Northeastern University
Khoury College of
Computer Sciences

Classification

DS 4400 | Machine Learning and Data Mining I

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Recap Continuation

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

- Batch Gradient Descent
  - Use **entire training set per epoch**
  - The whole training dataset is used to compute a single parameter update

$$\theta_t = \theta_{t-1} - \alpha \frac{1}{m} \sum_{i=1}^{m} \nabla \ell_{\theta_{t-1}}(x_i, y_i)$$

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Sum over the whole training dataset

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

- Stochastic Gradient Descent
  - Use **one** randomly selected training data point at each step
  - Parameters are updated after looking at each data point
  - One epoch leads to **m** parameter updates

$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}(x_i, y_i)$$

Train / Test Splits

- Generally data is split into a training dataset and a testing data
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y	x_0	x_1	x_2

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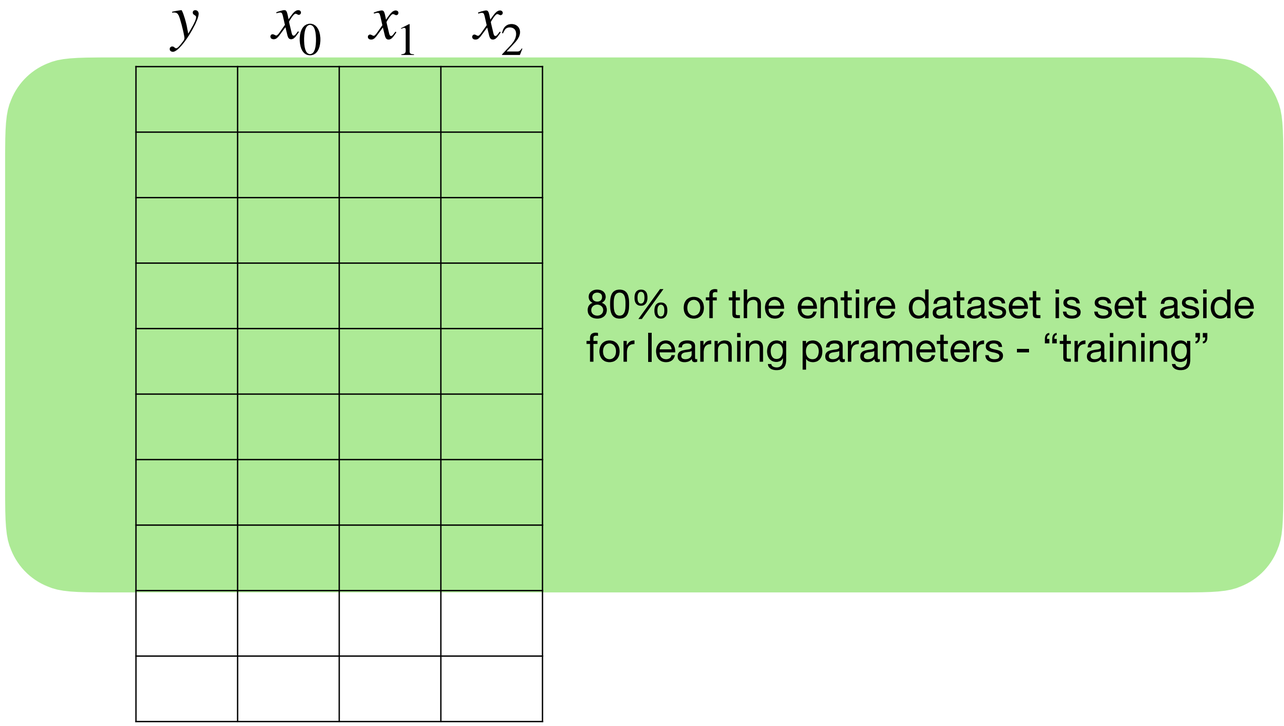

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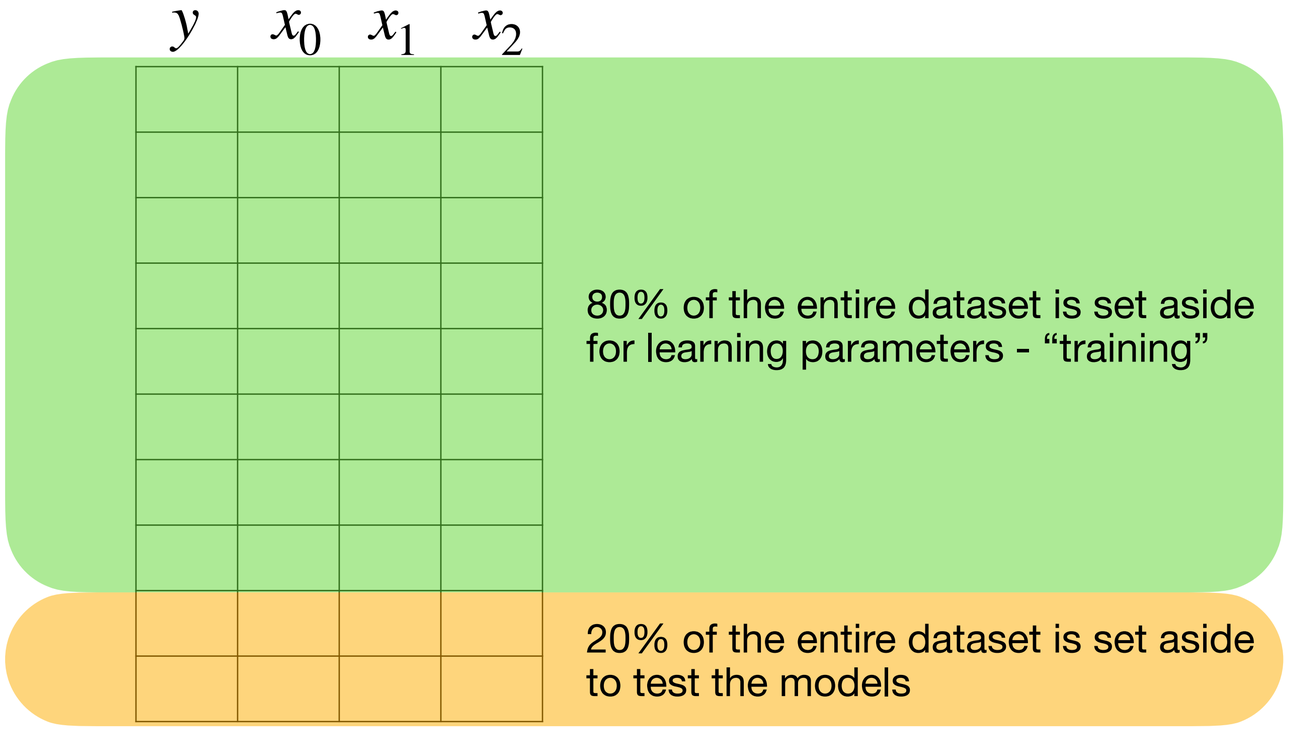


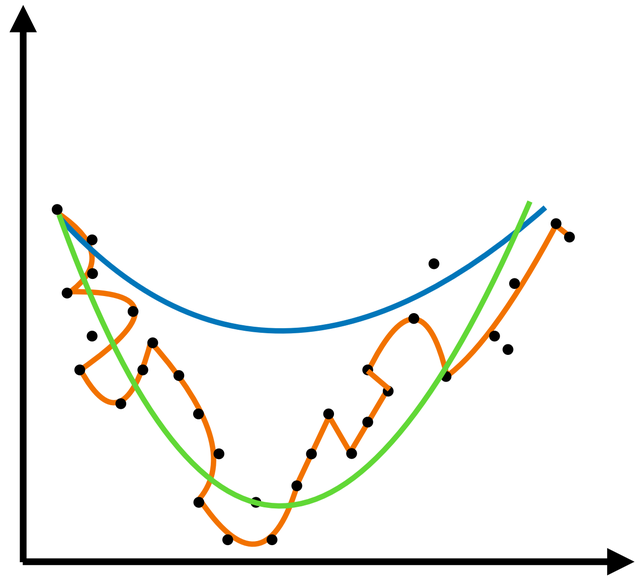
This is **unseen** data and tells you if the model can generalize well

Train / Test Splits

- However, in practice, if you are given only one train and test set, its easy to accidentally pick model architectures that work well on the test set, even though test set data is unseen
- To counter this, we use two unseen datasets - “validation” set and “test” set
- The split is generally of the form 80-10-10 where 80% is training data, 10% is validation data and 10% is test data

Practical Issues in Linear Regression

Overfitting vs Underfitting



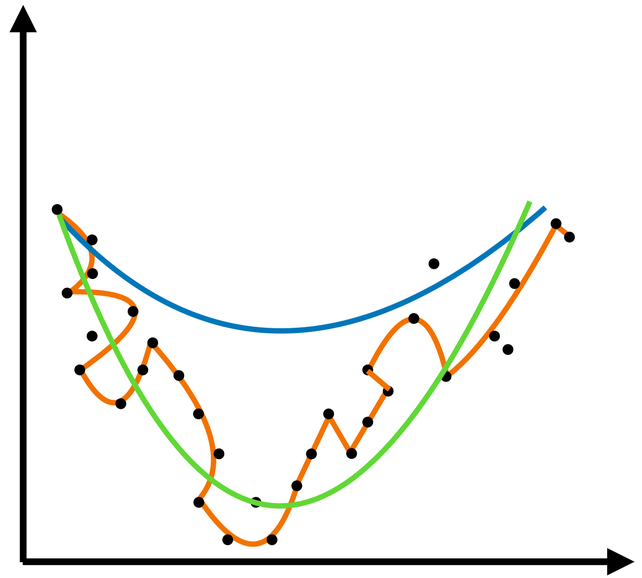
Practical Issues in Linear Regression

Overfitting vs Underfitting

The blue model is **underfitting** the data

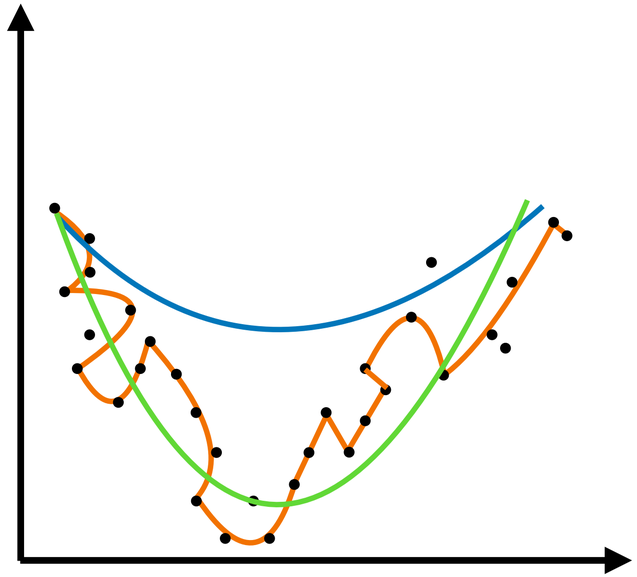
The orange model is **overfitting** the data

The green model is a good fit of the data



Practical Issues in Linear Regression

Underfitting



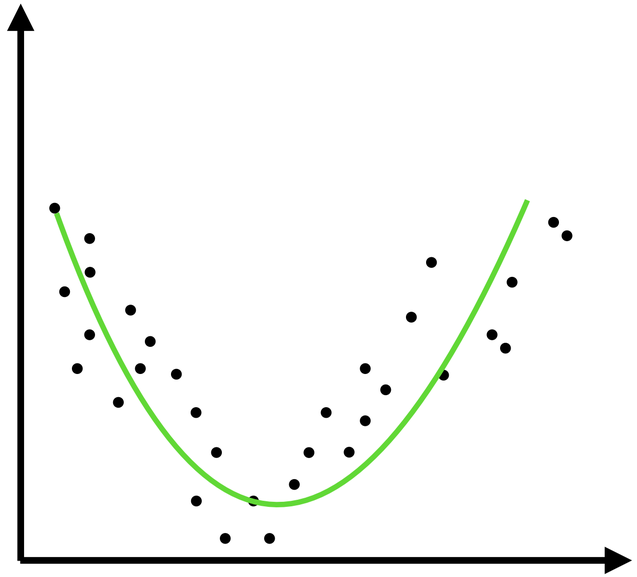
- What is happening?
  - The model is too simple to be able to capture the data
- How do you identify it?
  - Training loss is **high**
  - Test loss is **high**
- Solutions
  - Add more features
  - Add polynomial features ($x_1^2, x_2^2, x_1 x_2, \cdots$)
  - Use a more complex model

Practical Issues in Linear Regression

Quick Aside

- Add polynomial features $(x_1^2, x_2^2, x_1 x_2, \cdots)$

$$f_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$$



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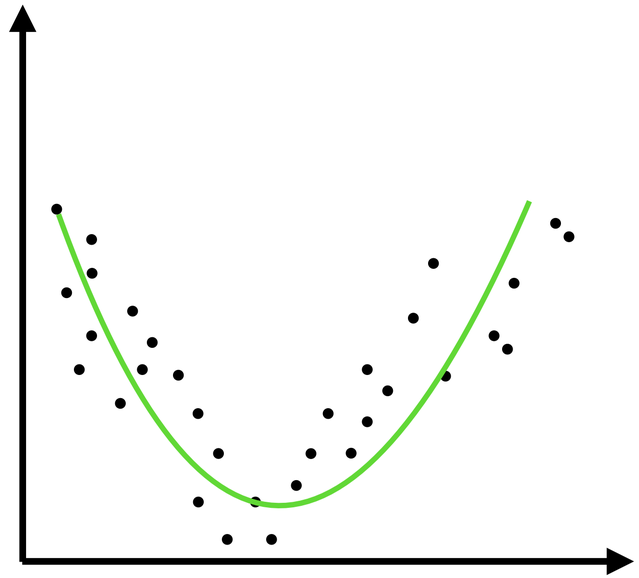


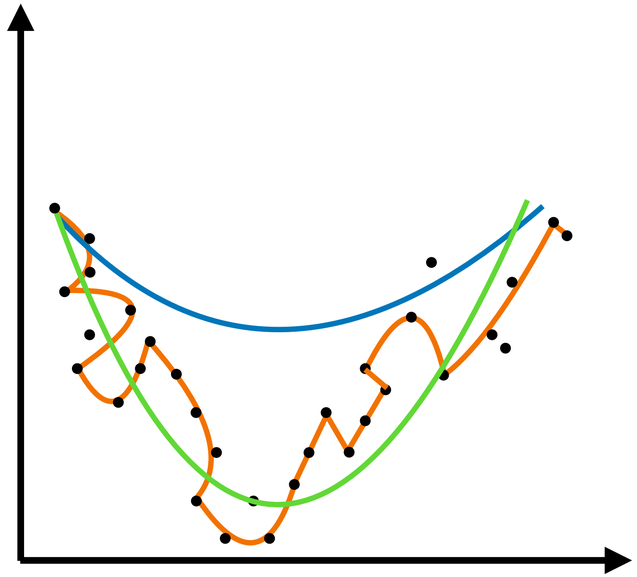
What about these models?

$$f_\theta(x) = \theta_0^{x_0} + \theta_1^{x_1}$$

$$f_\theta(x) = x_0^{\theta_0} + x_1^{\theta_1}$$

Practical Issues in Linear Regression

Overfitting



- What is happening?
  - The model is too complex, so it learns the noise distribution and outliers and hence does not generalize well to new data points
- How do you identify it?
  - Training loss is **low**
  - Test loss is **high**
  - Coefficients have **large** magnitudes
- Solutions
  - Regularization (L_1, L_2)
  - Cross-validation for model selection
  - Reduce number of features
  - Get more training data

Practical Issues in Linear Regression

A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

$$\text{Expected Loss} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Noise}$$

Practical Issues in Linear Regression

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Error from wrong assumptions due to the model being too simple

Practical Issues in Linear Regression

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Every model's prediction error/loss can be decomposed into three parts:

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Error from high sensitivity to each data point and noise due to the model being too complex

Practical Issues in Linear Regression

A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

$$\text{Expected Loss} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Noise}$$

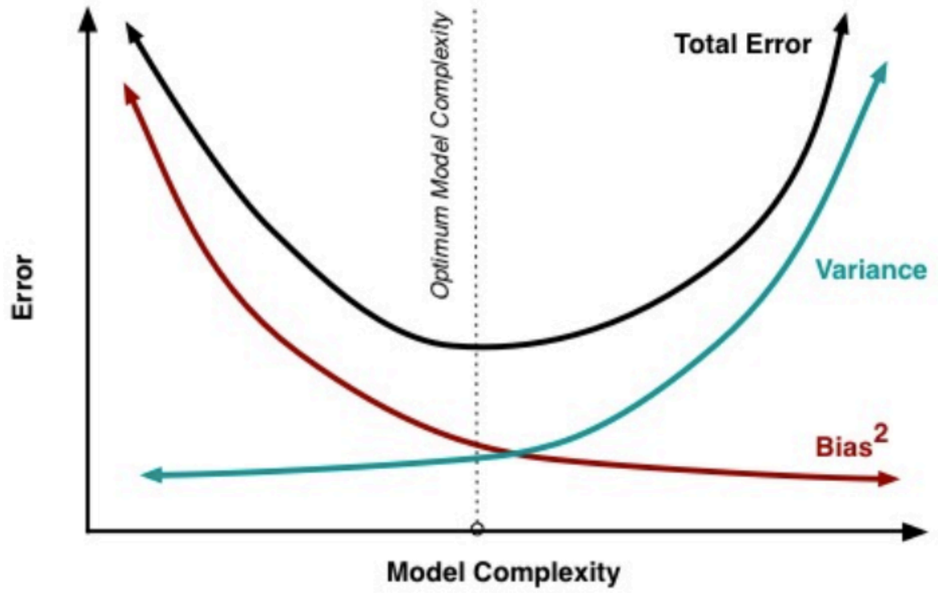
Inherent randomness in data. Cannot be removed.

Practical Issues in Linear Regression

Bias / Variance Tradeoff

Why is it called a **tradeoff**?

Model Complexity	Bias	Variance	Train Error	Test Error
Too Simple	High	Low	High	High
Sweet Spot	Medium	Medium	Medium	Medium
Too Complex	Low	High	Low	High

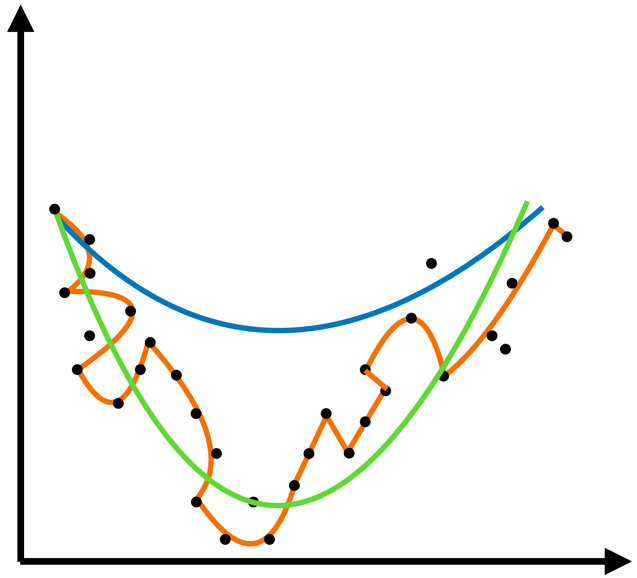


Practical Issues in Linear Regression

Regularization

- Regularization explicitly trades bias for variance.

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$



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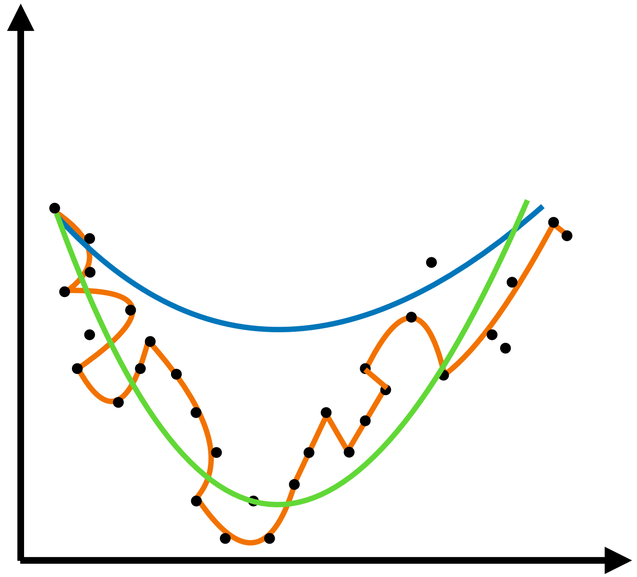

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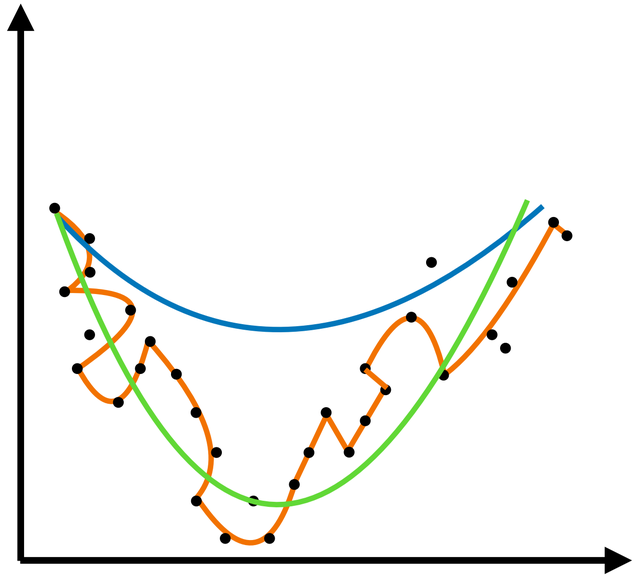
$$\theta = (X^T X + \lambda I)^{-1} X^T Y$$



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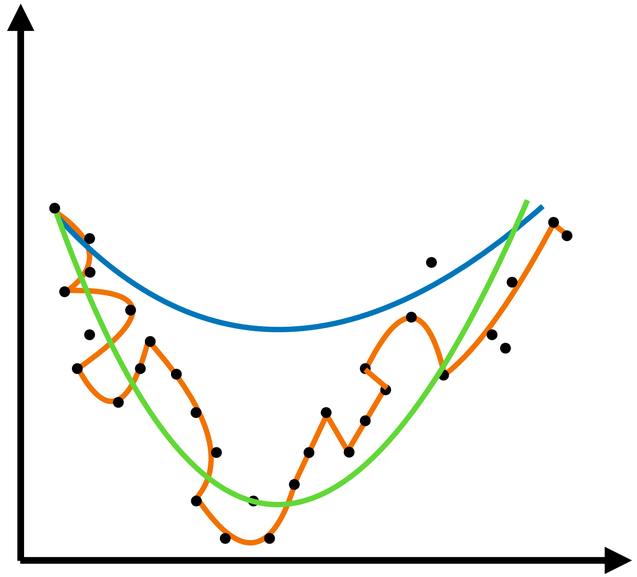

- As λ increases:
  - Coefficients shrink toward zero
  - Bias increases (we're constraining the model)
  - Variance decreases (less sensitive to data)
  - At some λ^*, test error is minimized

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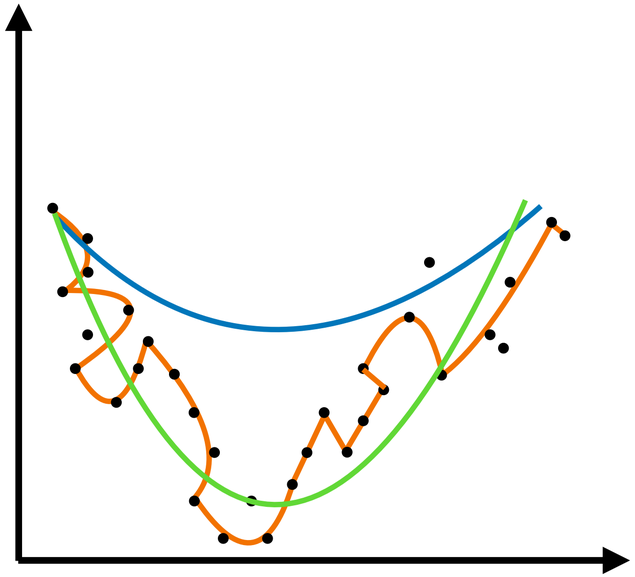
These sort of parameters are usually called **hyper-parameters**

They are **not learnable** but are human defined



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Feature Normalization

Why Normalize?

- If feature x_1 ranges from 0 to 1 and feature x_2 ranges from 0 to 1,000,000, this could lead to numerical instability in the solving process
  - This is particular relevant to gradient descent
- Regularization unfairness
  - If x_2 is much larger, θ_2 must be much smaller to produce similar predictions.
  - The regularization penalty then affects features unequally based on arbitrary scale choices.
- Distance-based algorithms

Feature Normalization

Normalization Methods

1. Min-Max Normalization
2. Mean-Variance Normalization
3. Max-Absolute Normalization
4. Robust Normalization

Feature Normalization

Min-Max Normalization

- For every column in the input data, i.e., for each x_0, x_1, x_2, x_4 etc., this normalization method will scale each column to 0 and 1

$$x' = \frac{x - min(x)}{max(x) - min(x)}$$

- This method preserves zero entries in sparse data
- But is very sensitive to **outliers**

Feature Normalization

Mean-Variance Normalization

- For every column in the input data, i.e., for each x_0, x_1, x_2, x_4 etc., this normalization method will scale to have mean 0 and standard deviation 1

$$x' = \frac{x - \mu(x)}{\sigma(x)}$$

- Most common in practice
- Less sensitive to outliers than min-max
- Does not bound the range to 0 and 1

Feature Normalization

Max-Absolute Normalization

- For every column in the input data, i.e., for each x_0, x_1, x_2, x_4 etc., this normalization method will scale each column to -1 and 1

$$x' = \frac{x}{|max(x)|}$$

- Good for sparse data since it preserves sparsity (zeros stay zero)

Feature Normalization

Robust Normalization

- For every column in the input data, i.e., for each x_0, x_1, x_2, x_4 etc., this normalization method will scale each column as

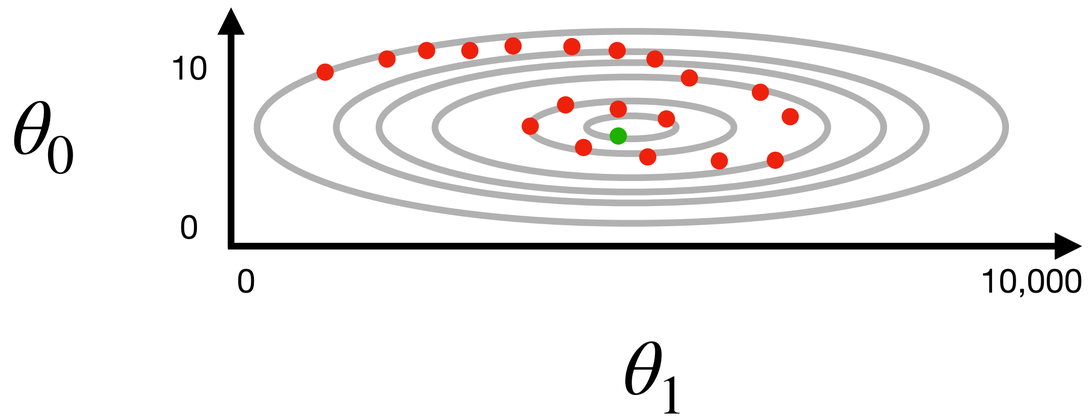
$$x' = \frac{x - median(x)}{IQR(x)}$$

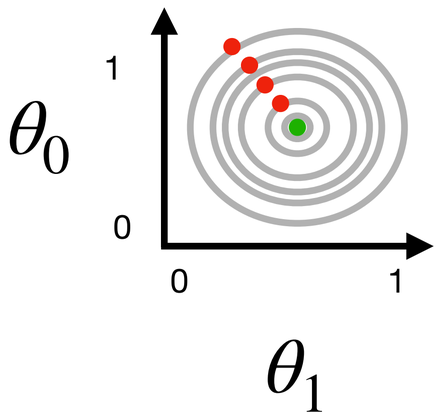
- Robust to outliers
- Use when data has many outliers

Optimizing Loss Functions

Gradient Descent - Practical Fixes

- Feature Scaling
  - Remember we want all input features $x_1, x_2 \cdots x_n$ to be in similar ranges
  - When features have different scales, the loss surface becomes elongated (ill-conditioned).





This dramatically accelerates the optimization process

This also allows having one single learning rate for all parameters

Optimizing Loss Functions

Gradient Descent - Practical Fixes

- Feature Scaling

NOTE: Scaling parameters (mean, standard deviation, min, max) must be computed **only on training data** and then applied to validation and test data to prevent data leakage.

  - Remember we want all input features $x_1, x_2 \cdots x_n$ to be in similar ranges
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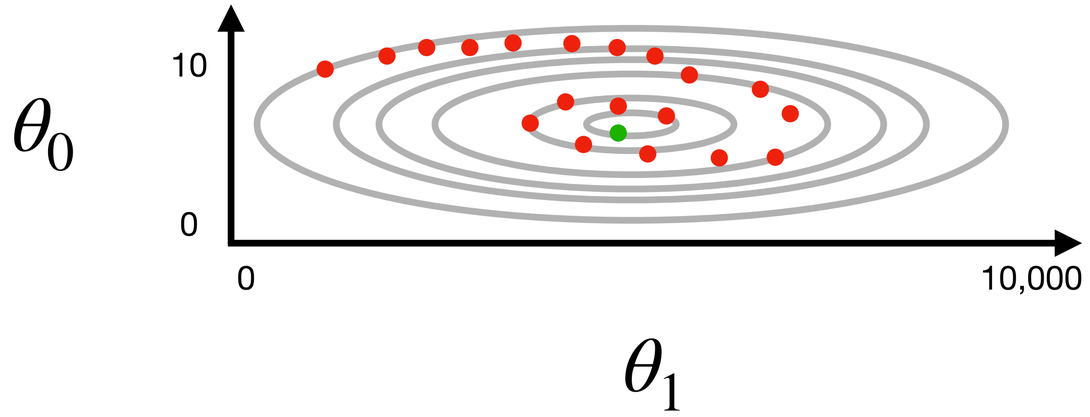

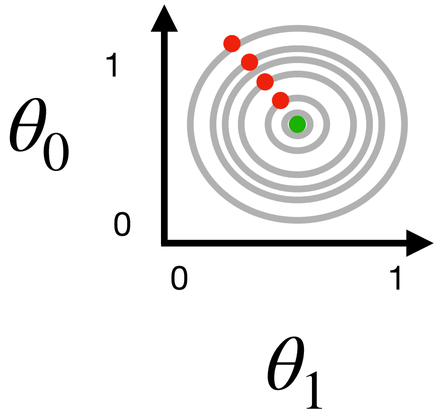

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Today’s Outline

- Classification
- Metrics
- k-Nearest Neighbors

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- k-Nearest Neighbors

Classification

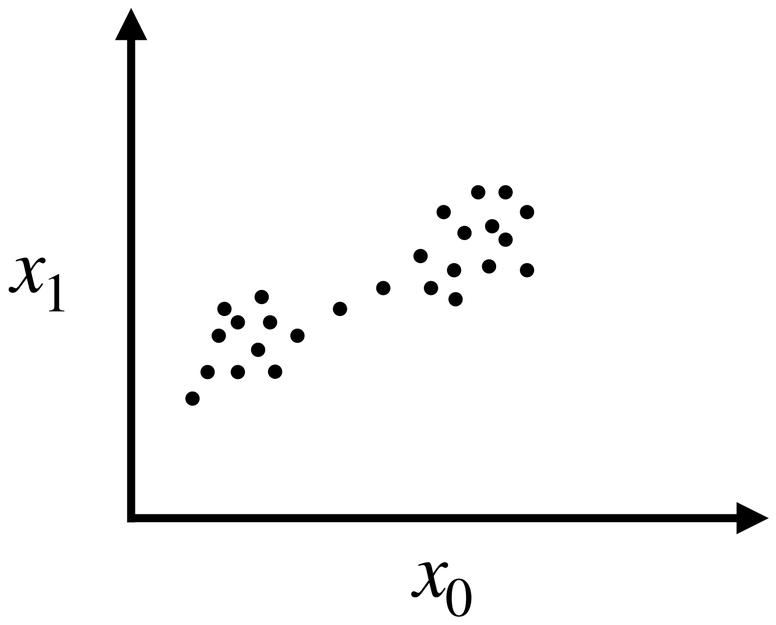
Introduction

- 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, $y \in \{1, 2, \ldots, k\}$ where $k > 2$

Classification

Decision Boundary

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



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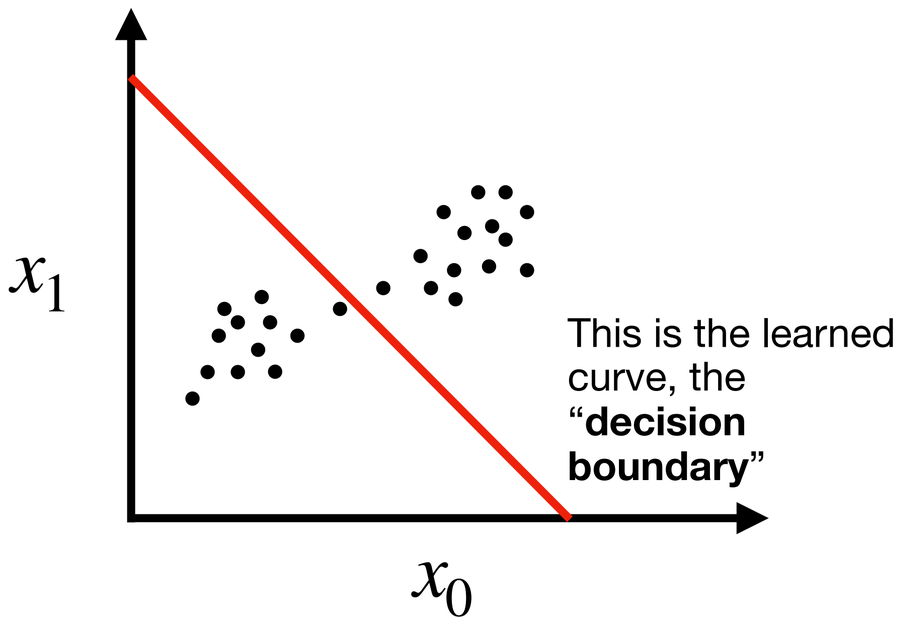
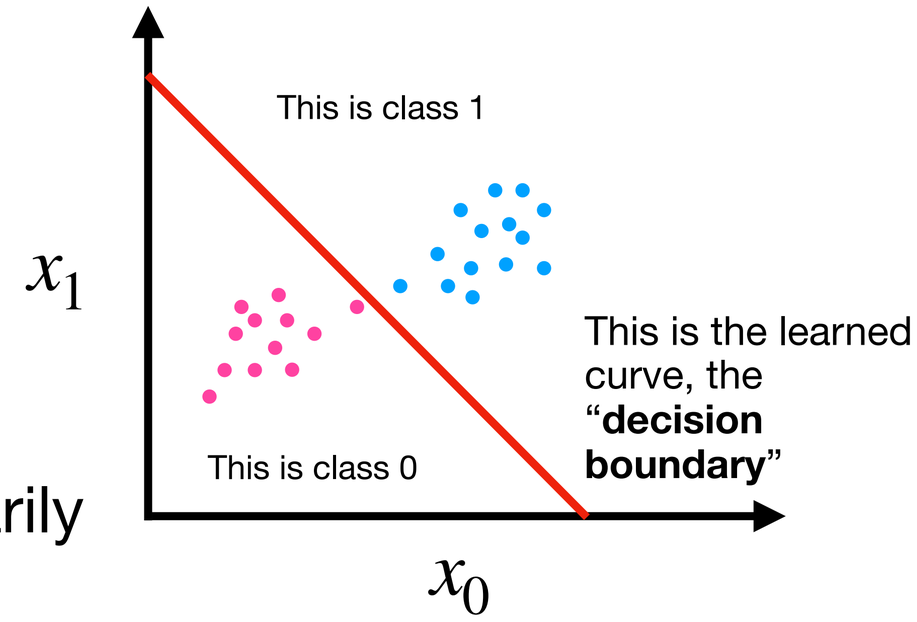


Classification

Decision Boundary

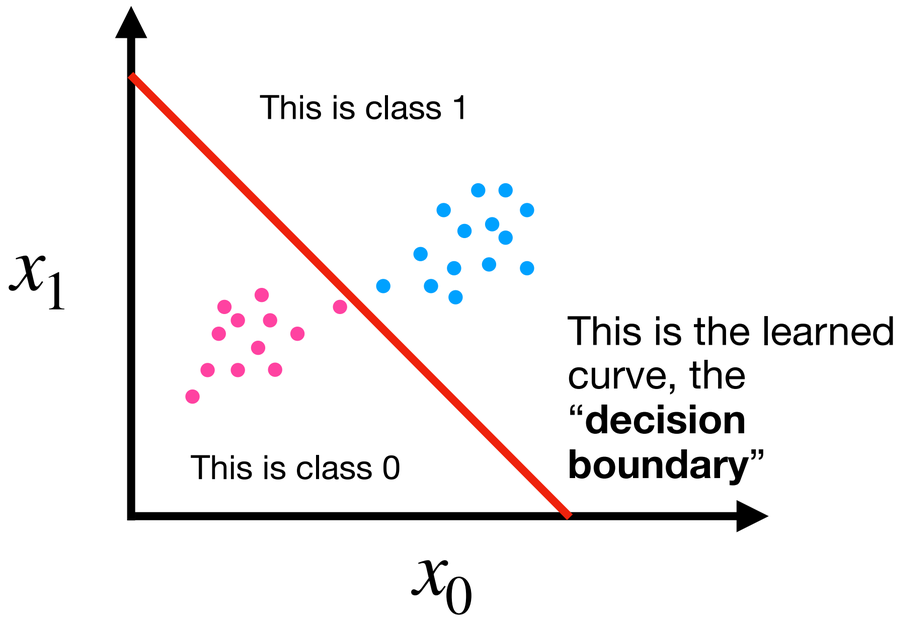
- A classifier partitions space into multiple sections, each section corresponding to a class.
- Different algorithms produce different boundary shapes
  - Linear classifiers produce hyperplanes
  - Non-linear classifiers can produce arbitrarily complex boundaries.



Classification

Decision Boundary

- But practically speaking, your classifier will output a probability value between 0 and 1
- Example:
  - $\mathbb{P}(cat \mid image_1) = 0.61$
  - $\mathbb{P}(cat \mid image_2) = 0.52$



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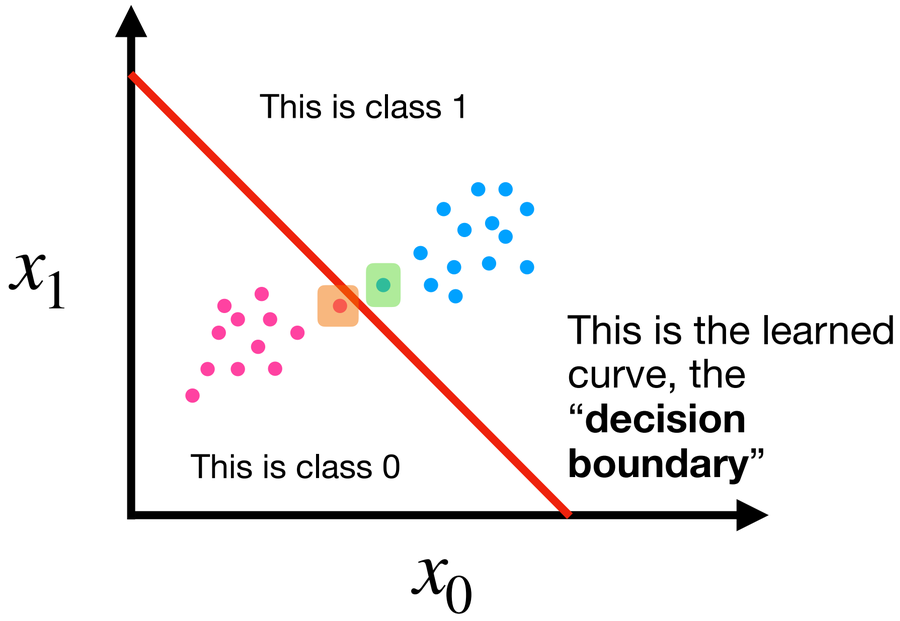

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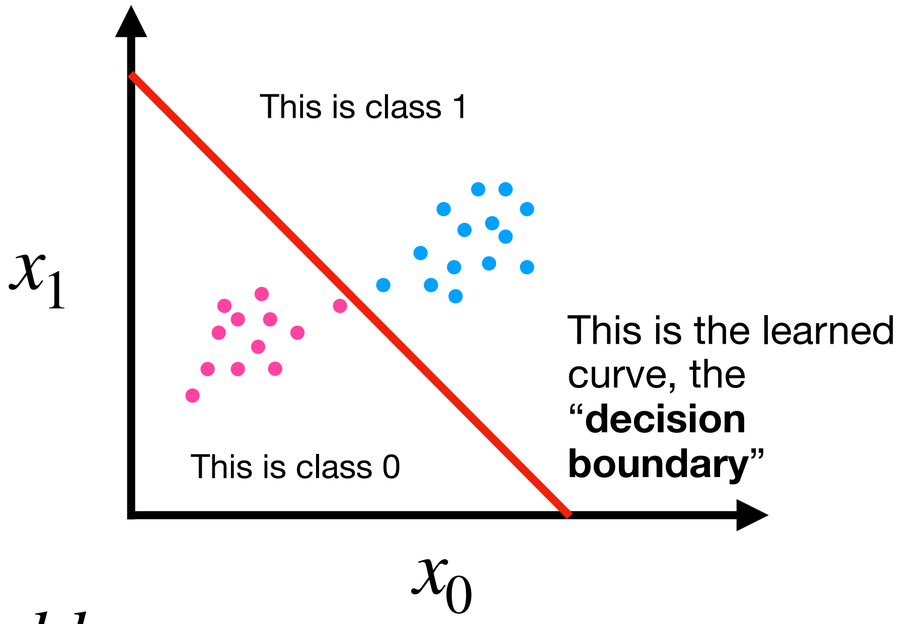
- Example:
  - $\mathbb{P}(cat \mid image_1) = 0.61$
  - $\mathbb{P}(cat \mid image_2) = 0.52$
- Practitioner needs to also set a **threshold**
  - $image_i$ is a cat if $\mathbb{P}(cat \mid image_i) \geq Threshold$



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:** Is accuracy a good metric in this case?

Metrics

Confusion Matrix

	Predicted Positive	Predicted Negative
Actual Positive		
Actual Negative		

Metrics

Confusion Matrix

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

Metrics

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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

	Predicted Positive	**Predicted Negative**
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Metrics

Precision and Recall

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

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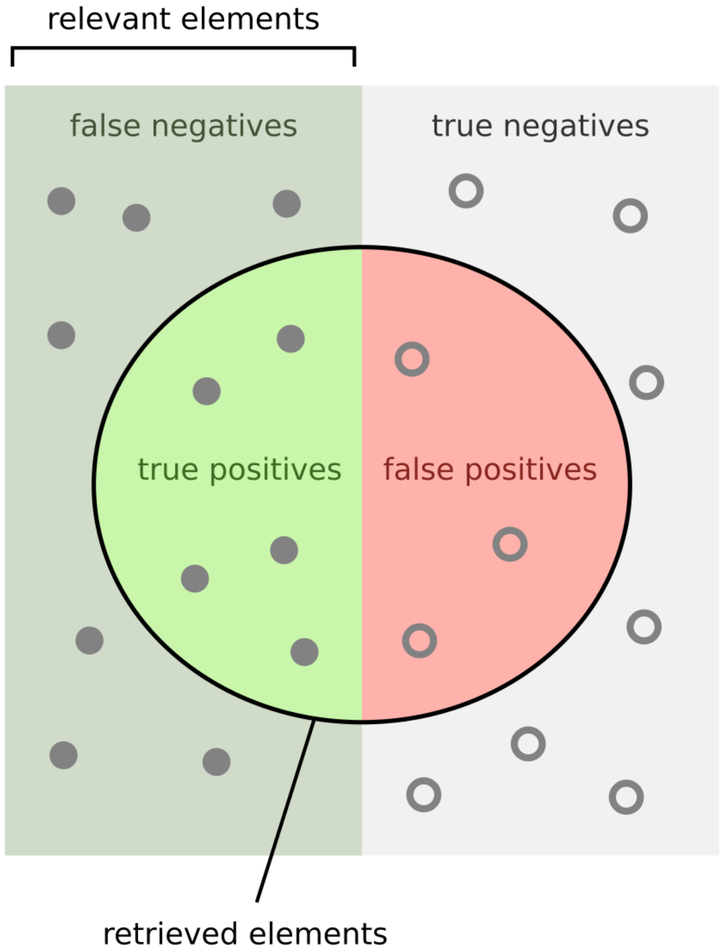

How many retrieved items are relevant?

Precision = 

How many relevant items are retrieved?

Recall = 

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Metrics

Precision and Recall

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

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.

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

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).

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Actual Negative	False Positive (FP)	True Negative (TN)

Metrics

Precision vs Recall Tradeoff - F1 Score

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

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

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

Increasing the threshold for positive classification typically **increases precision but decreases recall**.

Decreasing the threshold has the opposite effect.

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

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

Metrics

Precision vs Recall Tradeoff - F1 Score

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

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

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

The harmonic mean of precision and recall

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

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

Metrics

Precision vs Recall Tradeoff - F1 Score

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

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

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

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

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

Metrics

Precision vs Recall Tradeoff - F1 Score

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

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

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

	Predicted Positive	**Predicted Negative**
Actual Positive	True Positive (TP)	False Negative (FN)
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$$\text{Specificity} = \frac{TN}{TN + FP}$$

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

Same denominator

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

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Precision vs Recall Tradeoff - F1 Score

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

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

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

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

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

Same denominator

FPR = 1 - Specificity

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

Metrics

Precision vs Recall Tradeoff - F1 Score

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

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

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

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

Recall is the True Positive Rate

Metrics

Why so many metrics?

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

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

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

	Predicted Positive	**Predicted Negative**
Actual Positive	True Positive (TP)	False Negative (FN)
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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?

Metrics

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

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

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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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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?

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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?

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

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Answer: By changing the threshold

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- Cat in image if $\mathbb{P}(cat \mid image_i) \geq 0$
  - Precision goes [redacted], Recall goes [redacted]

Metrics

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  - Precision goes down, Recall goes up

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$$\text{Precision} = \frac{TP}{TP + FP} \qquad \text{Recall} = \frac{TP}{TP + FN}$$

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How would you increase/decrease the true positives?

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  - Precision goes  Recall goes 

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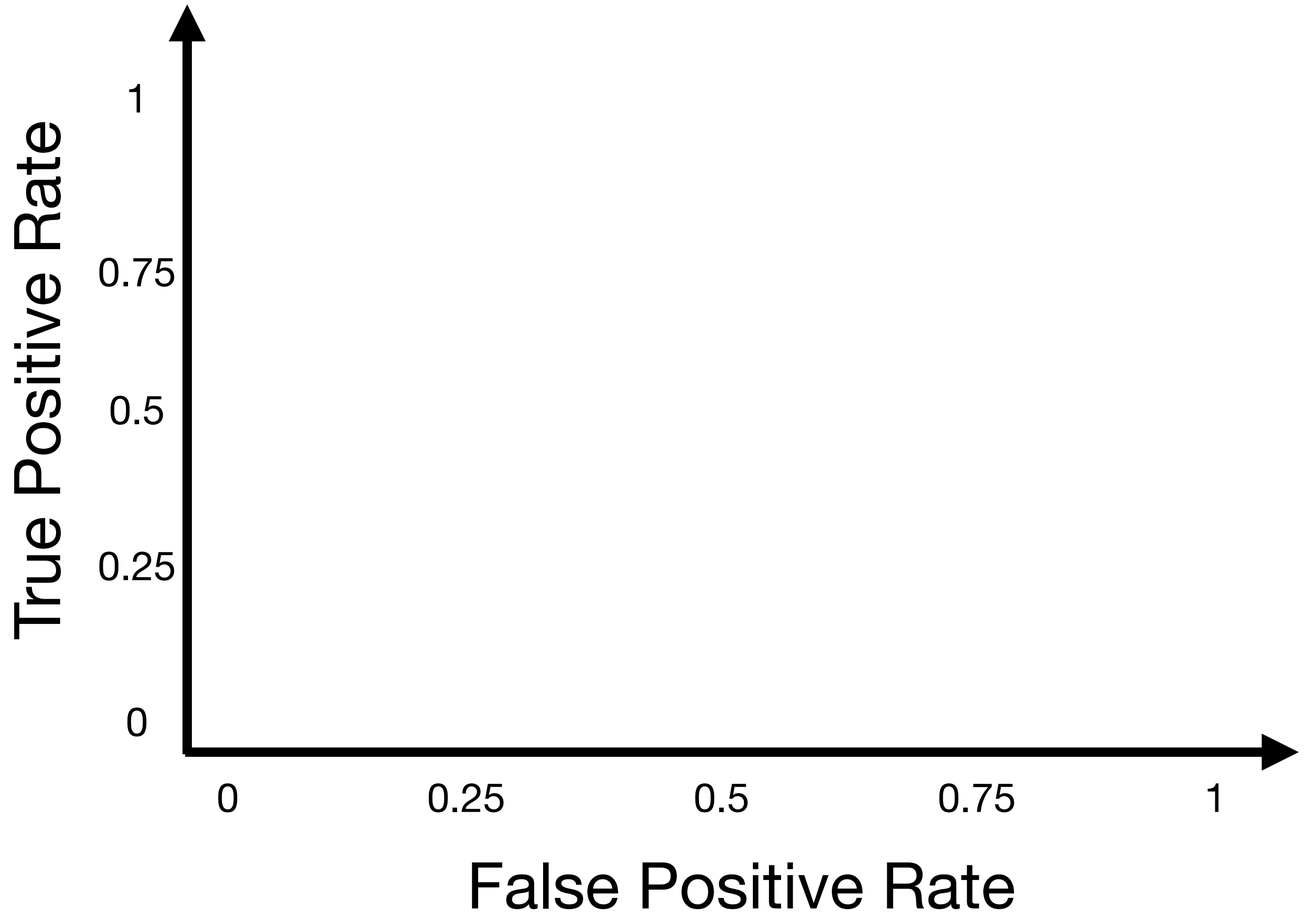
- Cat in image if $\mathbb{P}(cat \mid image_i) \geq 0.999$
  - Precision goes up, Recall goes down

Metrics

AUC-ROC Curve

$$\text{TPR} = \frac{TP}{TP + FN} \qquad \text{FPR} = \frac{FP}{TN + FP}$$



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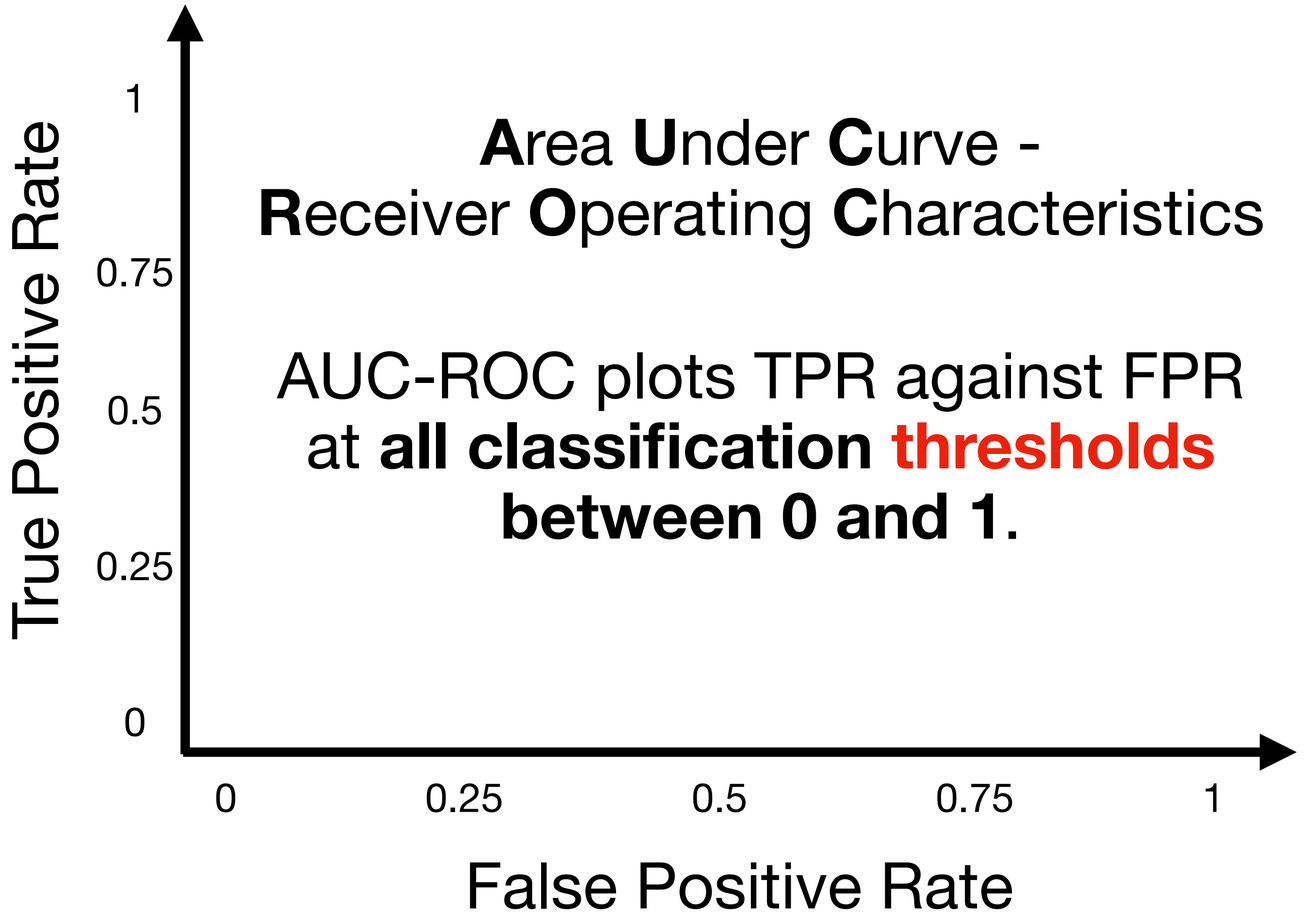

Area **U**nder **C**urve -
Receiver **O**perating **C**haracteristics

AUC-ROC plots TPR against FPR
at **all classification thresholds**
between 0 and 1.

Metrics

AUC-ROC Curve

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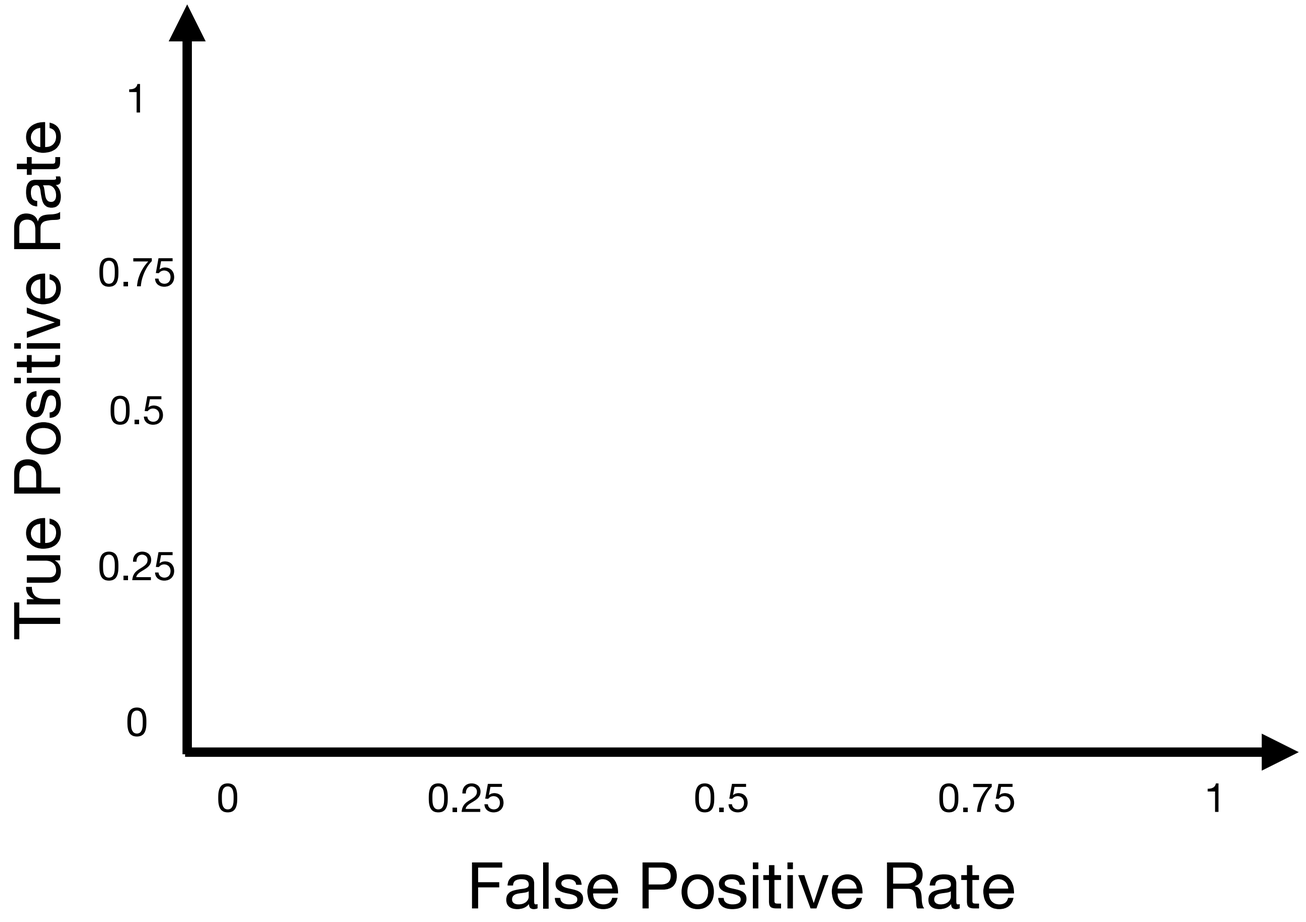

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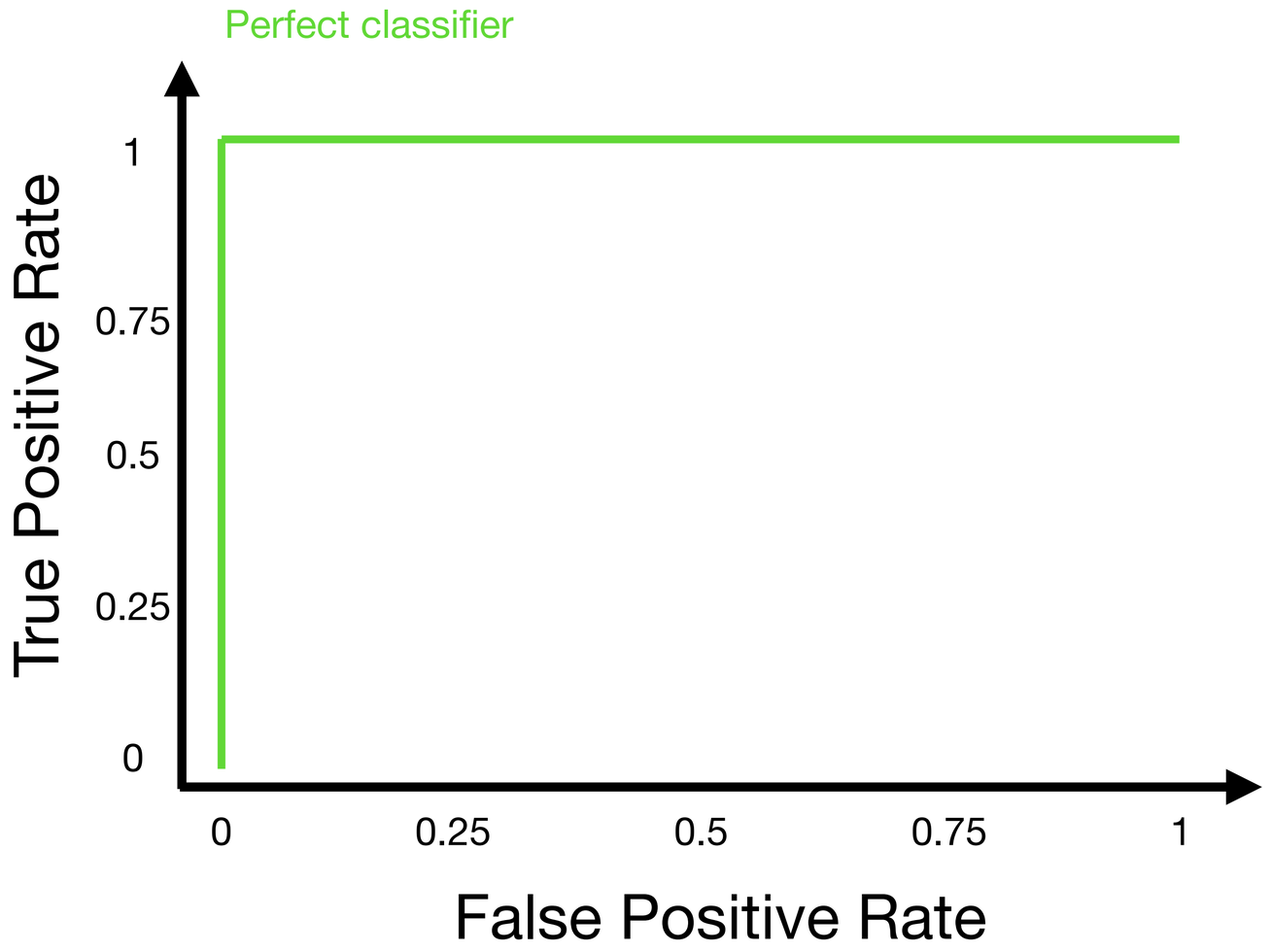

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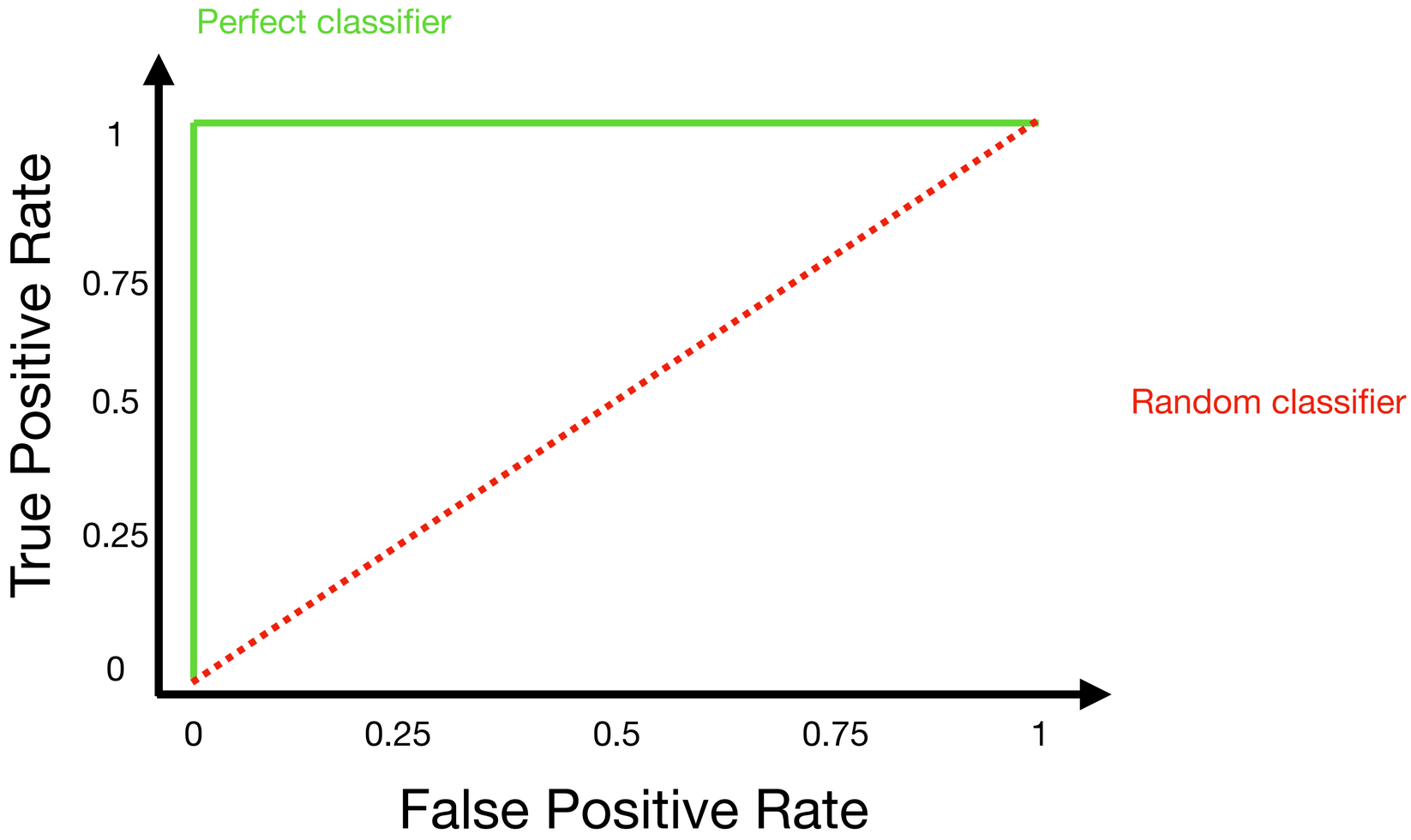

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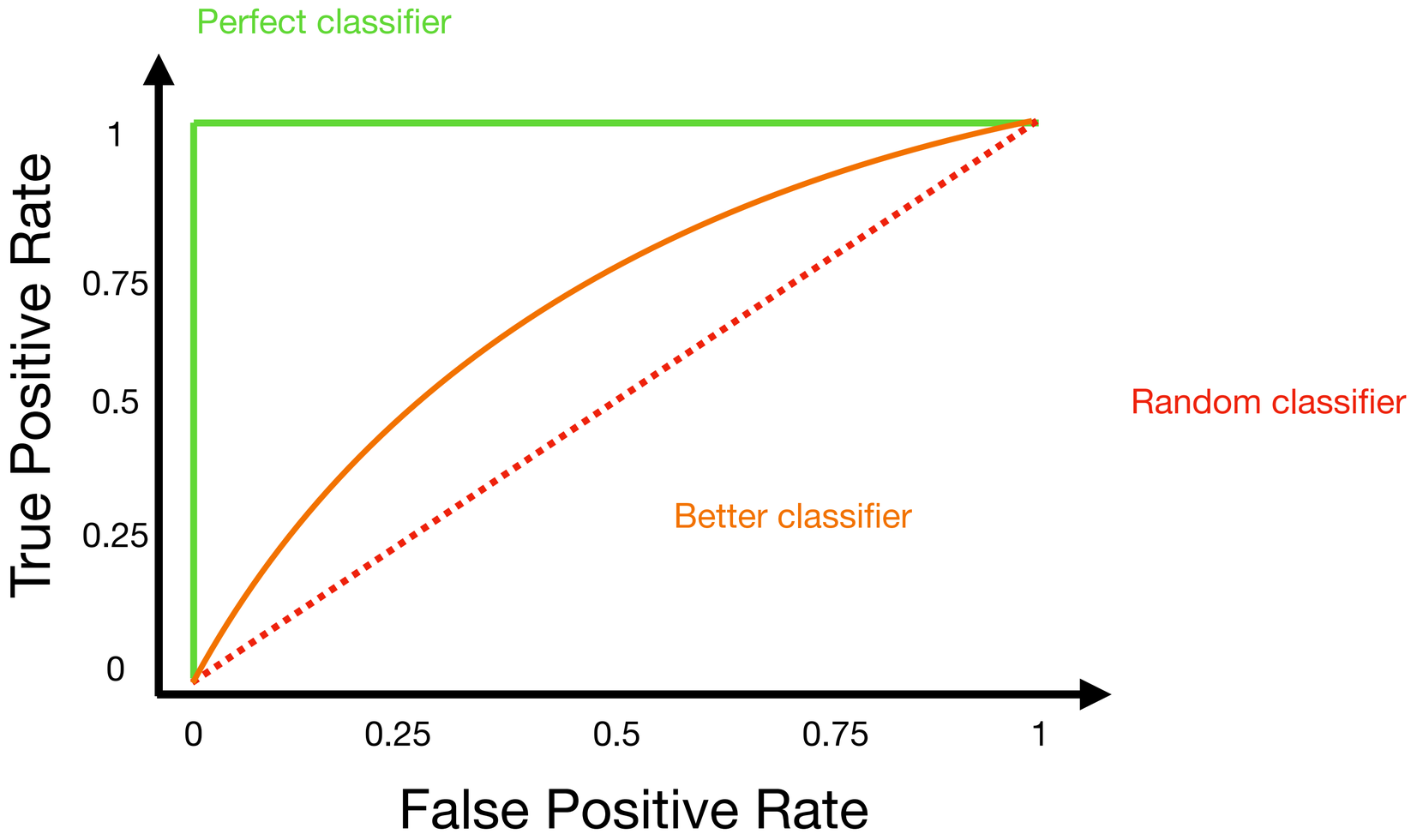

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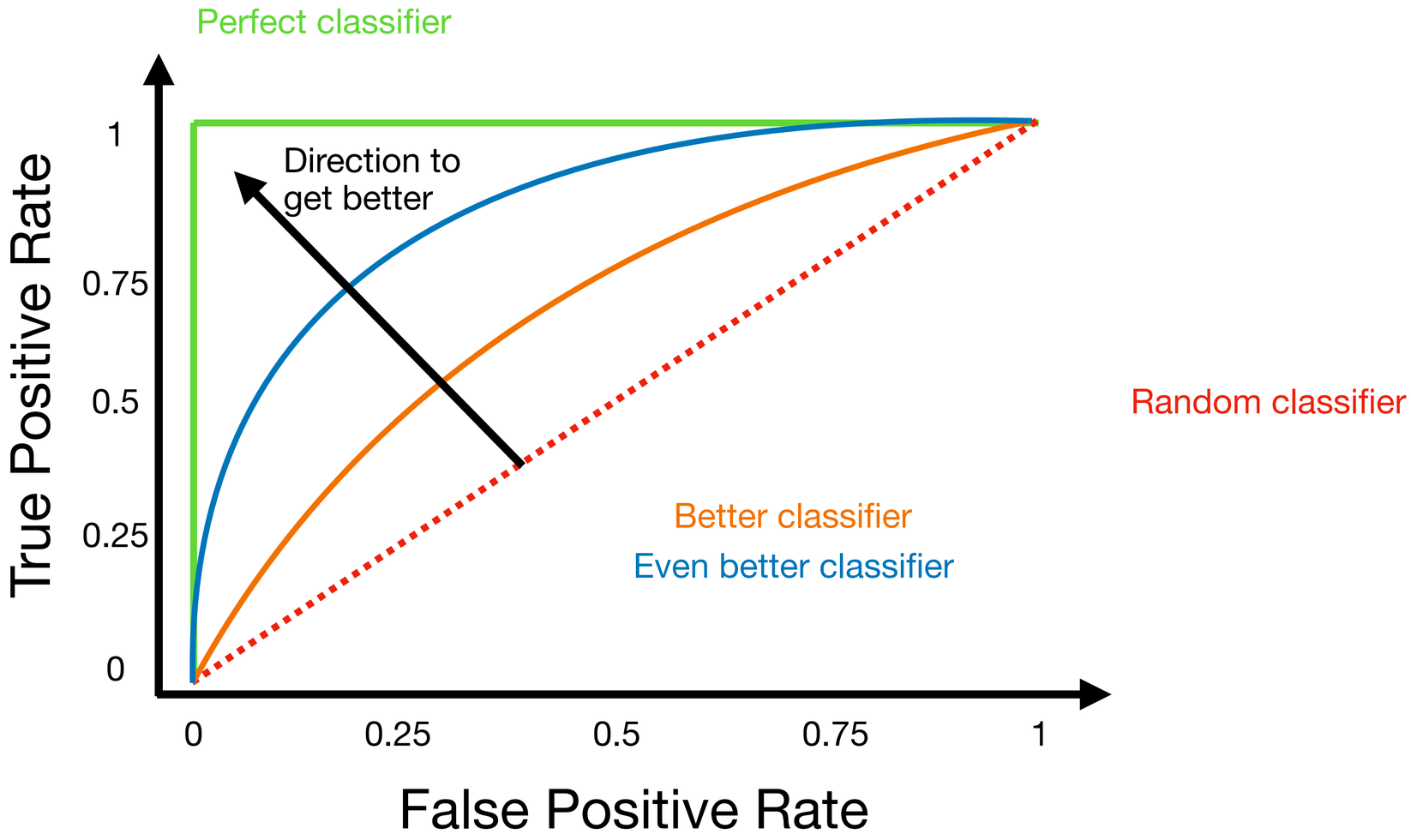

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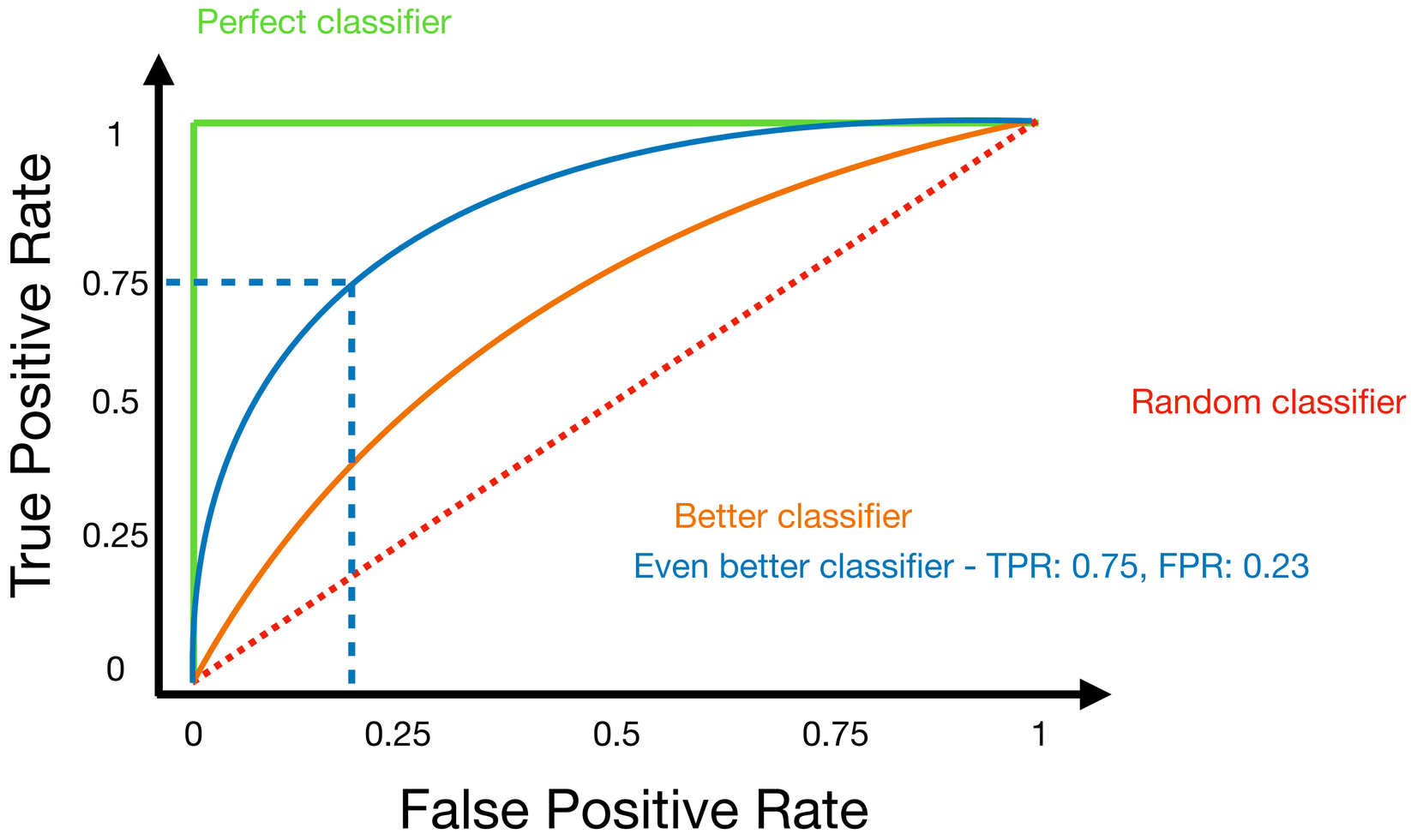

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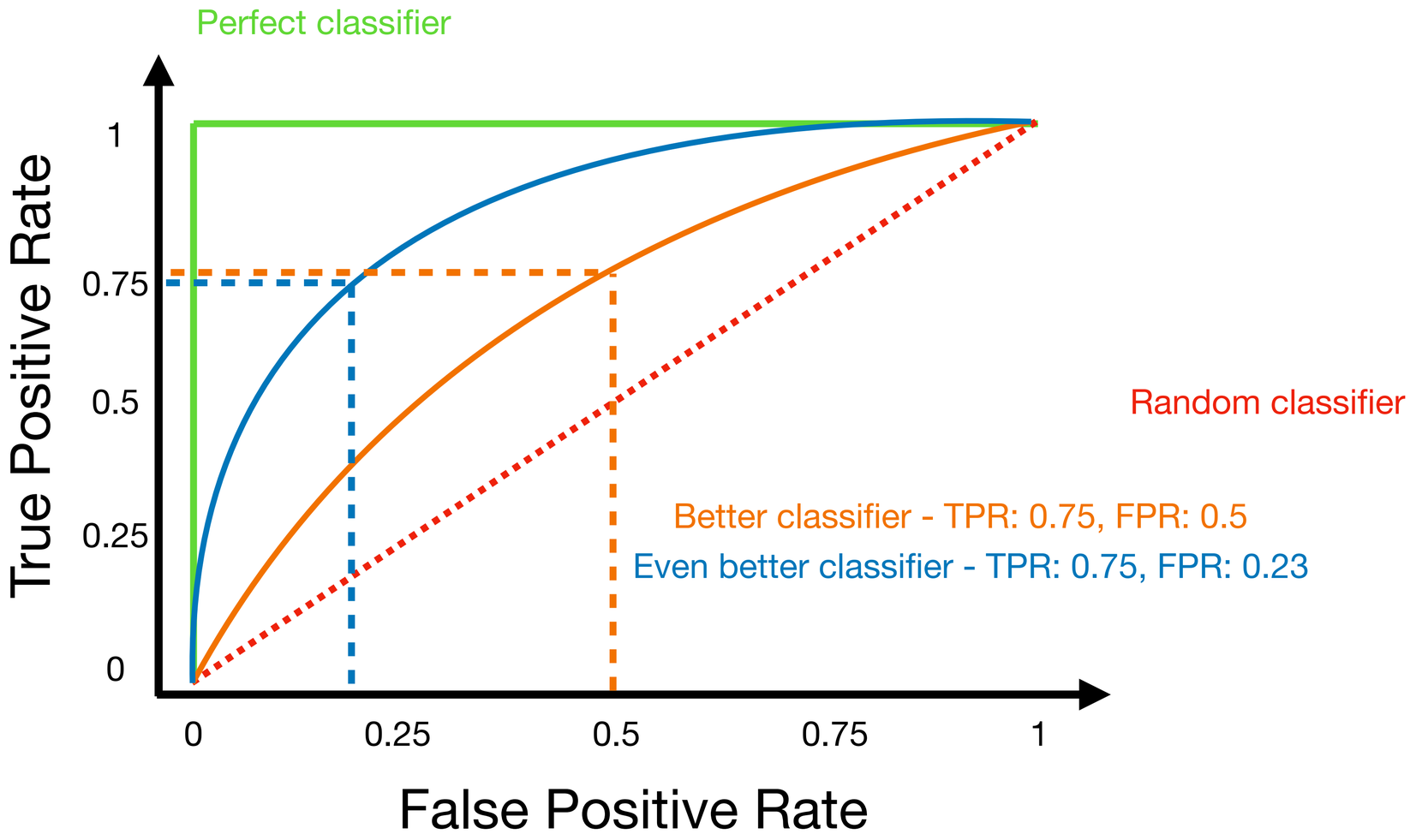

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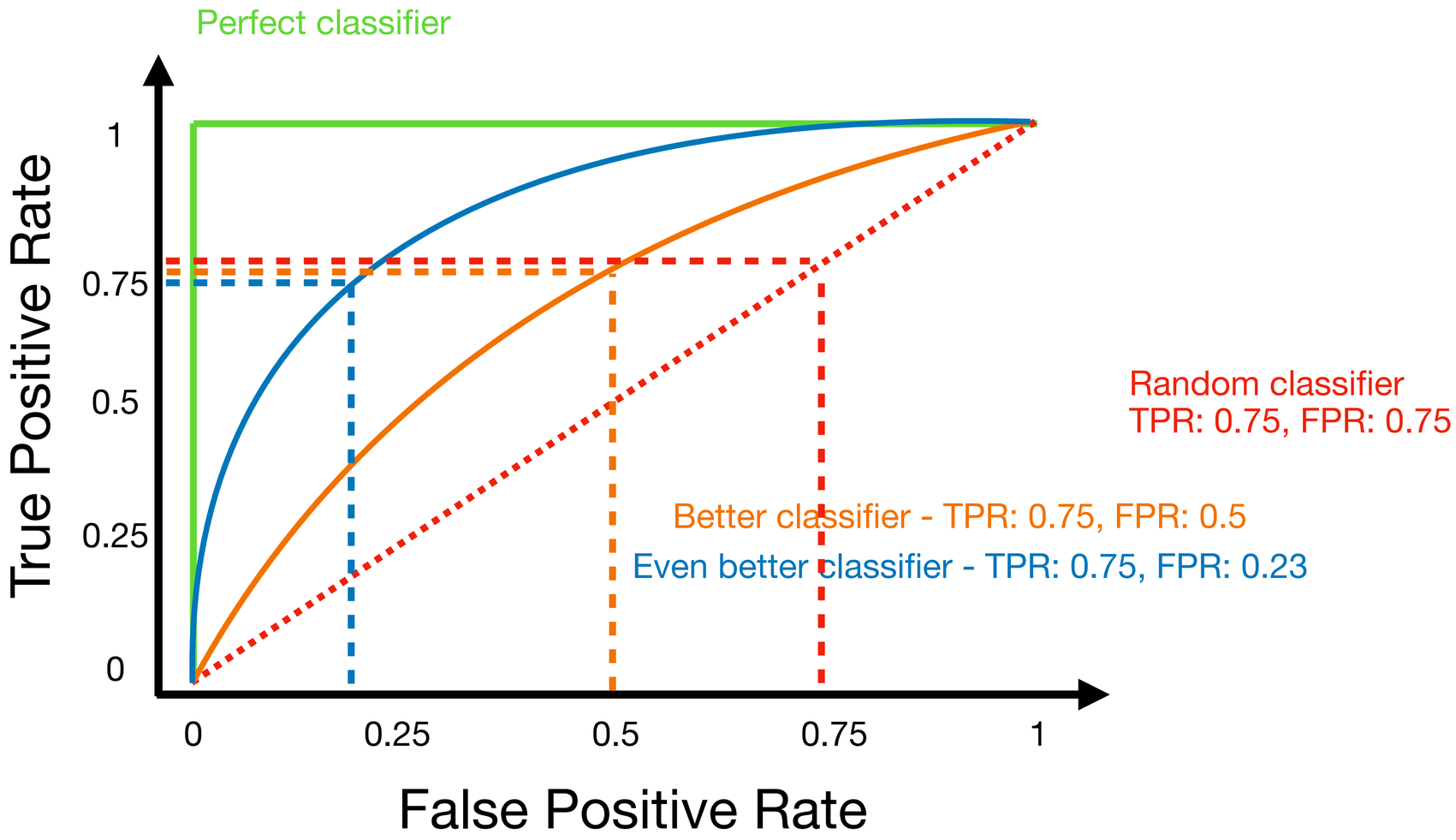

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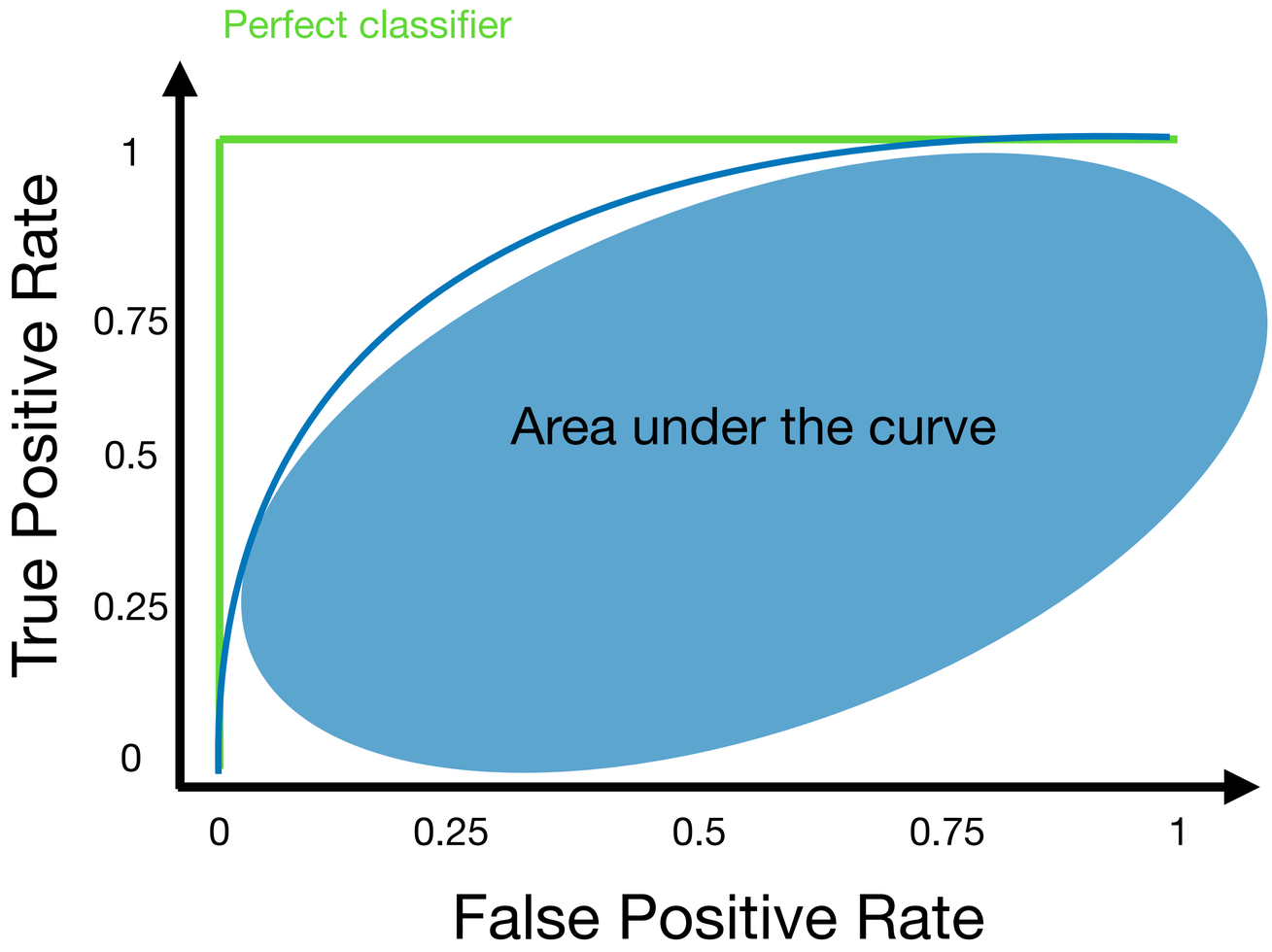

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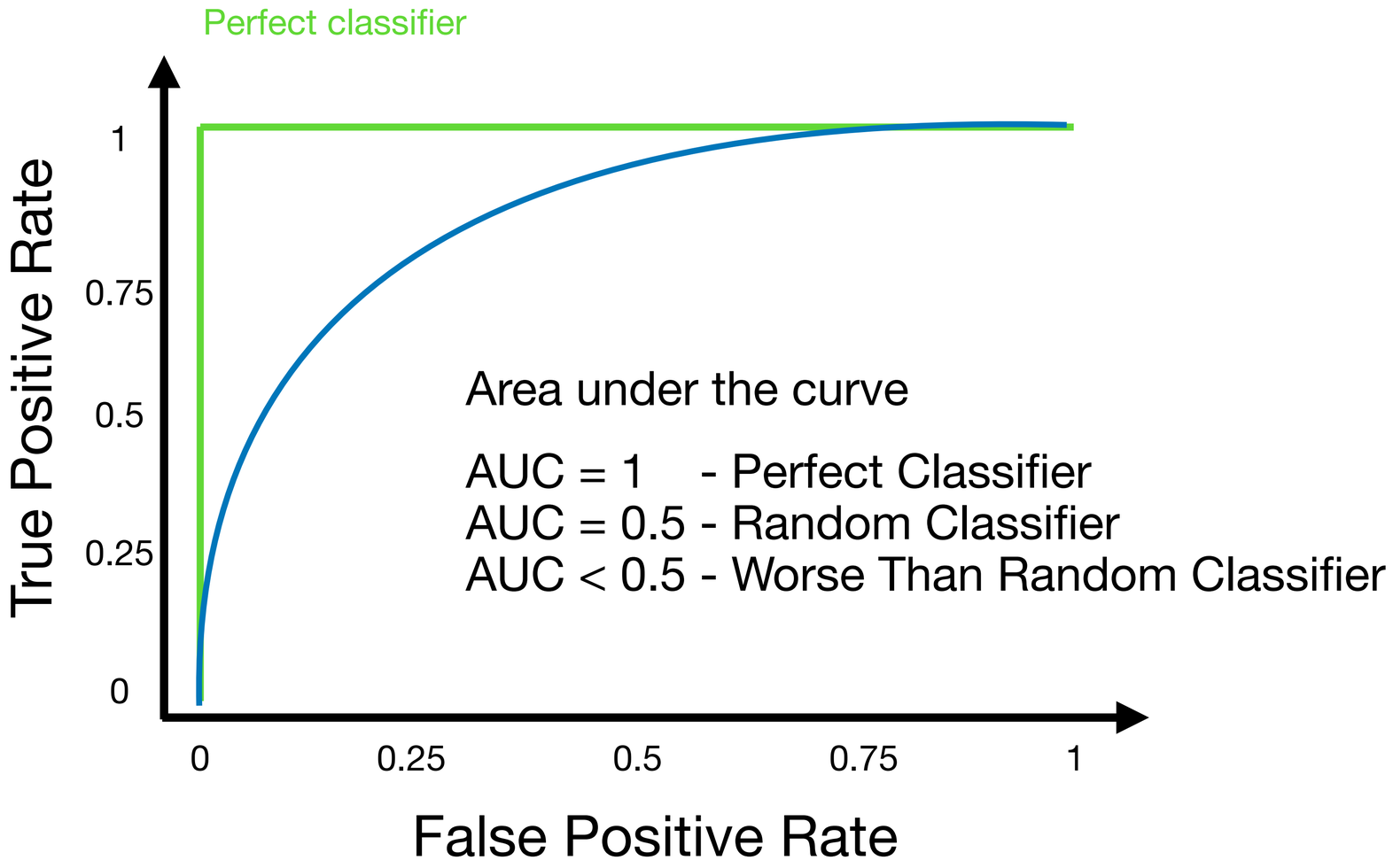
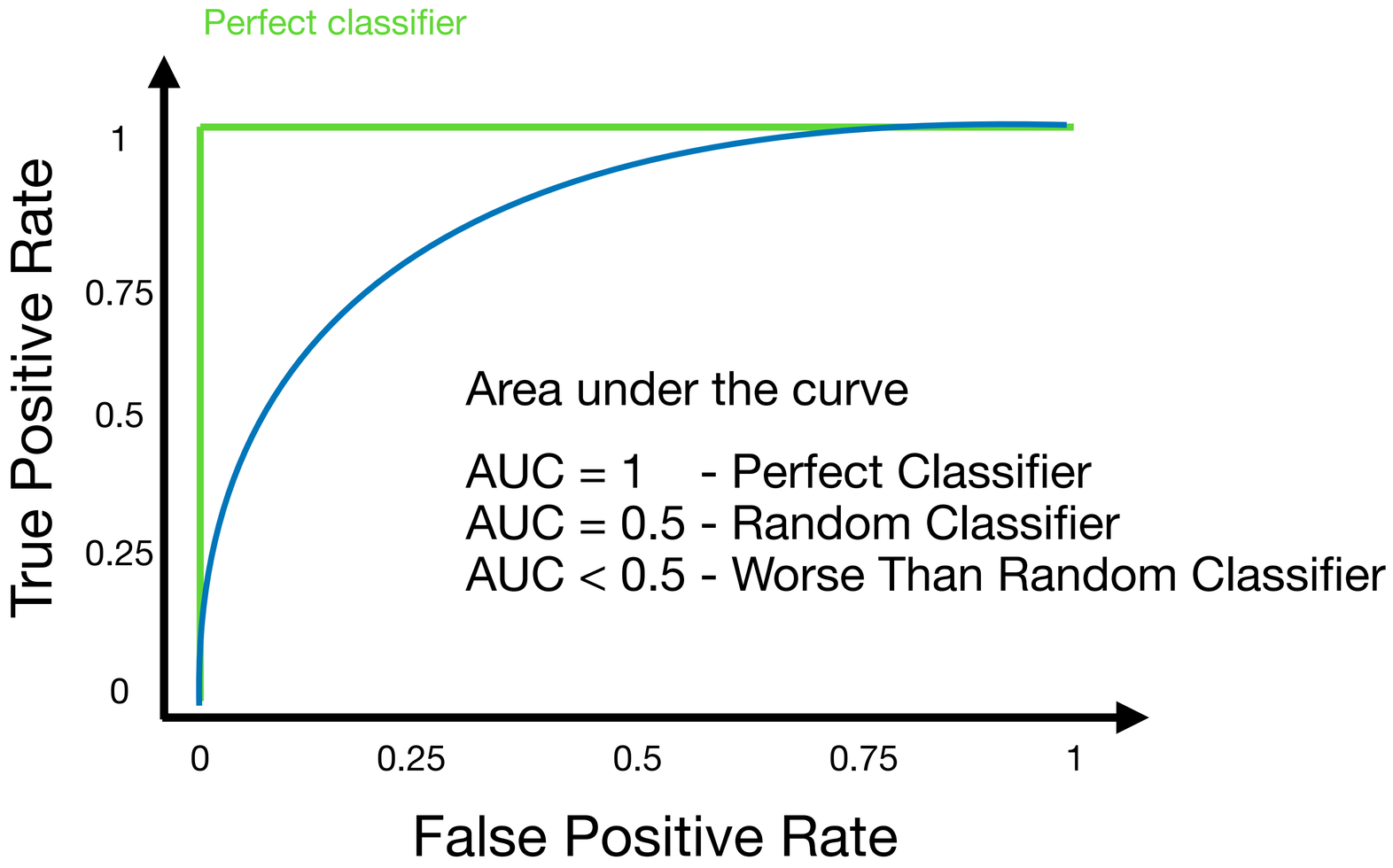


Metrics
AUC-ROC Curve

$$\text{TPR} = \frac{TP}{TP + FN} \qquad \text{FPR} = \frac{FP}{TN + FP}$$

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.



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AUC-ROC Curve

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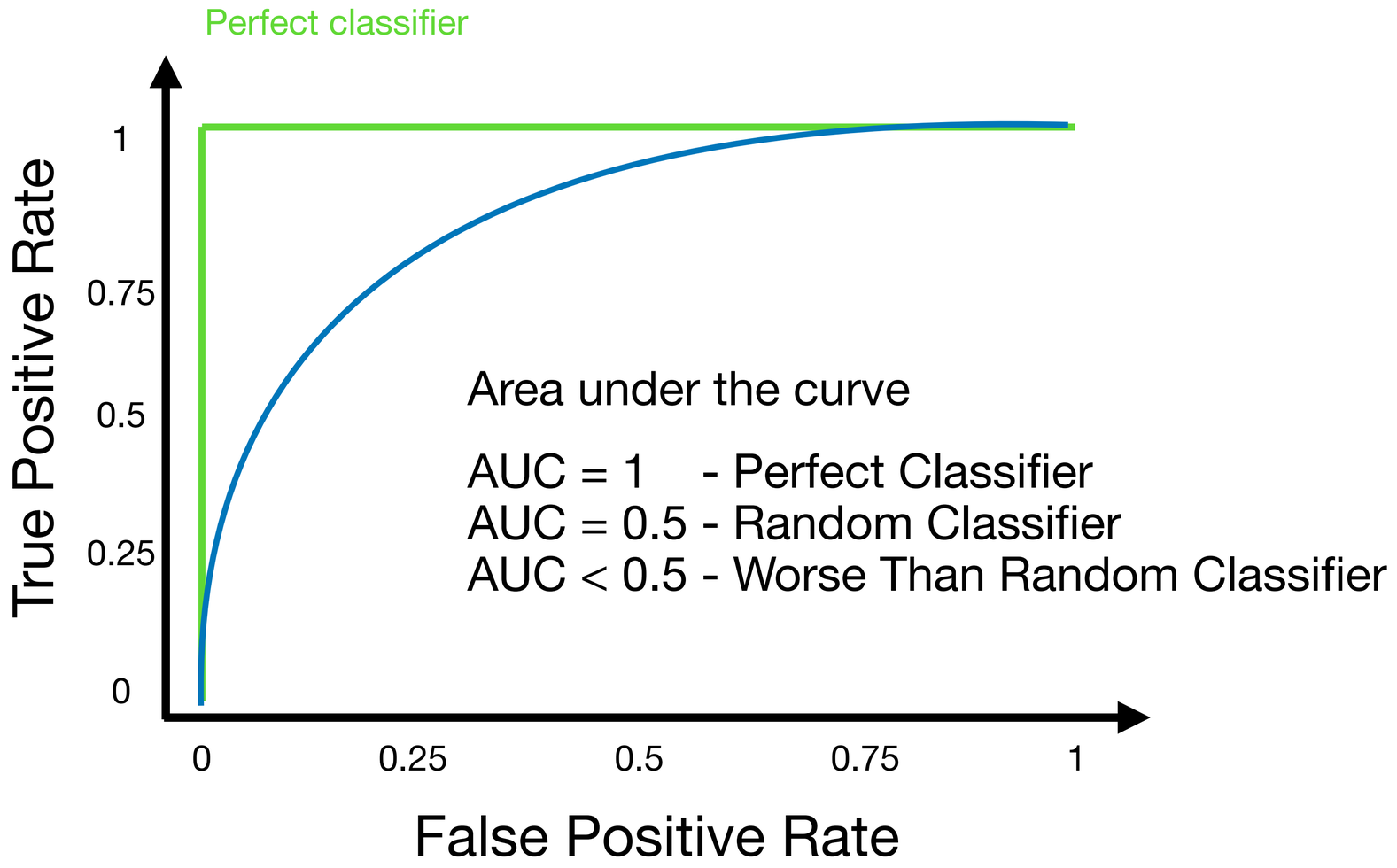
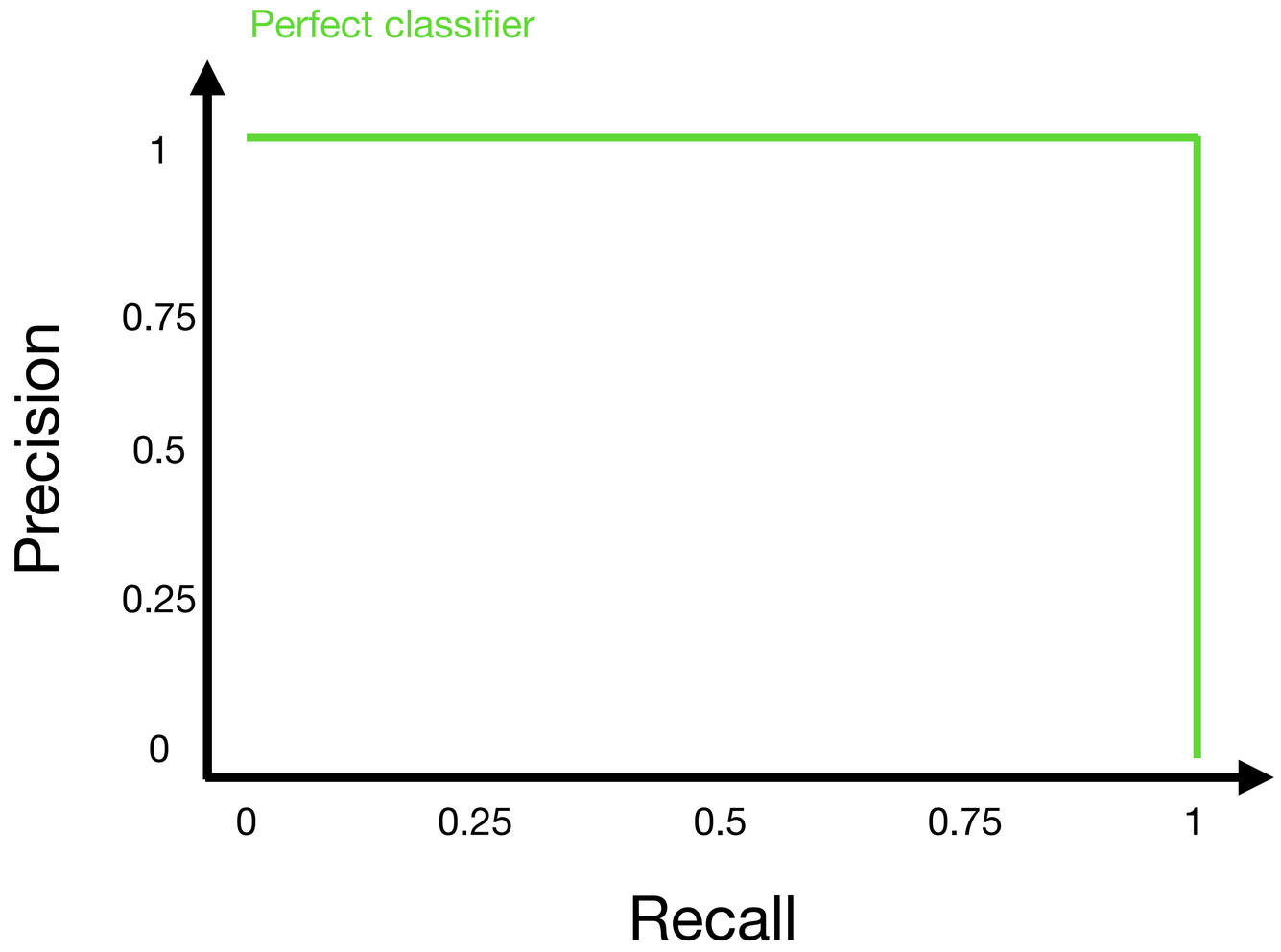
Intuition:
AUC equals the probability that a randomly chosen positive instance is **ranked higher** than a randomly chosen negative instance by the classifier's scores.

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



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.

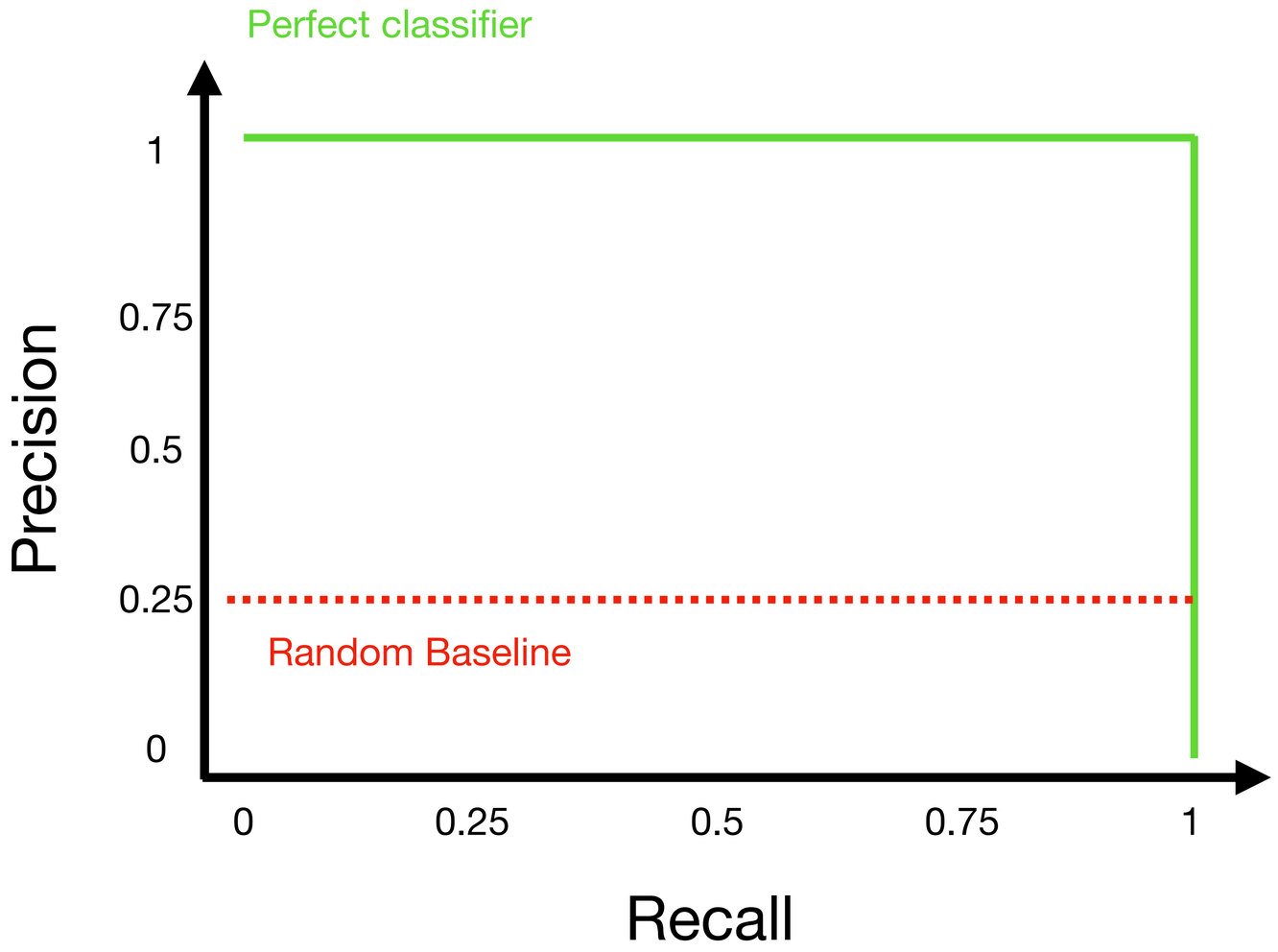
Metrics

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.



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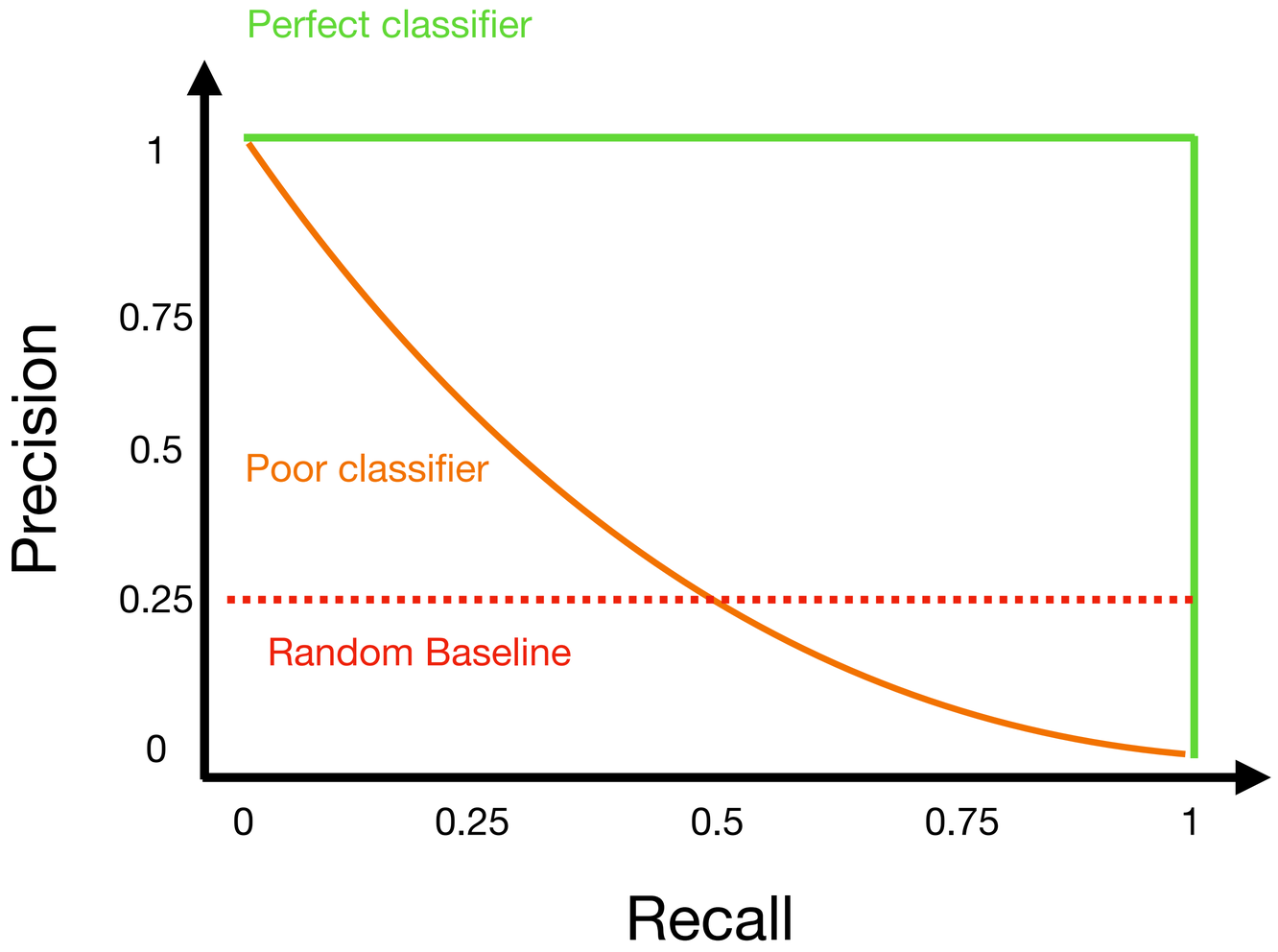
Precision drops steadily as recall increases.

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



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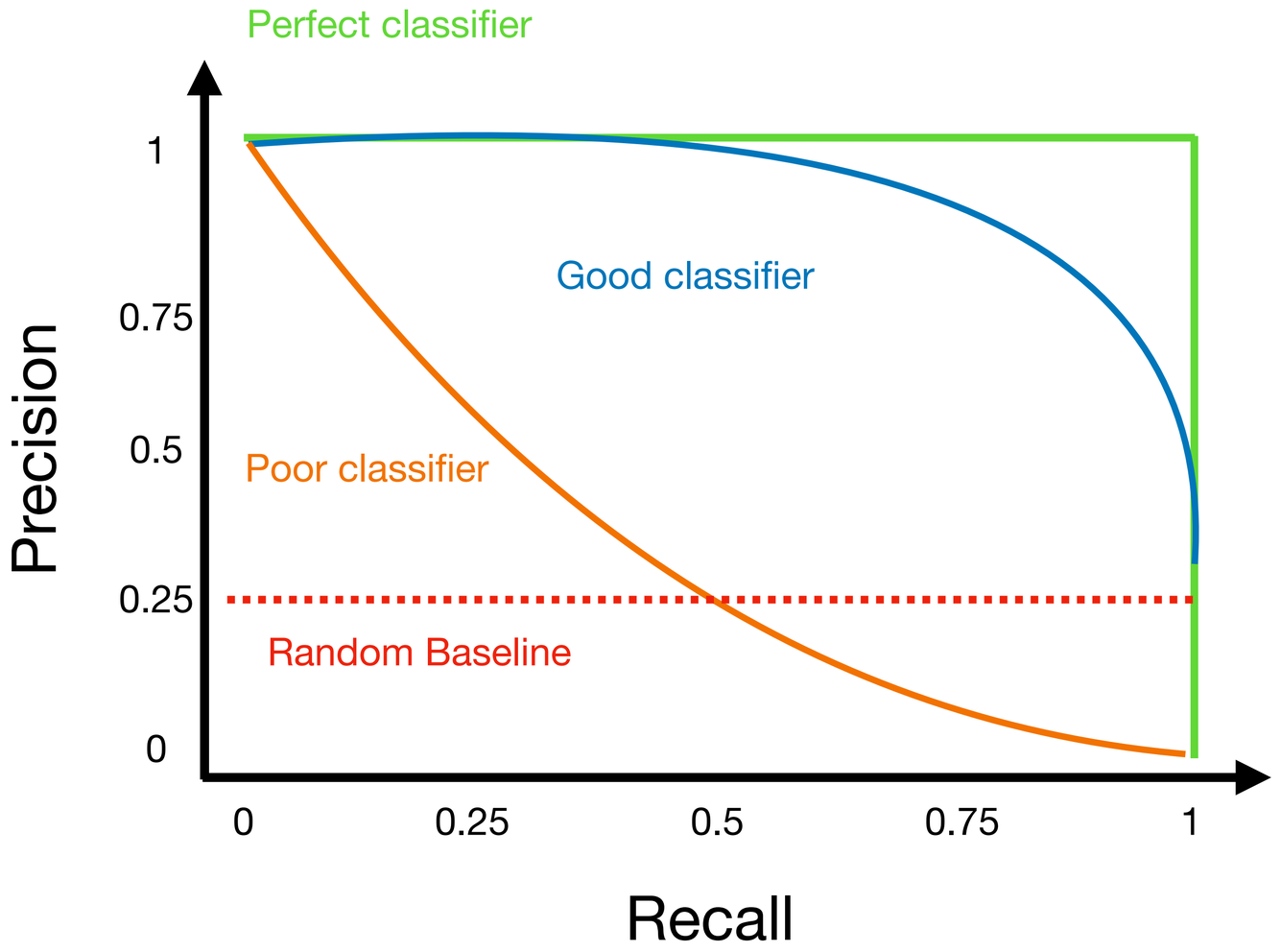

Perfect classifier:

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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

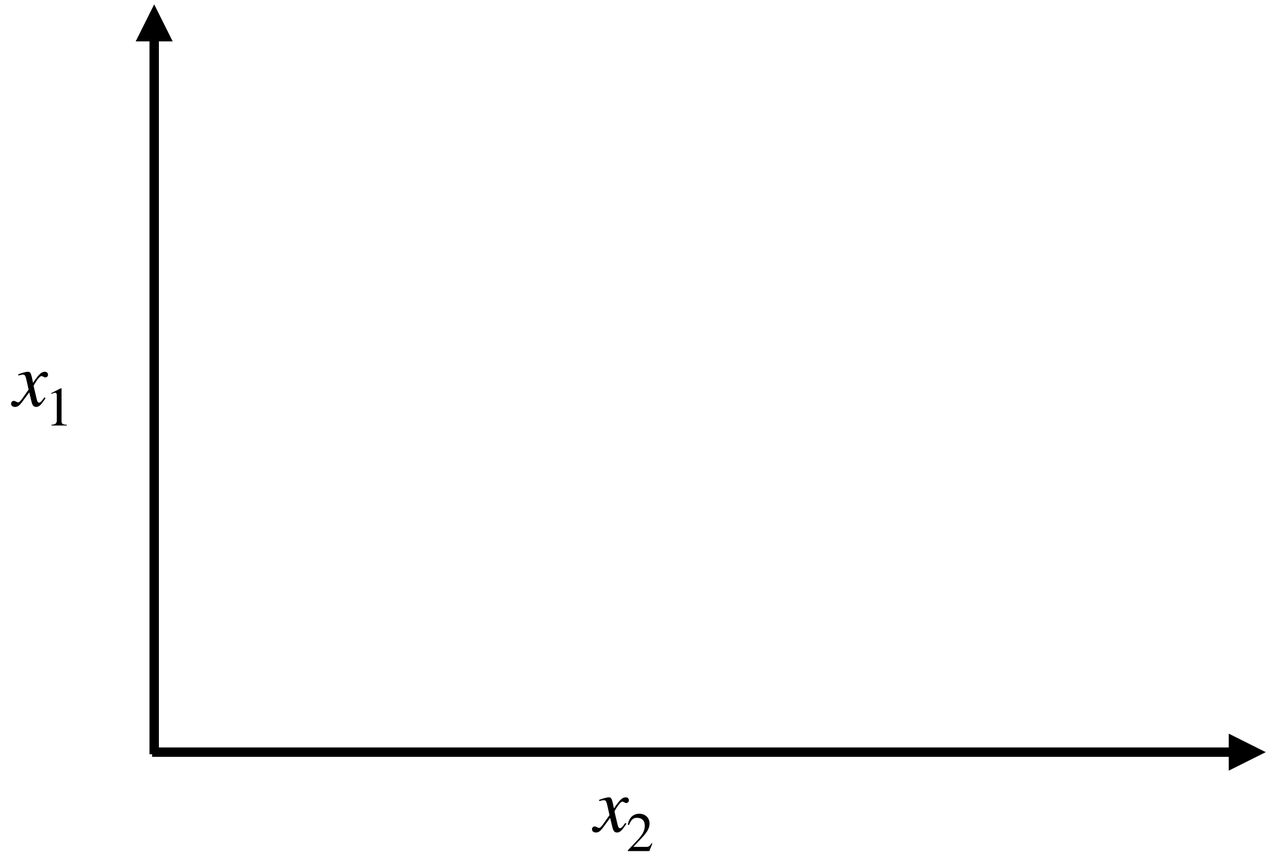
- KNN is a **non-parametric**, instance-based (lazy) learning algorithm.
- It makes no assumptions about the underlying data distribution and stores all training instances **rather than learning explicit parameters**.

k-Nearest Neighbors

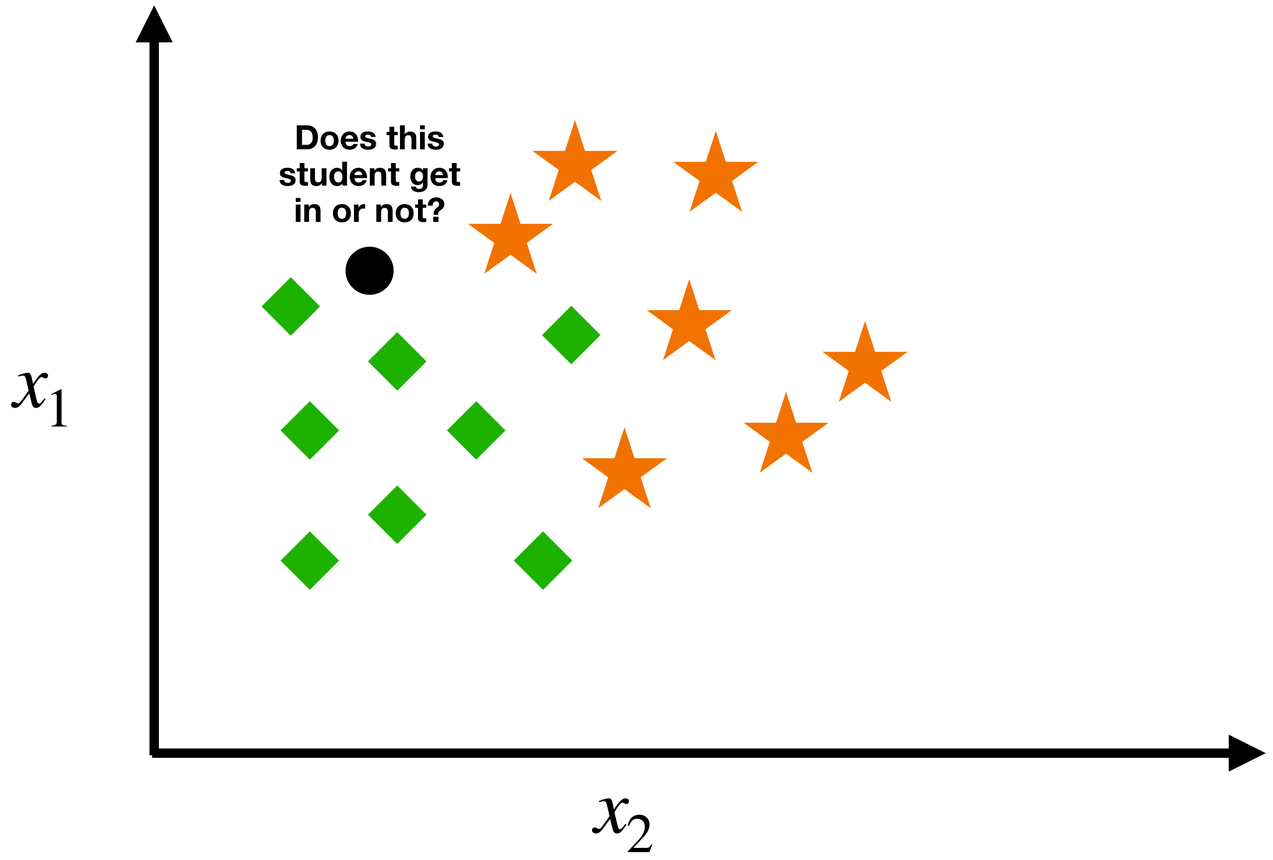
- KNN is a **non-parametric**, instance-based (lazy) learning algorithm.
- It makes no assumptions about the underlying data distribution and stores all training instances **rather than learning explicit parameters**.
- **Key Idea**:
  - Similar instances have similar labels.
  - To classify a new point,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

k-Nearest Neighbors

	High School GPA x_1	SAT Scores x_2	Get Into College? 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**	**?**



k-Nearest Neighbors



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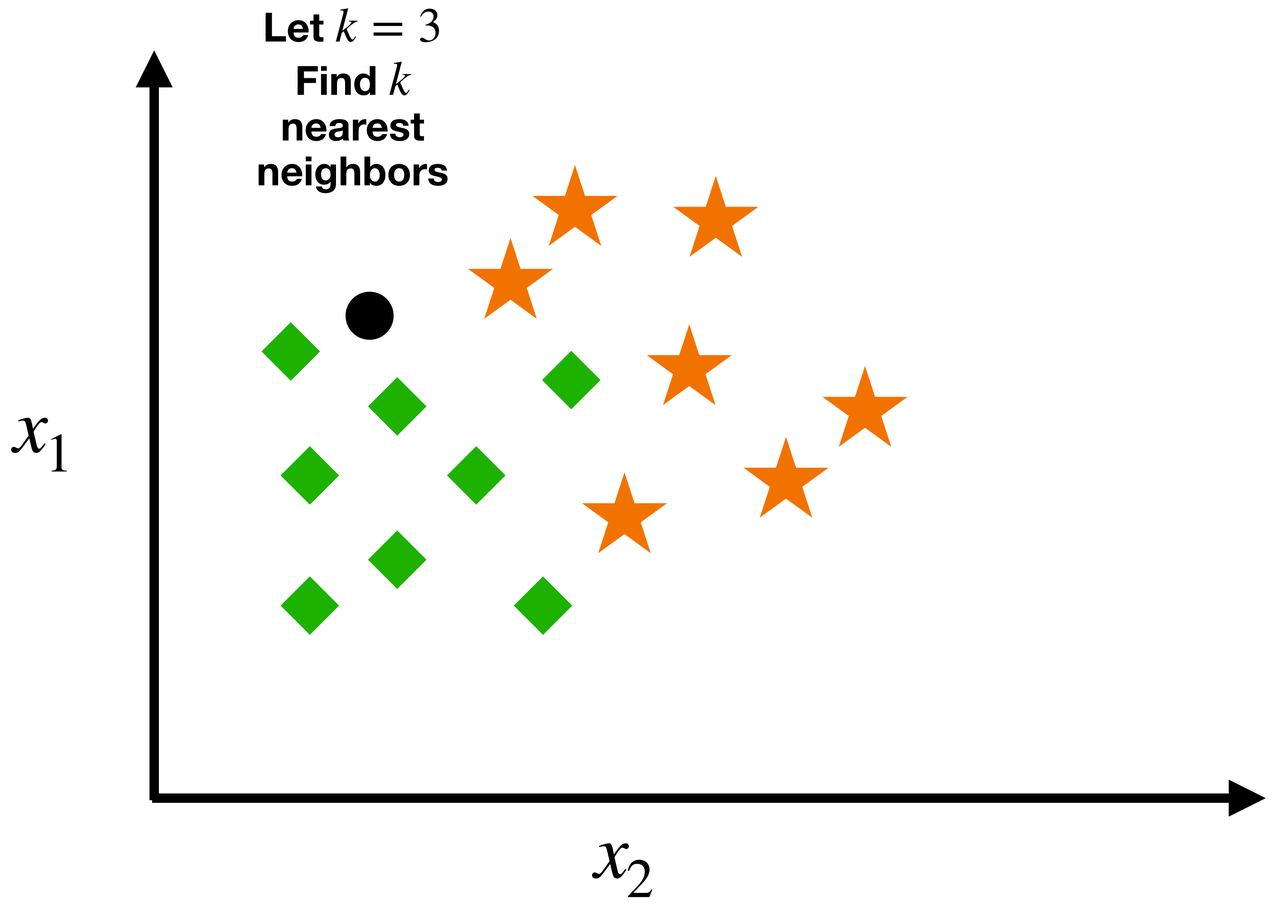
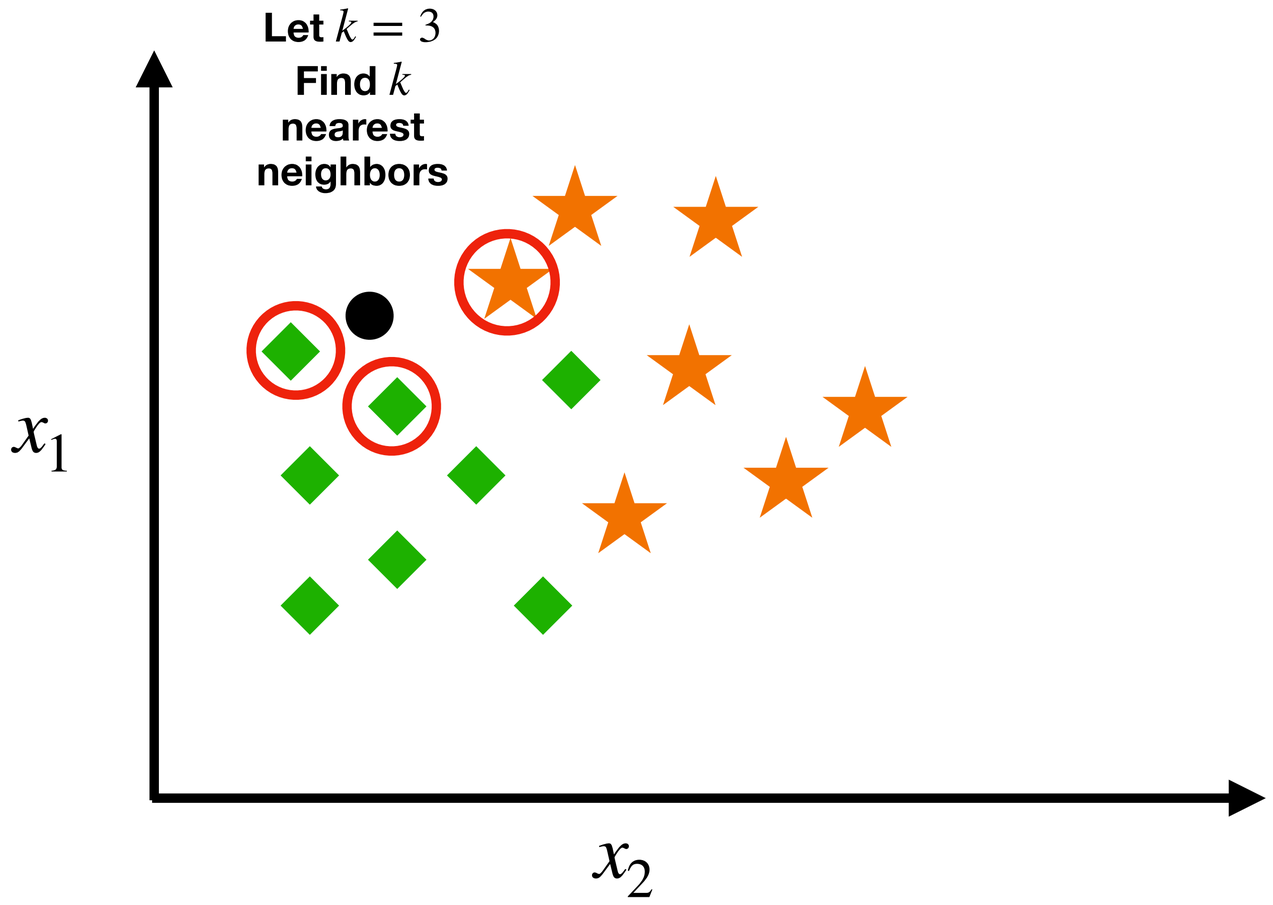
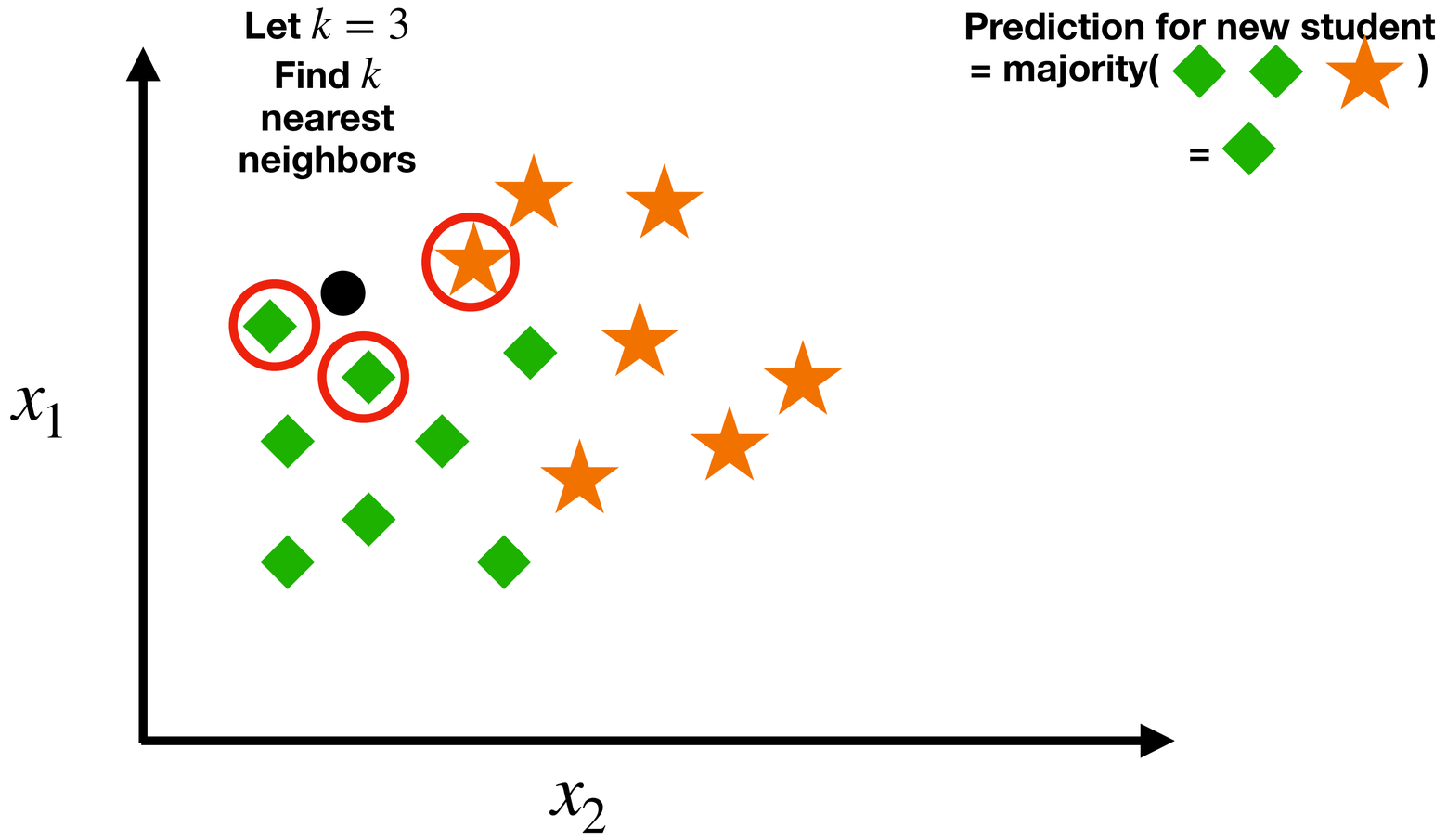


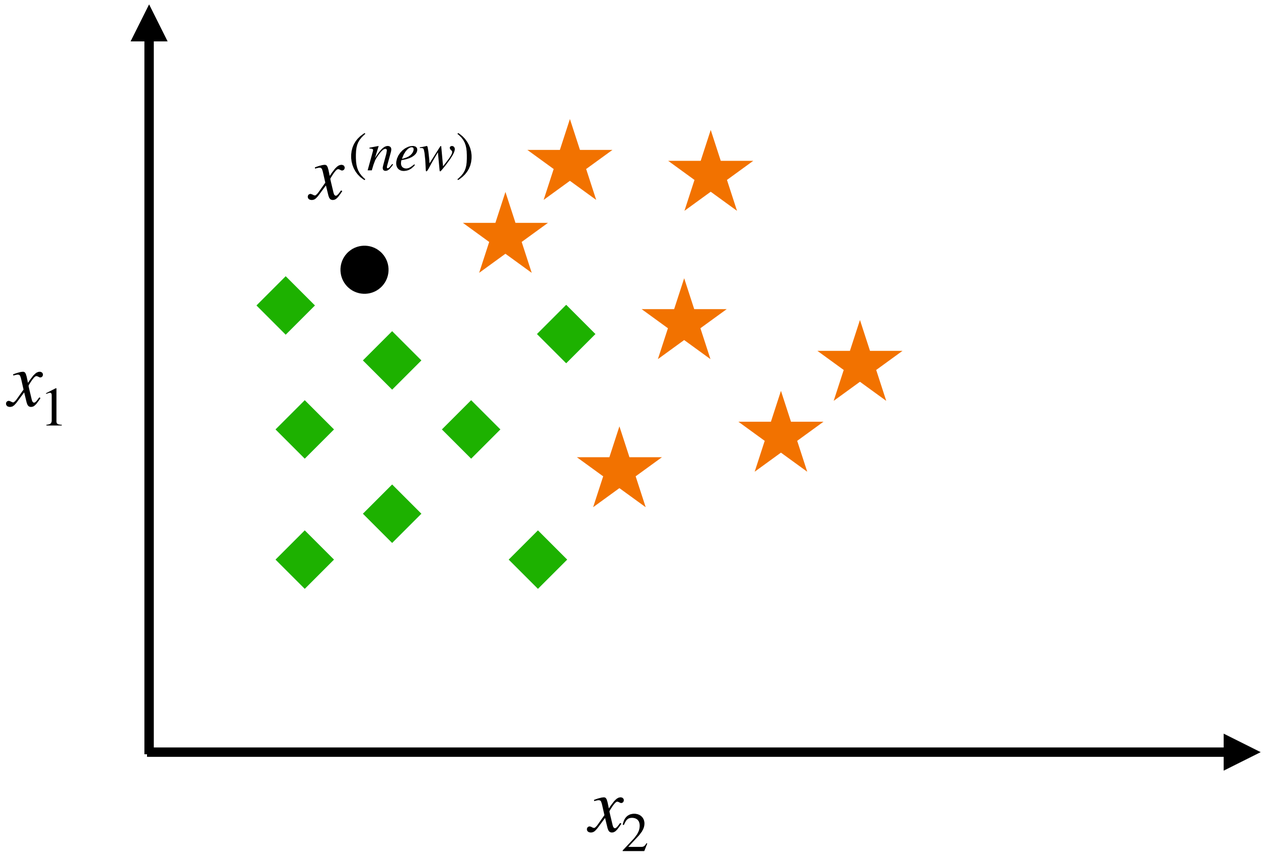
k-Nearest Neighbors



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 x_1	SAT Scores x_2	Get Into College? 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:

Training Phase:

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

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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

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

Euclidean Distance (L_2 Norm):

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

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

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:

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k-Nearest 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):

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

Sum of **absolute** differences.
More **robust to outliers** than Euclidean.
Appropriate when features represent fundamentally different quantities.

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:

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k-Nearest Neighbors

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Cosine Similarity:

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

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

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})
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

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.

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
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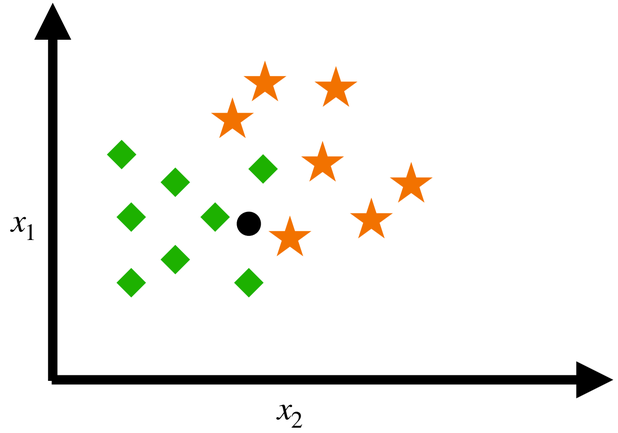
k-Nearest Neighbors

Choosing k



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

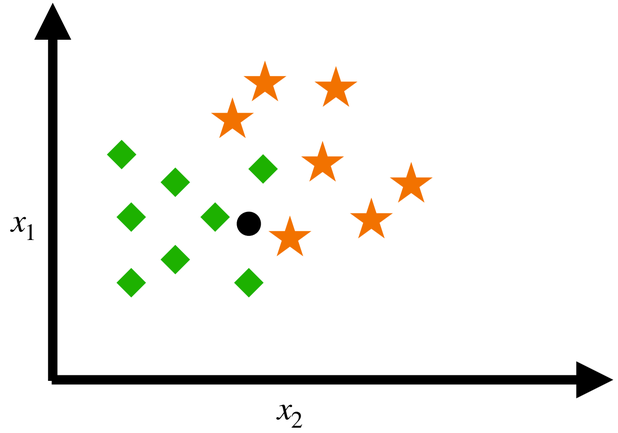
Small k (e.g. $k = 1$)

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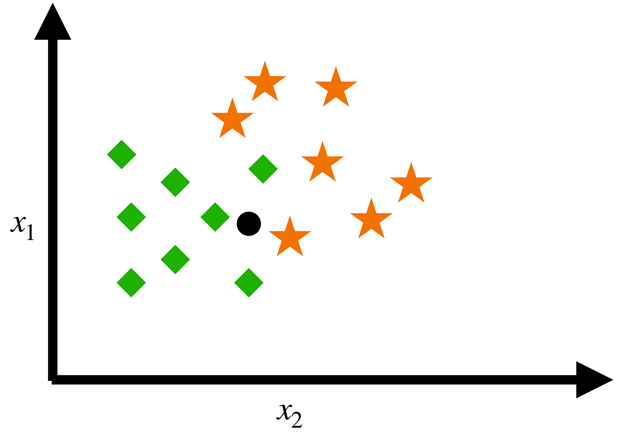
Large k (e.g. $k = m$)

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

Practical Tips

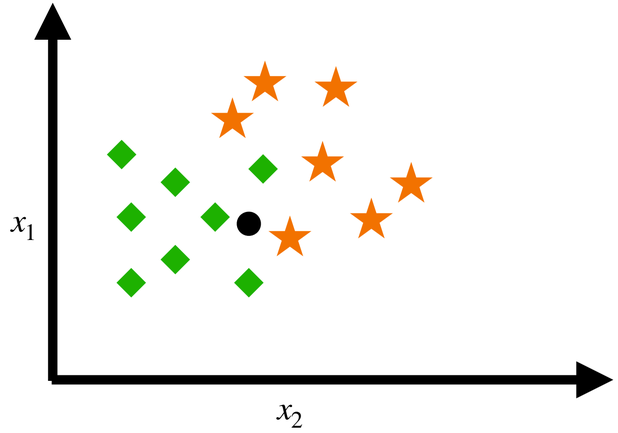
- Start with $k = \sqrt{m}$
- Use cross-validation to select optimal k
- If k is odd, it avoids ties in binary classification
- k should be smaller than the smallest class size

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

- 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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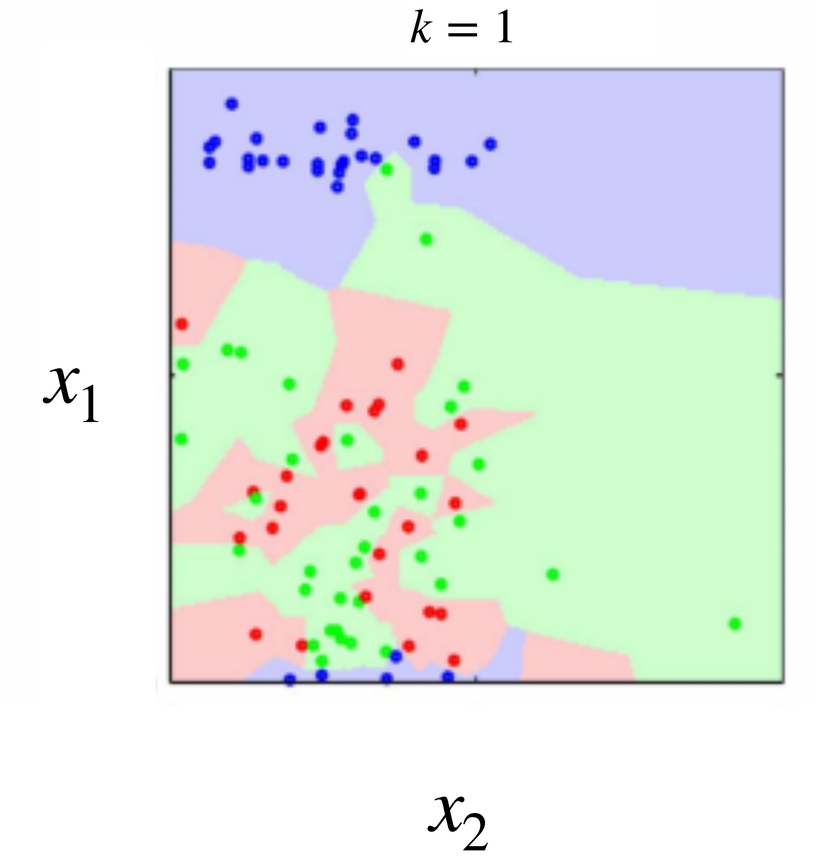
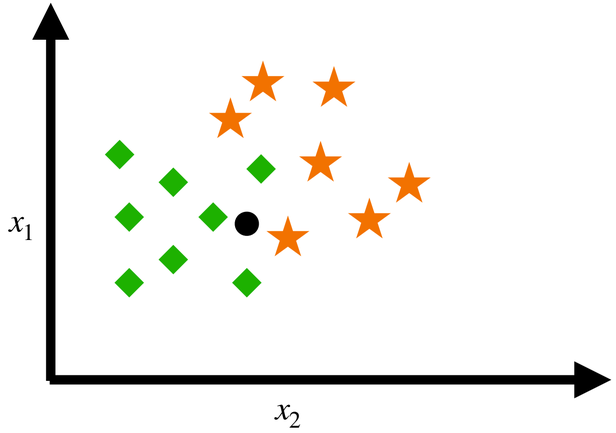


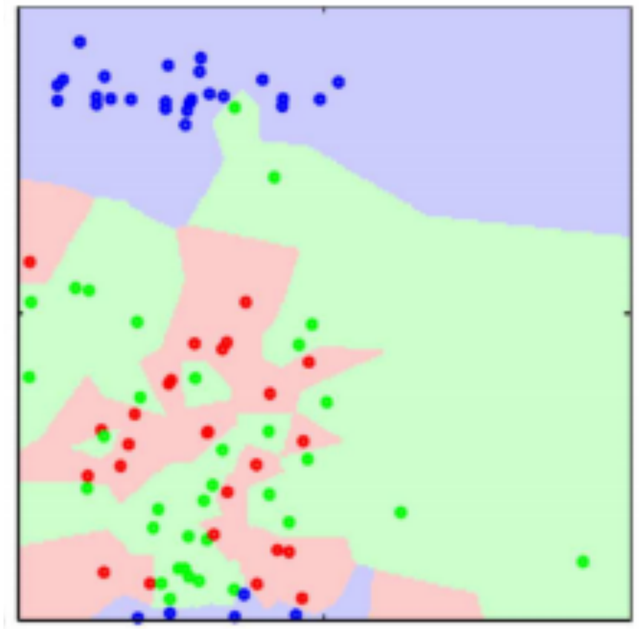
k-Nearest Neighbors

Choosing k

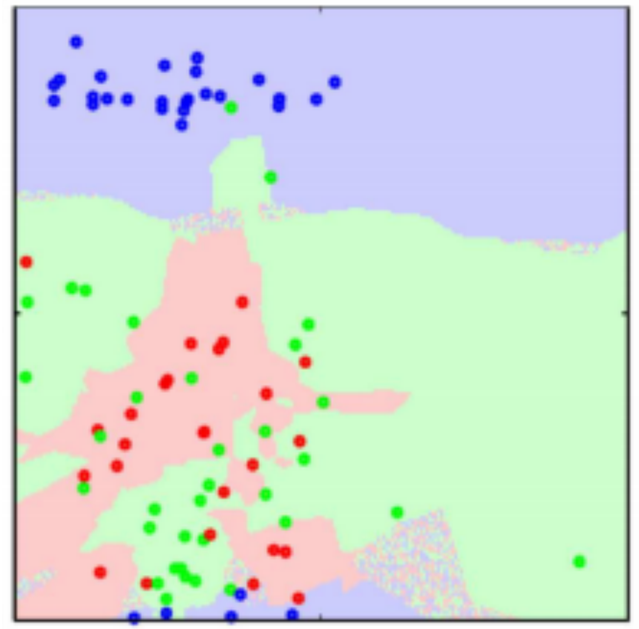


- k is the primary hyper-parameter controlling the bias-variance tradeoff

$k = 1$

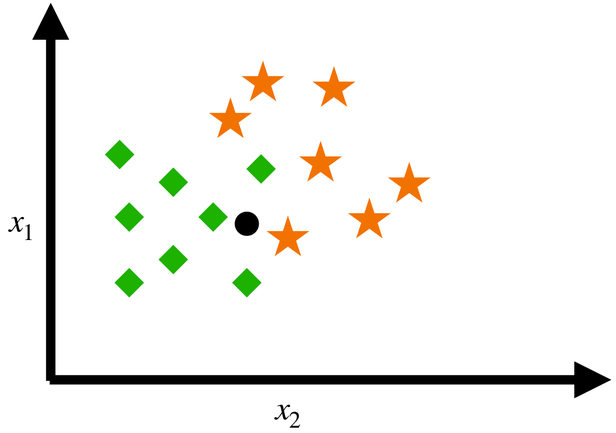


$k = 3$



k-Nearest Neighbors

Choosing k



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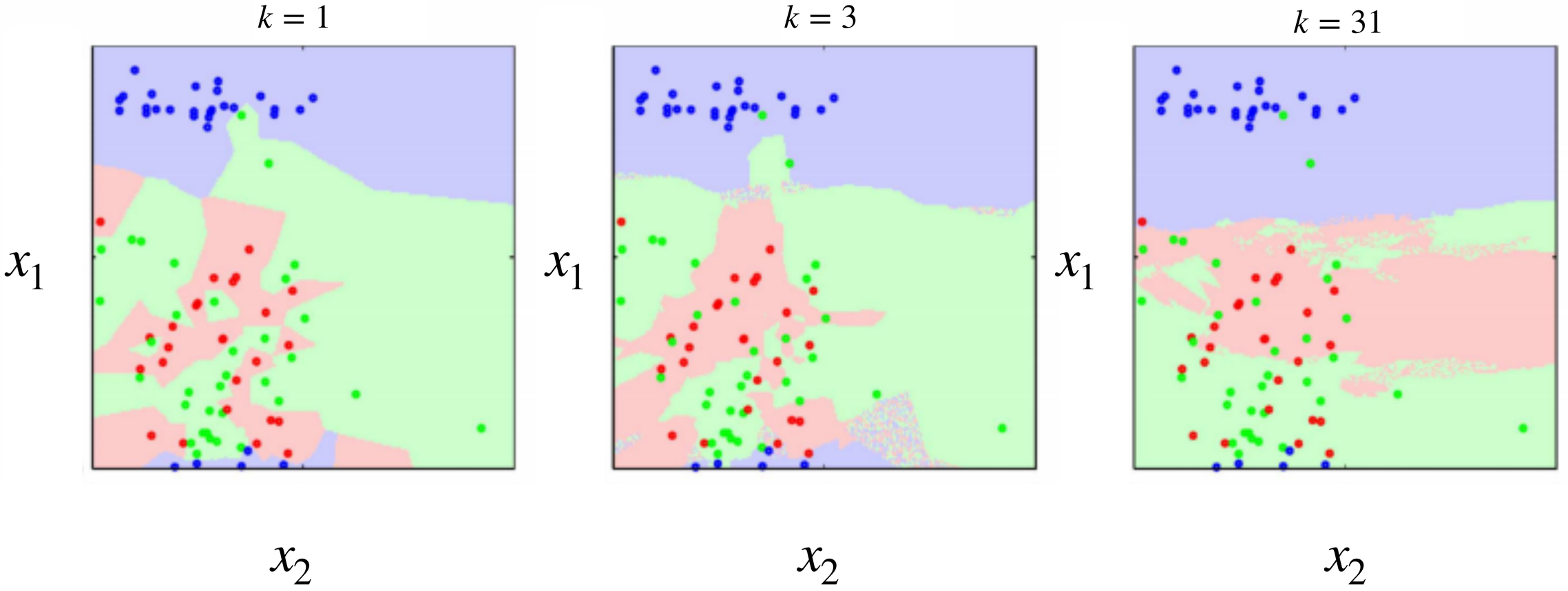

k-Nearest Neighbors

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 $i = 1, 2, \ldots, k$:

    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

Algorithm

1. Shuffle the dataset randomly

2. Split data into k equally-sized folds (or partitions)

3. for each fold $i = 1, 2, \ldots, k$:

    3a. Use fold i as the validation set

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    3c. Train the model on the training set

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k-Fold Cross Validation

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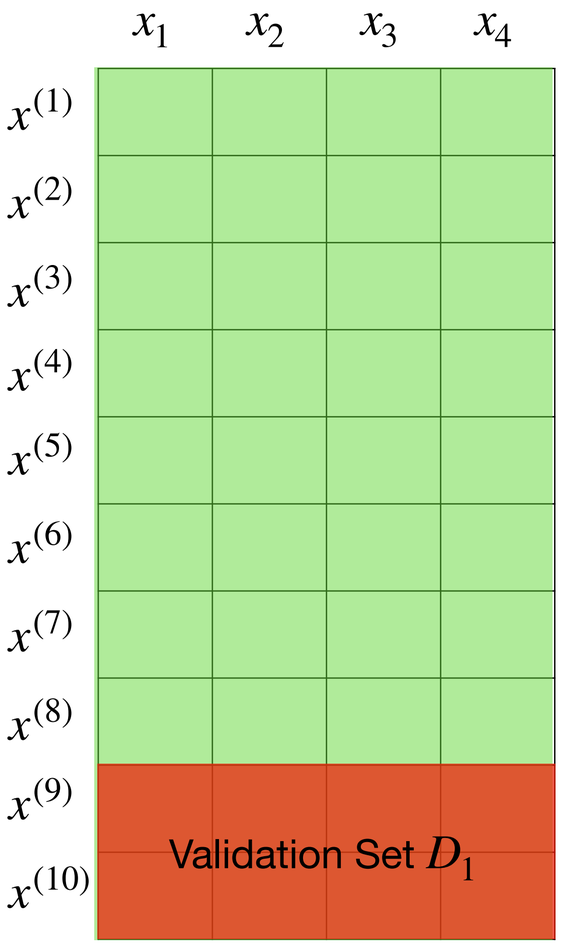


Let's say we want to run $k = 5$-fold cross validation

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

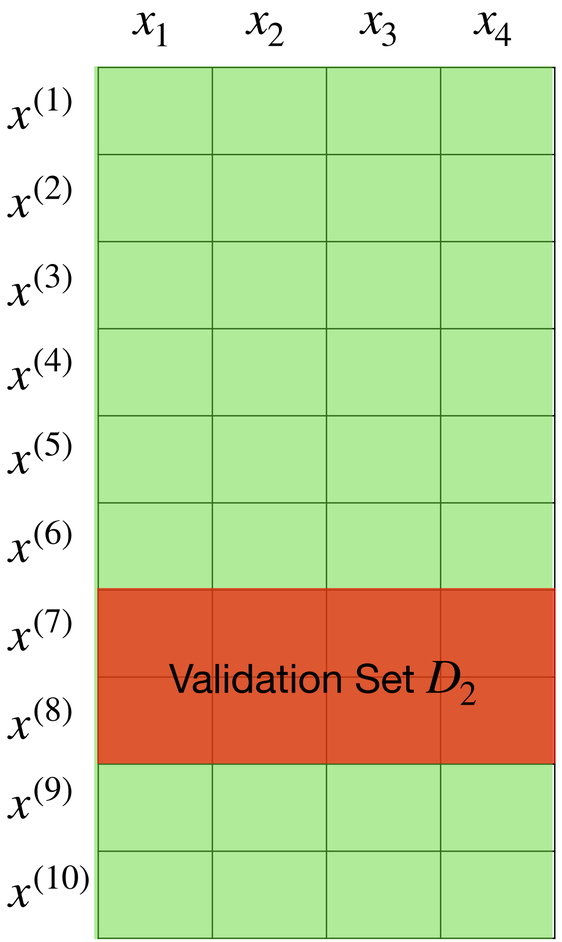
$$CV_1 = \frac{1}{D_1} \sum_{D_1} \ell(y_{D_1}, f_\theta(D_1))$$

Algorithm

1. Shuffle the dataset randomly
2. Split data into k equally-sized folds (or partitions)
3. for each fold $i = 1, 2, \ldots, k$:
   - 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



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

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

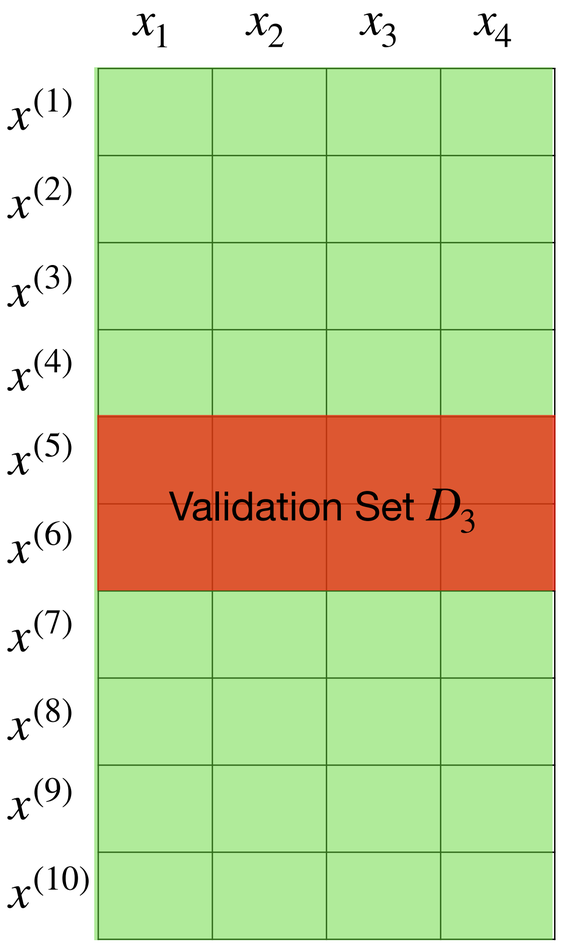
$$CV_2 = \frac{1}{D_2} \sum_{D_2} \ell(y_{D_2}, f_\theta(D_2))$$

Algorithm

1. Shuffle the dataset randomly
2. Split data into k equally-sized folds (or partitions)
3. for each fold $i = 1, 2, \ldots, k$:
   - 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



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

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

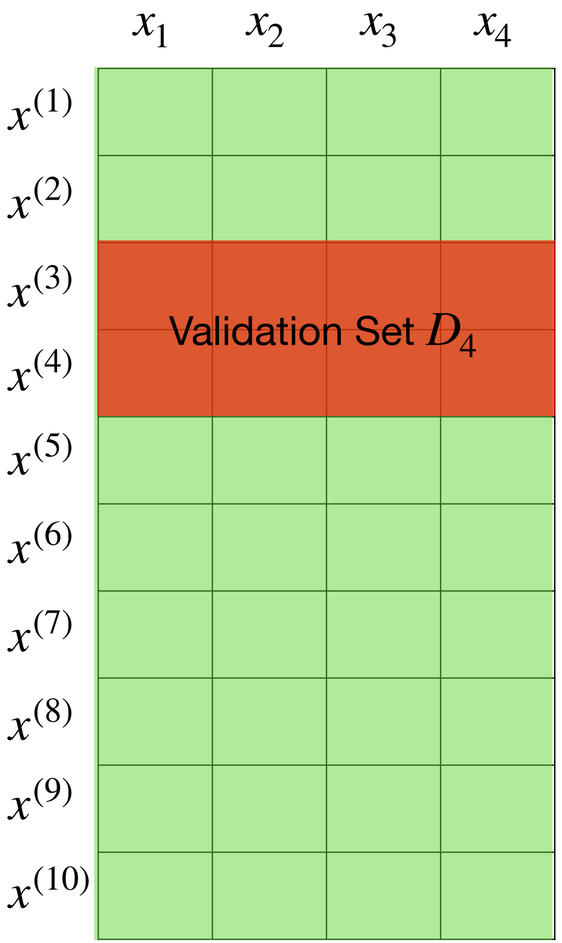
$$CV_3 = \frac{1}{D_3} \sum_{D_3} \ell(y_{D_3}, f_\theta(D_3))$$

Algorithm

1. Shuffle the dataset randomly
2. Split data into k equally-sized folds (or partitions)
3. for each fold $i = 1, 2, \ldots, k$:
   - 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



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)
3. for each fold $i = 1, 2, \ldots, k$:
   - 3a. Use fold i as the validation set
   - 3b. Use the remaining $k - i$ folds as the training set
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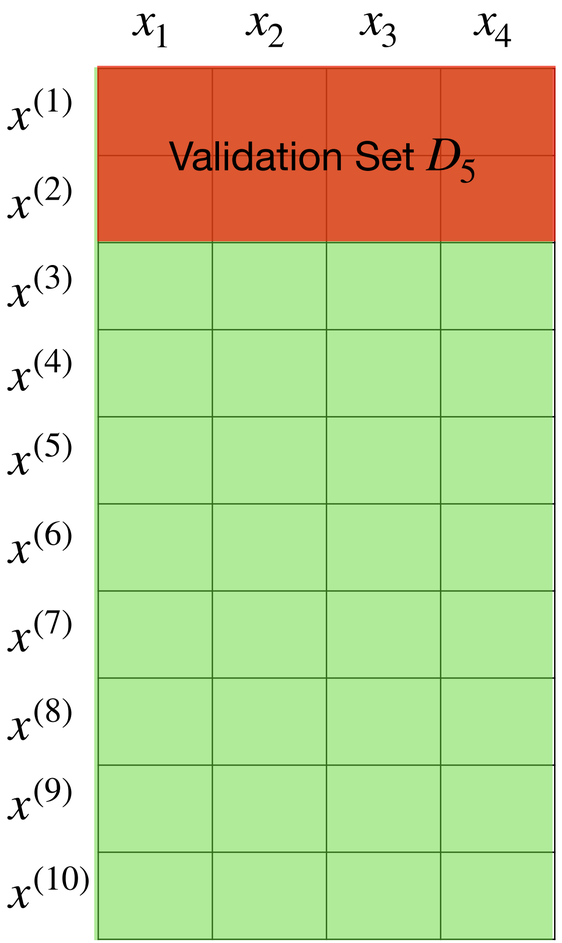
k-Fold Cross Validation

Algorithm



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

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

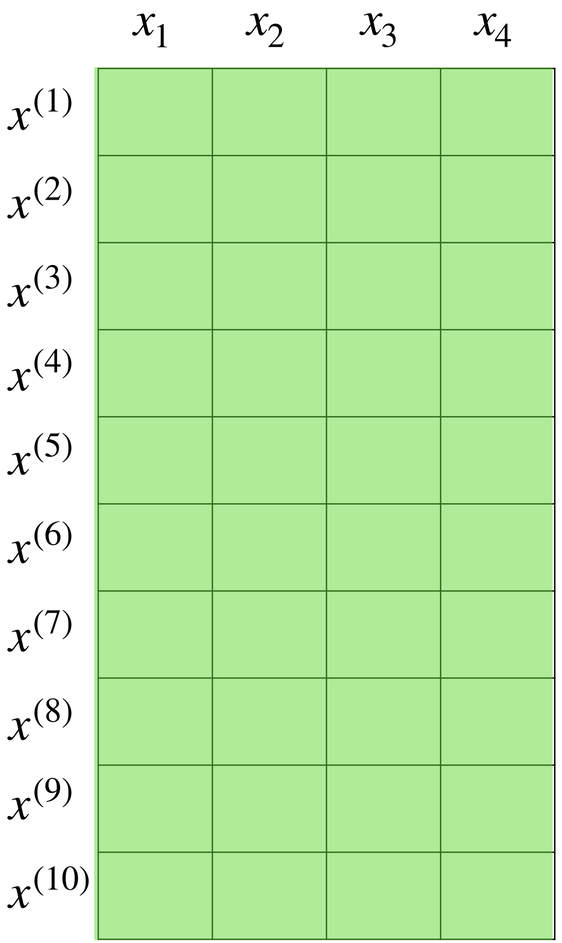
$$CV_5 = \frac{1}{D_5} \sum_{D_5} \ell(y_{D_5}, f_\theta(D_5))$$

Algorithm

1. Shuffle the dataset randomly
2. Split data into k equally-sized folds (or partitions)
3. for each fold $i = 1, 2, \ldots, k$:
   - 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



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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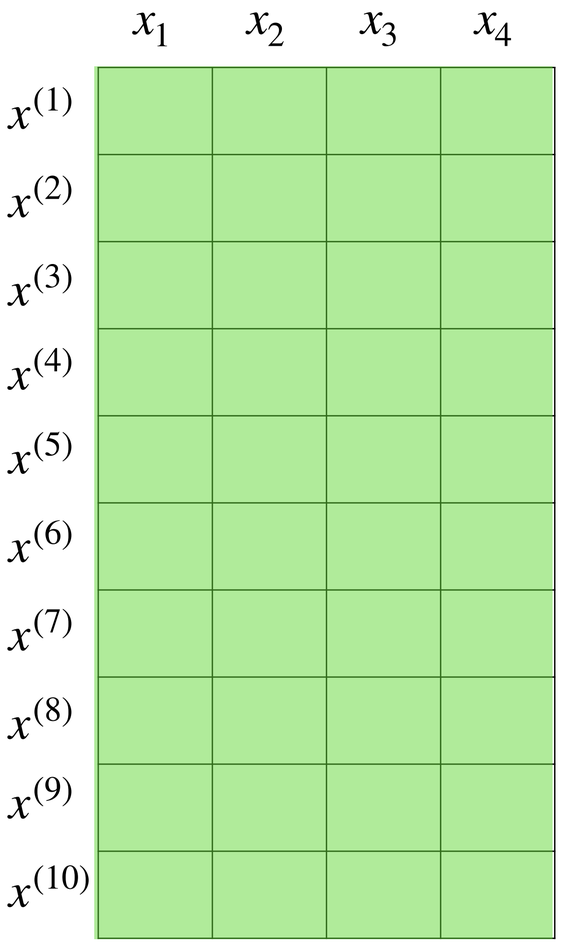
k-Fold Cross Validation

Algorithm



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

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

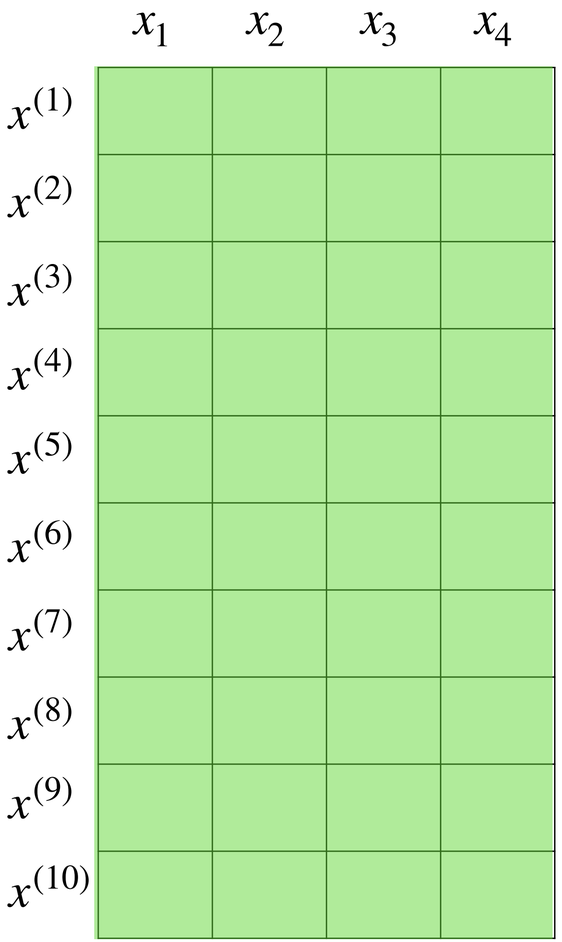
Mean CV Score:

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

k-value	Training Size	Properties
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



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

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

Mean CV Score:

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

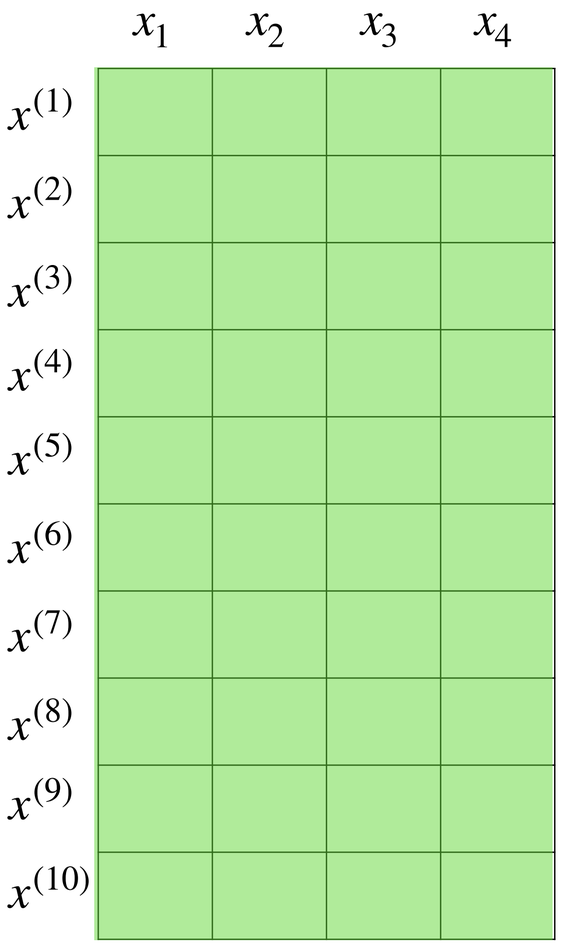
k-fold CV requires **training k models**.

If training is expensive, smaller k is preferred.

k-value	Training Size	Properties
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



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

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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.

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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 $d > 20$

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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: $O(nlogm)$ 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.

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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

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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