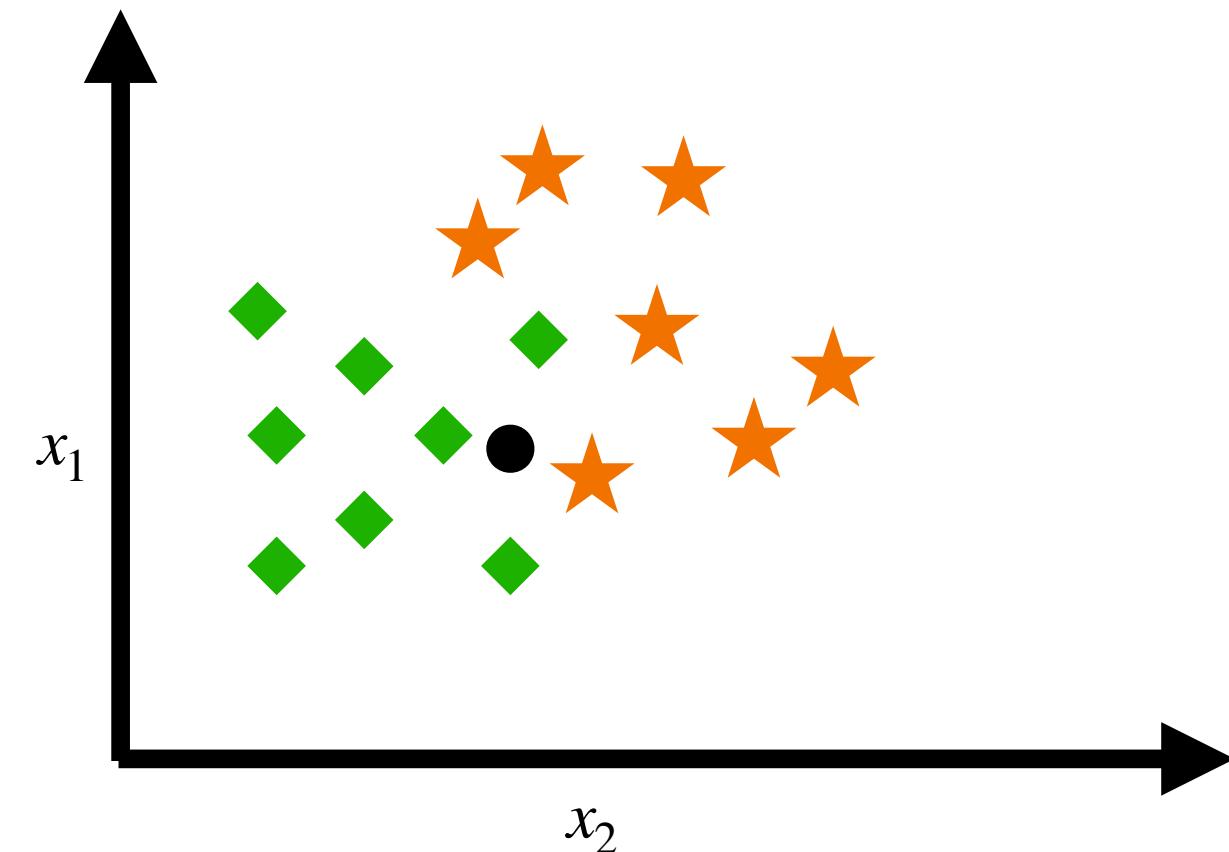
- High variance, low bias
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### Large $k$ (e.g. $k = m$ )

- High bias, low variance
- Decision boundary is very smooth
- Robust to noise, but may miss local patterns
- At the extreme of  $k = m$ , always predicts majority class

# k-Nearest Neighbors

## Choosing $k$



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### Small $k$ (e.g. $k = 1$ )

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### Practical Tips

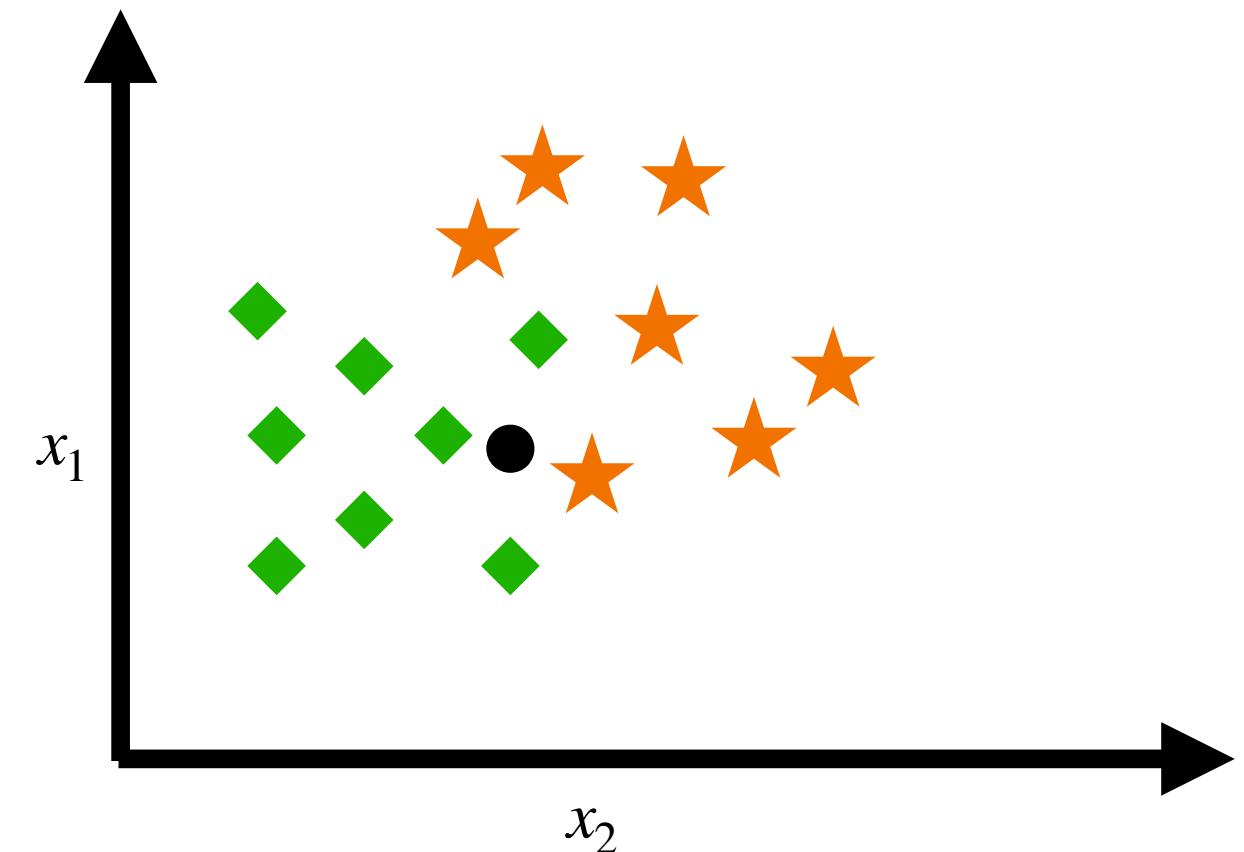
- Start with  $k = \sqrt{m}$
- Use cross-validation to select optimal  $k$
- If  $k$  is odd, it avoids ties in binary classification
- $k$  should be smaller than the smallest class size

### Large $k$ (e.g. $k = m$ )

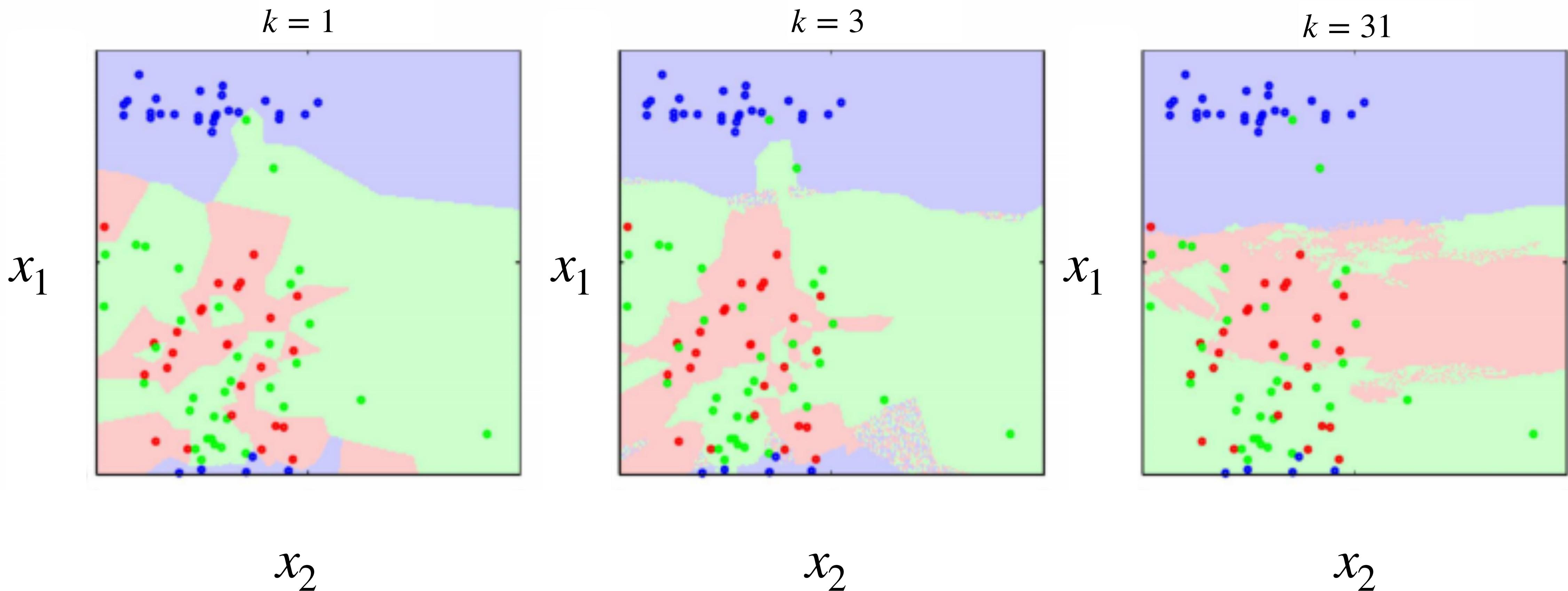
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# k-Nearest Neighbors

## Choosing $k$



- $k$  is the primary hyper-parameter controlling the bias-variance tradeoff



# k-Nearest Neighbors

## Choosing k - Cross-validation

- Why Not Just Use Training Error?
  - A model that memorizes the training data achieves zero training error but fails on new data.
  - Training error is a biased (optimistic) estimate of true generalization performance.
  - We need to estimate how well our model will perform on **unseen data**.

# k-Nearest Neighbors

## Choosing k - Cross-validation

- Naive Solution - Train/Test Split
  - Split data into training set (say 80%) and test set (20%).
  - Train on training set, evaluate on test set.
  - Issues:
    - Wastes data - 20% of precious labeled data is never used for training
    - High variance - Performance estimate depends heavily on **which points land in the test set**
    - No hyperparameter tuning: If we use the test set to select hyperparameters, we're overfitting to the test set - (using **validation set** is a possible fix for this issue)

# k-Nearest Neighbors

## Choosing k - Cross-validation

- Naive Solution - Train/Test Split
  - **Data Leakage Issue**
    - If we repeatedly evaluate on the test set while tuning hyperparameters, information about the test set **leaks** into our model selection process.
    - The test error becomes optimistically biased - no longer a valid estimate of **generalization**

# k-Nearest Neighbors

## Choosing k - Cross-validation

- **Solution!**
- Use cross-validation
  - Use **all data** for both training and validation
  - Get **reliable performance estimates** with uncertainty quantification
  - Select hyperparameters **without contaminating the final test set**

# k-Fold Cross Validation

## Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
3. for each fold  $i = 1, 2, \dots, k$ :
  - 3a. Use fold  $i$  as the validation set
  - 3b. Use the remaining  $k - i$  folds as the training set
  - 3c. Train the model on the training set
  - 3d. Evaluate on the validation set, record performance metric
4. Aggregate the  $K$  performance estimates

# k-Fold Cross Validation

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$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

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# k-Fold Cross Validation

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$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$	Validation Set $D_1$			
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

$$CV_1 = \frac{1}{D_1} \sum_{D_1} \ell(y_{D_1}, f_\theta(D_1))$$

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
3. for each fold  $i = 1, 2, \dots, k$ :
  - 3a. Use fold  $i$  as the validation set
  - 3b. Use the remaining  $k - i$  folds as the training set
  - 3c. Train the model on the training set
  - 3d. Evaluate on the validation set, record performance metric
4. Aggregate the  $K$  performance estimates

# k-Fold Cross Validation

## Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$	Validation Set $D_2$			
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

$$CV_2 = \frac{1}{D_2} \sum_{D_2} \ell(y_{D_2}, f_\theta(D_2))$$

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
3. for each fold  $i = 1, 2, \dots, k$ :
  - 3a. Use fold  $i$  as the validation set
  - 3b. Use the remaining  $k - i$  folds as the training set
  - 3c. Train the model on the training set
  - 3d. Evaluate on the validation set, record performance metric
4. Aggregate the  $K$  performance estimates

# k-Fold Cross Validation

## Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
Validation Set $D_3$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

$$CV_3 = \frac{1}{D_3} \sum_{D_3} \ell(y_{D_3}, f_\theta(D_3))$$

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
3. for each fold  $i = 1, 2, \dots, k$ :
  - 3a. Use fold  $i$  as the validation set
  - 3b. Use the remaining  $k - i$  folds as the training set
  - 3c. Train the model on the training set
  - 3d. Evaluate on the validation set, record performance metric
4. Aggregate the  $K$  performance estimates

# k-Fold Cross Validation

## Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$	Validation Set $D_4$			
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

$$CV_4 = \frac{1}{D_4} \sum_{D_4} \ell(y_{D_4}, f_\theta(D_4))$$

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
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4. Aggregate the  $K$  performance estimates

# k-Fold Cross Validation

## Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

$$CV_5 = \frac{1}{D_5} \sum_{D_5} \ell(y_{D_5}, f_\theta(D_5))$$

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
3. for each fold  $i = 1, 2, \dots, k$ :
  - 3a. Use fold  $i$  as the validation set
  - 3b. Use the remaining  $k - i$  folds as the training set
  - 3c. Train the model on the training set
  - 3d. Evaluate on the validation set, record performance metric
4. Aggregate the  $K$  performance estimates

# k-Fold Cross Validation

## Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

Mean CV Score:

$$\bar{CV} = \frac{1}{k} \sum_{i=1}^k CV_i$$

### Algorithm

1. Shuffle the dataset randomly
2. Split data into  $k$  equally-sized folds (or partitions)
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# k-Fold Cross Validation Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

Mean CV Score:

$$\bar{CV} = \frac{1}{k} \sum_{i=1}^k CV_i$$

<b>k-value</b>	<b>Training Size</b>	<b>Properties</b>
k=2	50%	High Bias Low Variance Fast
k=5	80%	Good Balance Commonly Used
k=10	90%	Low Bias Commonly Used
k=m-1	m-1 samples	Low Bias Highest Variance Slow

# k-Fold Cross Validation Algorithm

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

Let's say we want to run  $k = 5$ -fold cross validation

Train on **8 rows**, test on **2 row**

Mean CV Score:

$$\bar{CV} = \frac{1}{k} \sum_{i=1}^k CV_i$$

$k$ -fold CV requires **training  $k$  models**.

If training is expensive, smaller  $k$  is preferred.

<b>k-value</b>	<b>Training Size</b>	<b>Properties</b>
k=2	50%	High Bias Low Variance Fast
k=5	80%	Good Balance Commonly Used
k=10	90%	Low Bias Commonly Used
k=m-1	m-1 samples	Low Bias Highest Variance Slow

# k-Fold Cross Validation

## Variants

	$x_1$	$x_2$	$x_3$	$x_4$
$x^{(1)}$				
$x^{(2)}$				
$x^{(3)}$				
$x^{(4)}$				
$x^{(5)}$				
$x^{(6)}$				
$x^{(7)}$				
$x^{(8)}$				
$x^{(9)}$				
$x^{(10)}$				

### Stratified Cross-Validation

- The Problem with Random Splits
  - For imbalanced classification, random splits may create folds with different class distributions.
  - One fold might have 40% positives while another has 20%, leading to unreliable estimates.
  - Stratified sampling ensures each fold has approximately the same class distribution as the full dataset.
- Algorithm:
  - Separate samples by class
  - For each class, distribute samples evenly across  $k$ –folds
  - Combine to form final folds

# Back to k-Nearest Neighbors

## Practical Issues

- Feature Scaling
- Curse of Dimensionality
- Space and computational complexity

# Back to k-Nearest Neighbors

## Practical Issues - Feature Scaling

- KNN is **highly sensitive** to feature scales because distance metrics are dominated by features with larger ranges.
- Example:
  - If feature A ranges from 0-1 and feature B ranges from 0-1000
  - Euclidean distance is almost **entirely determined by feature B**.
  - Solution: Always normalize or standardize features before applying kNN.

# Back to k-Nearest Neighbors

## Practical Issues - Curse of Dimensionality

- KNN suffers severely in high-dimensional spaces:
  - Distance concentration: As dimensionality increases, **distances between points become increasingly similar**.
  - **The ratio of nearest to farthest neighbor approaches 1**, making the concept of “nearest” meaningless.
- Sparsity: The volume of space grows exponentially with dimension. To maintain the same density of points, training set size must grow exponentially.
- Irrelevant features: In high dimensions, many features may be irrelevant, adding noise to distance calculations.
- Mitigation strategies:
  - Dimensionality reduction (PCA, feature selection)
  - **Feature weighting** based on relevance
  - Consider other algorithms for  $d > 20$

# Back to k-Nearest Neighbors

## Practical Issues - Computational Complexity

- Training:  $O(1)$  - just store the data
- Prediction (naive):
  - $O(nm)$  per query, where  $m$  is training set size and  $n$  is dimensionality.
  - Must compute distance to all  $m$  points.
- Prediction (optimized) - Data structures can accelerate nearest neighbor search:
  - KD-trees:  $O(n \log m)$  average case for low dimensions, but degrades to  $O(nm)$  in high dimensions
  - Ball trees: Better for high dimensions than KD-trees
  - Locality-sensitive hashing (LSH): Approximate nearest neighbors in  $O(n)$  with preprocessing
- Space complexity:  $O(nm)$  to store the training data.

# Back to k-Nearest Neighbors

## Practical Issues

### Pros

- Simple to understand and implement
- No training phase (fast to “train”)
- Naturally handles multi-class classification
- Non-parametric: makes no distributional assumptions
- Can capture arbitrarily complex decision boundaries
- Easily adapts to new training data (just add it)

### Cons

- Slow prediction for large datasets
- High memory requirement (stores all training data)
- Sensitive to irrelevant features and feature scaling
- Struggles in high dimensions (curse of dimensionality)
- No interpretable model or feature importance
- Requires meaningful distance metric

# Back to k-Nearest Neighbors

## When to use k-NN?

### Use

- Small to medium datasets
- Low to moderate dimensionality ( $n < 20$ )
- Non-linear decision boundaries expected
- Data arrives incrementally (online learning)
- Quick baseline model needed

### Don't Use

- Large datasets with real-time prediction requirements
- Very high-dimensional data
- Features have varying relevance
- Interpretability is required

# Conclusion

- We saw various classification metrics
- We saw one algorithm - k-nearest neighbors - for classification
- Next class - Logistic Regression