K Nearest Neighbors

KNN

- KNN (K nearest neighbors) is one of the simplest algorithms we will learn about!
- Section Overview
    - KNN Theory and Intuition
    - KNN Classification Coding Example
    - KNN Exercise Overview
    - KNN Exercise Solution

KNN

- While KNN can be used for regression tasks, its performance can be quite poor and less efficient than other algorithms, so we've decided not to exhibit its use for regression.
- However if you do want to use it for regression it is very easy to swap in the KNNRegressor model with scikit-learn.

KNN

- You may have also heard of K means algorithm.
- K means is unrelated to KNN, be careful not to confuse the two due to their similar sounding names!

KNN

- ISLR Relevant Reading
  - Chapter 2
  - Formula 2.12 starts discussion on KNN for classification.

$$\Pr(Y = j | X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j).$$

KNN Classification

Theory and Intuition

KNN

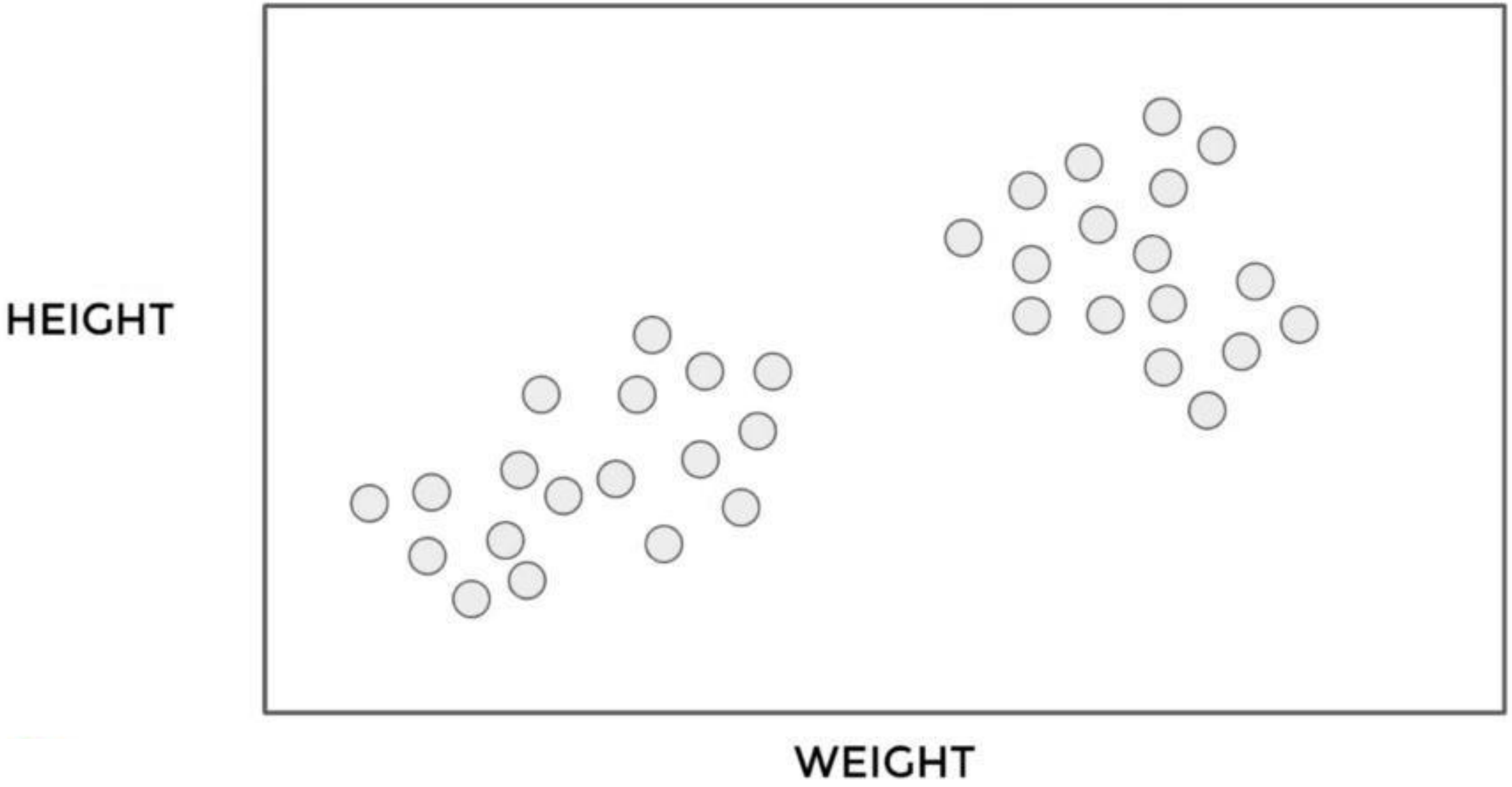
- K nearest neighbors is one of the simplest machine learning algorithms.
- It simply assigns a label to new data based on the **distance** between the old data and new data.
- Let's go through the intuition with an example use case...

KNN

- Sexing chicks is still a very manual process:
  - en.wikipedia.org/wiki/Chick_sexing
- Let's imagine we gathered a dataset of baby chick heights and weights.
- How could we train an algorithm to identify the sex of a new baby chick based on historical features?

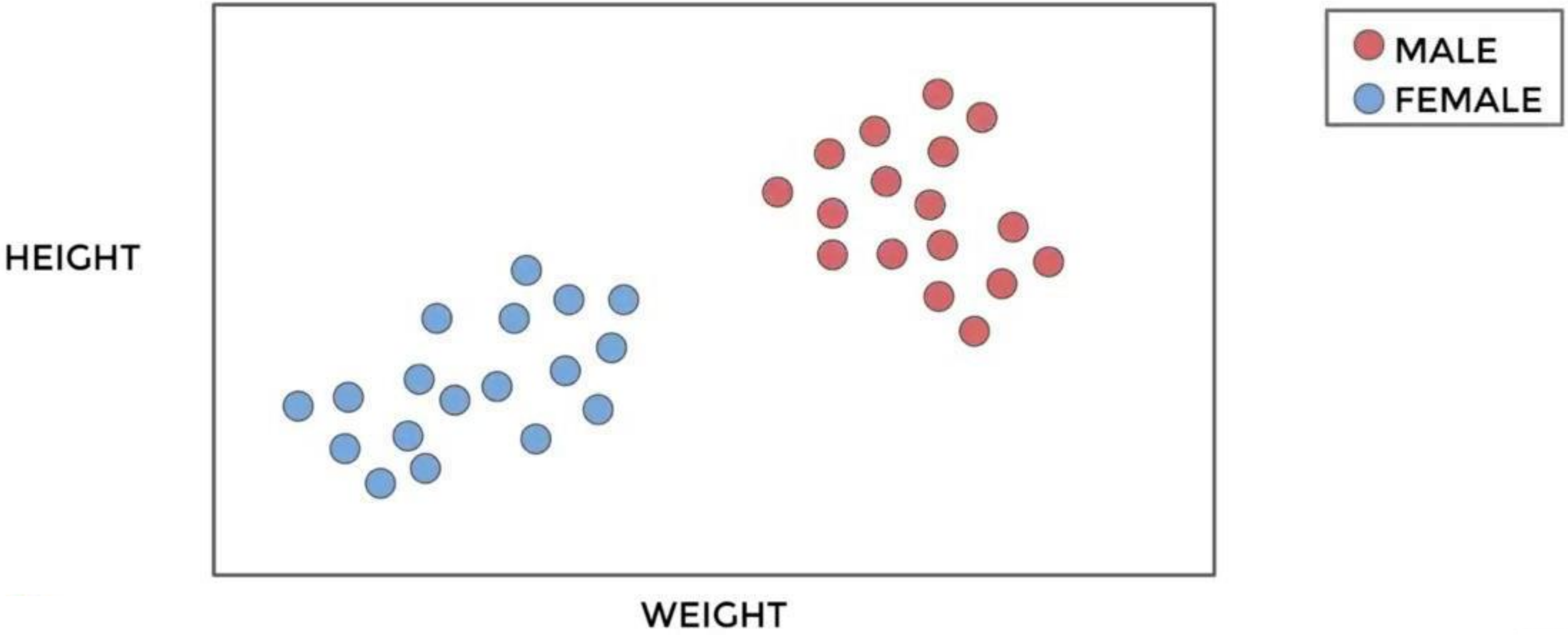
KNN

- Imagine a height and weight data set



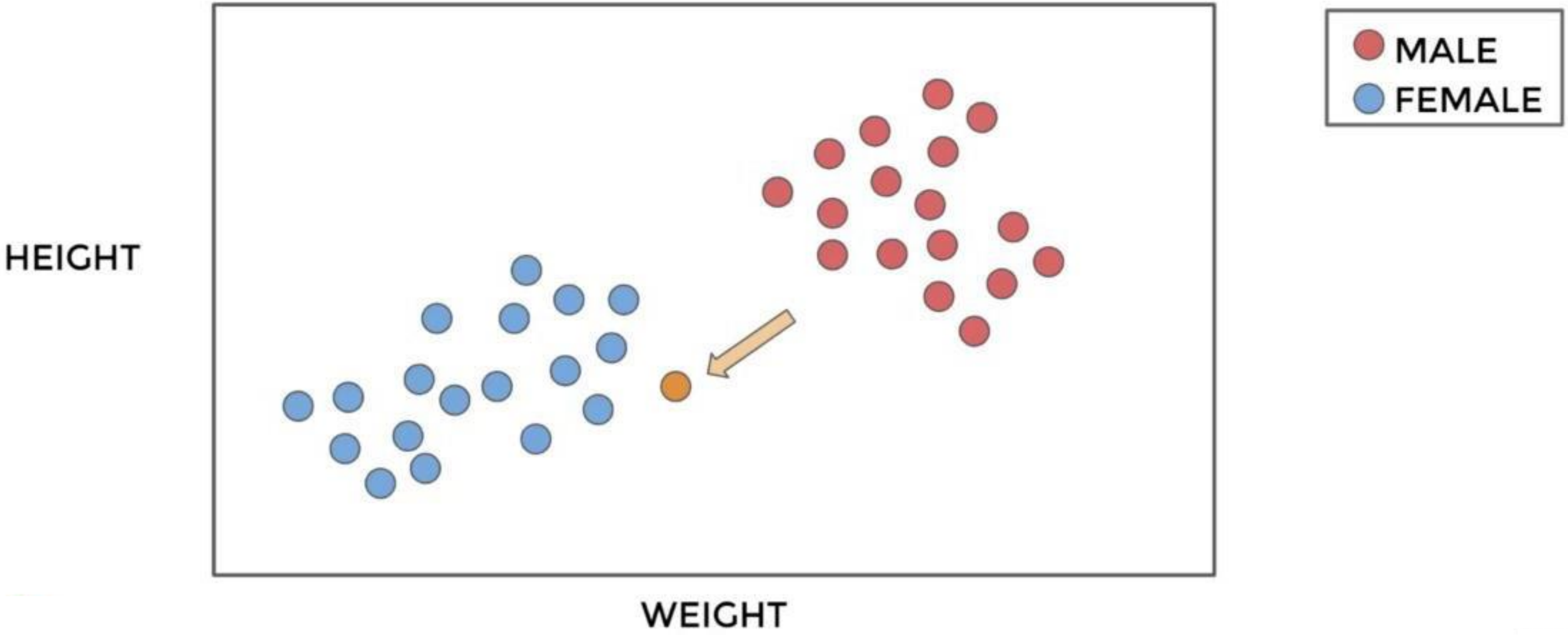
KNN

- We historically know the sex of the chicks:



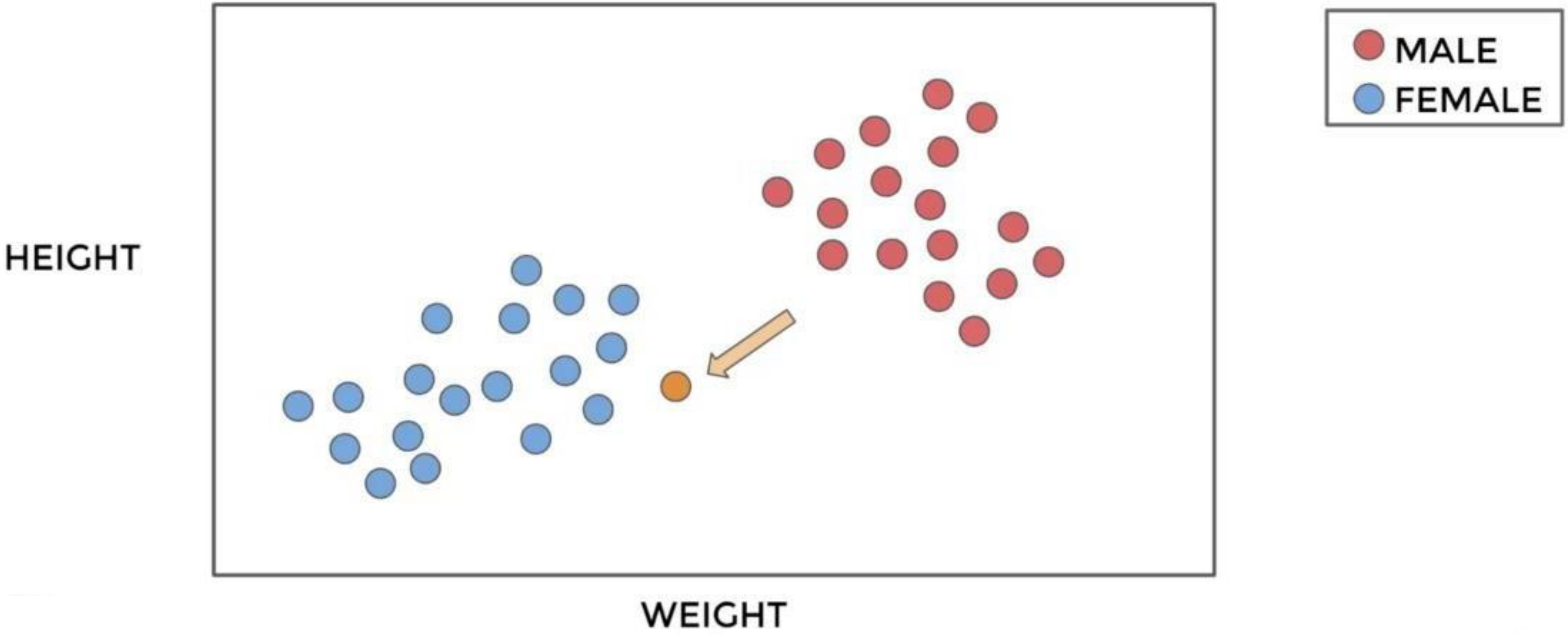
KNN

- How would we assign sex to a new point?



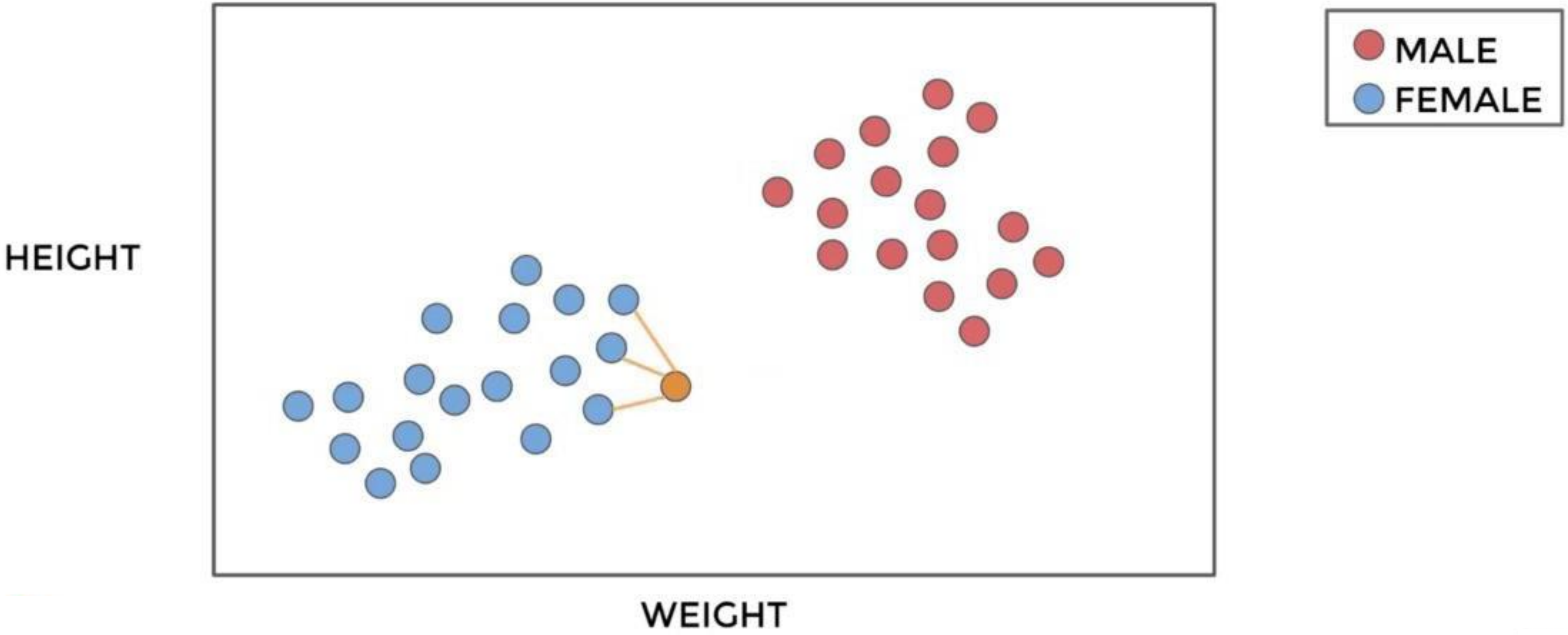
KNN

- We intuitively “know” this is likely female.



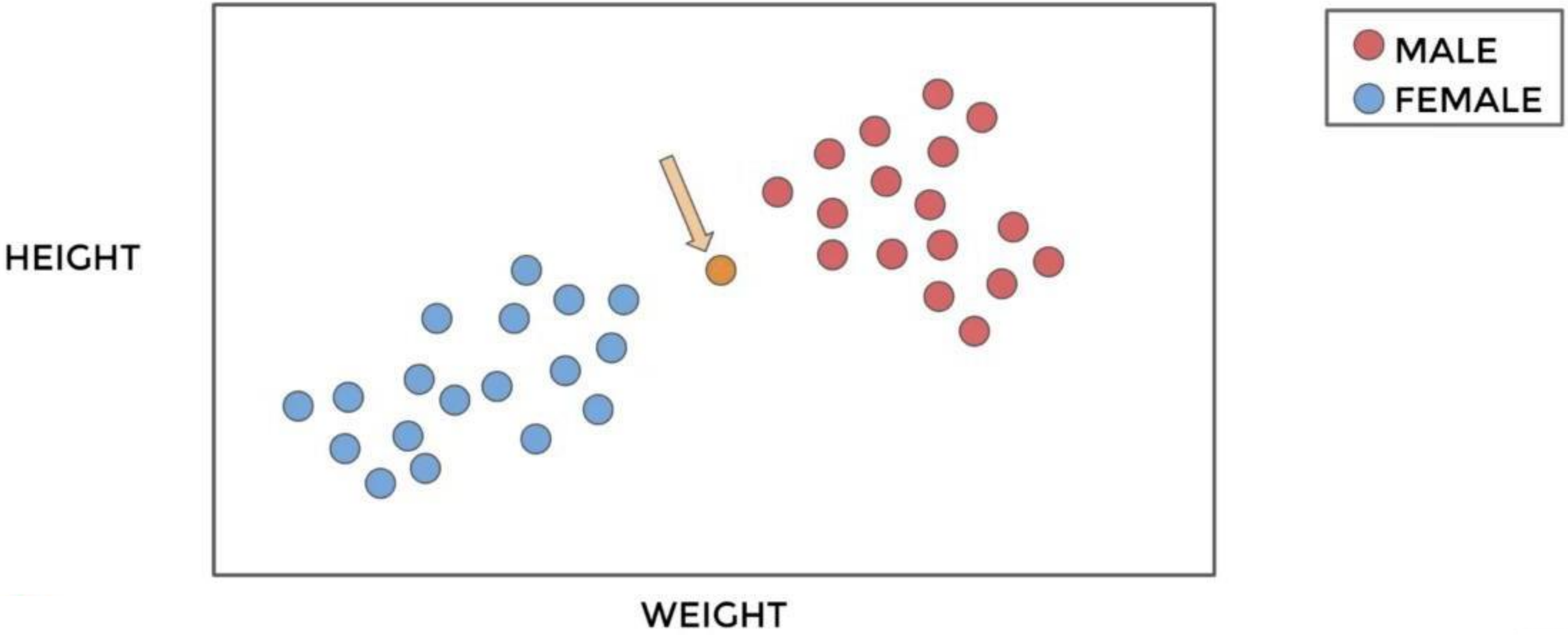
KNN

- Intuition comes from **distance** to points!



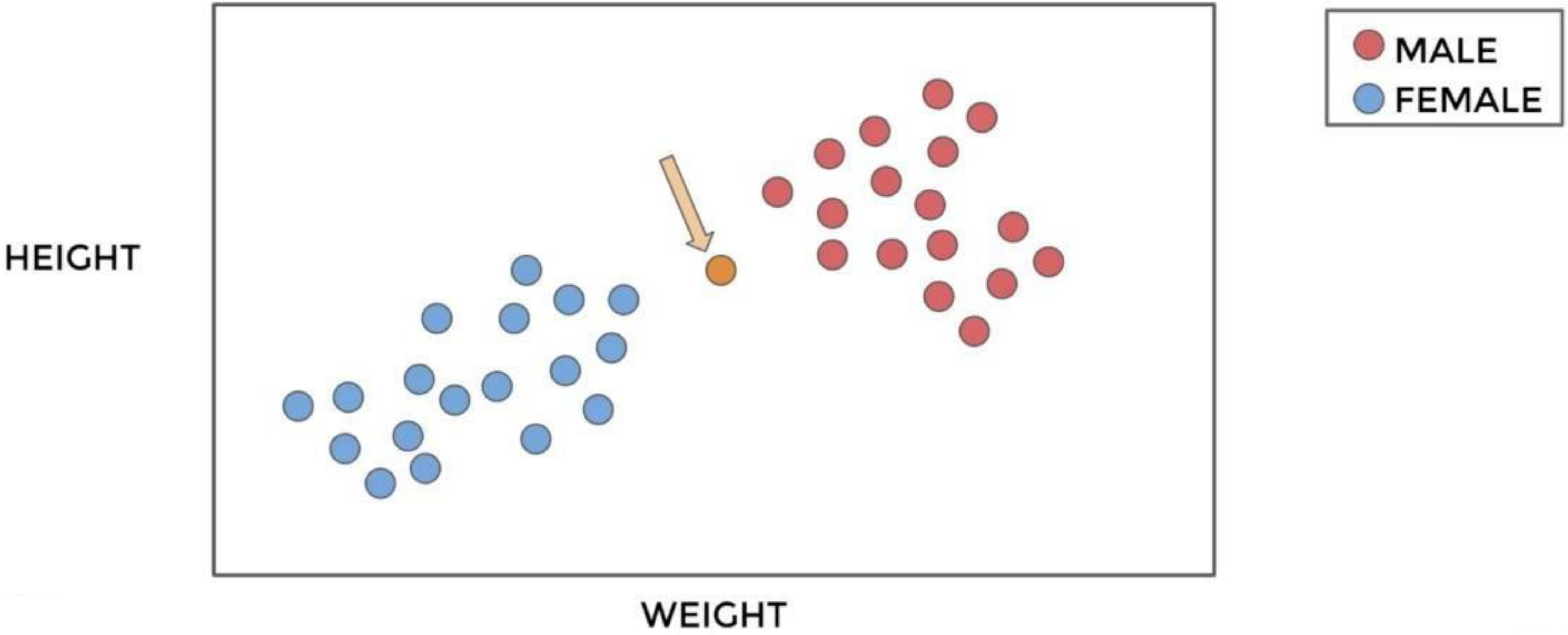
KNN

- What about a less obvious point?



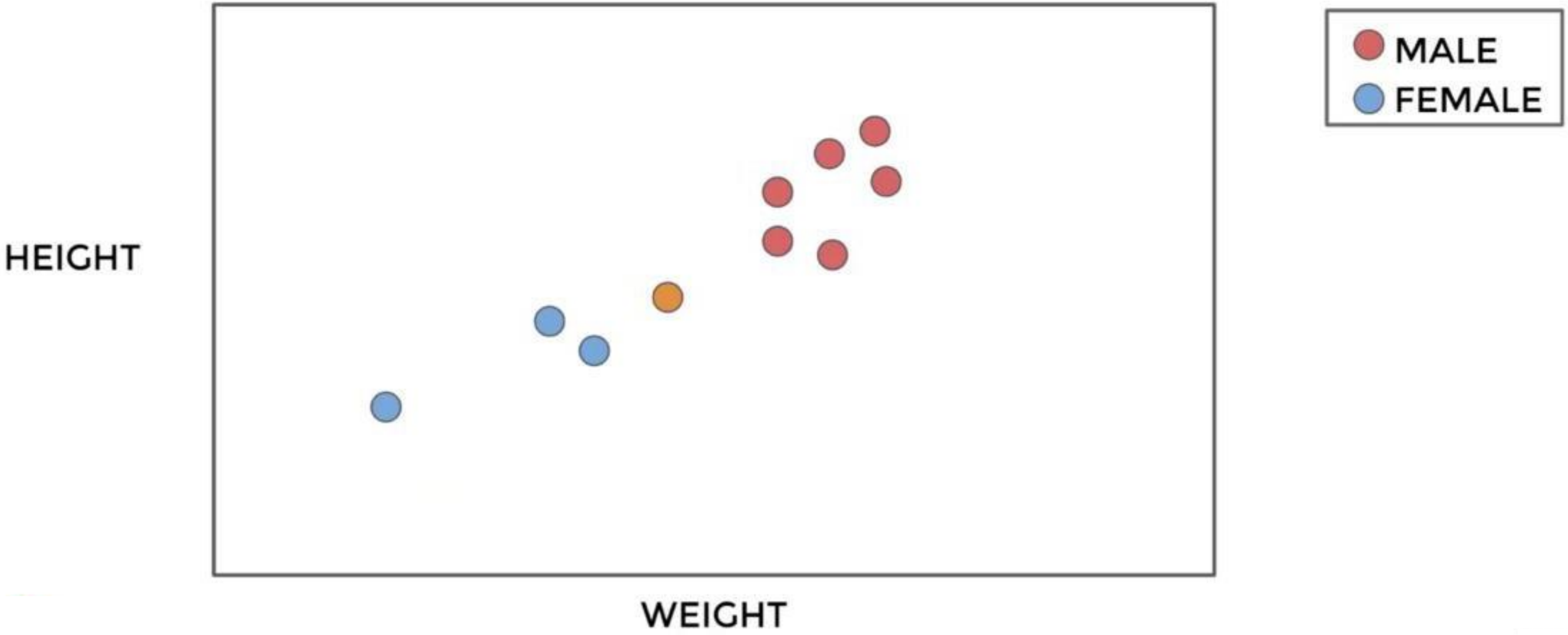
KNN

- How many points to we consider?



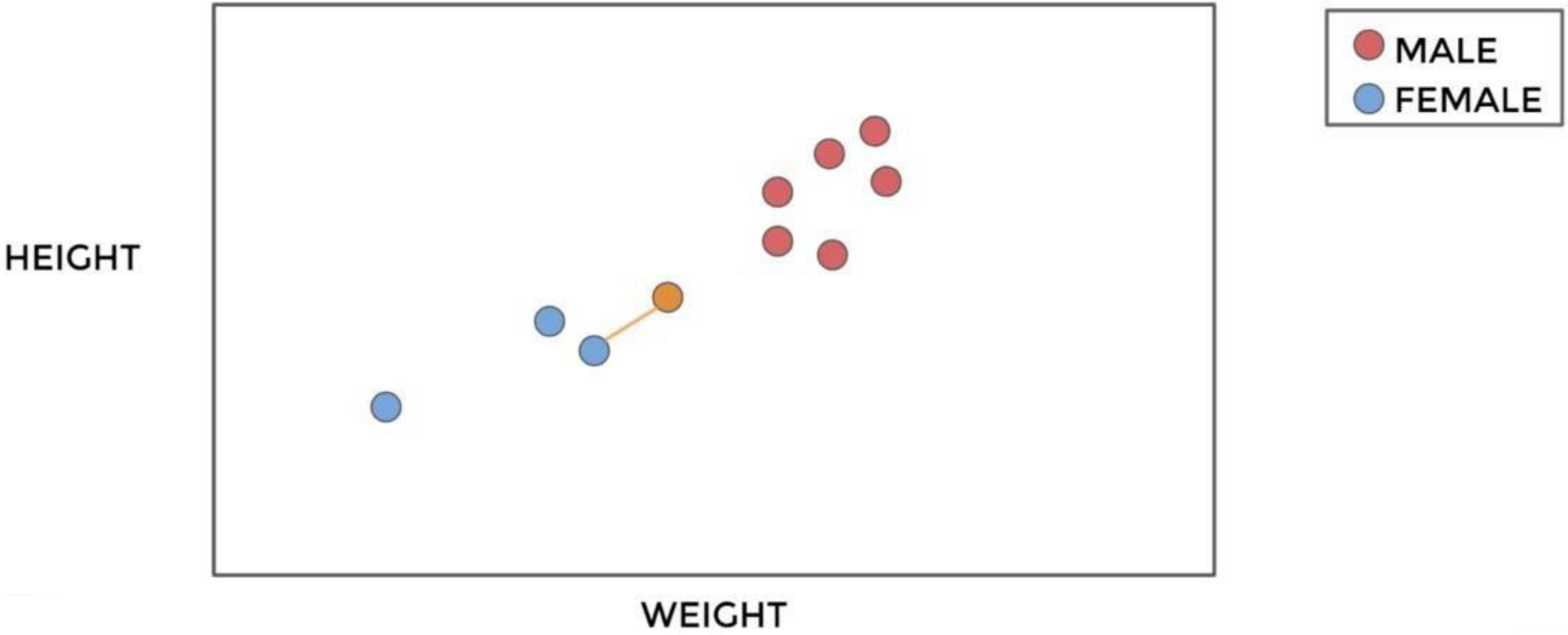
KNN

- Let's imagine a situation like this:



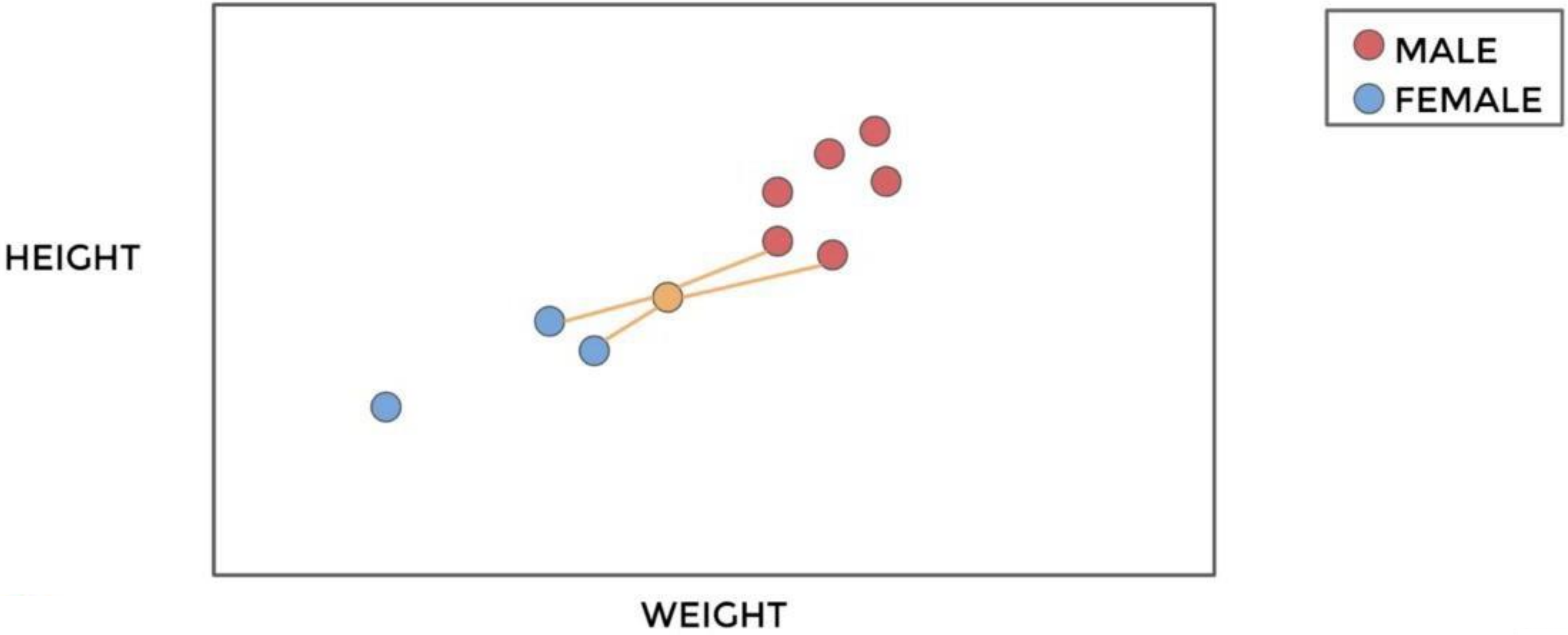
KNN

- K=1



KNN

- K=4 leads to a tie!



KNN

- Tie considerations and options:
  - Always choose an odd K.
  - In case of tie,simply reduce K by 1 until tie is broken.
  - Randomly break tie.
  - Choose nearest class point.

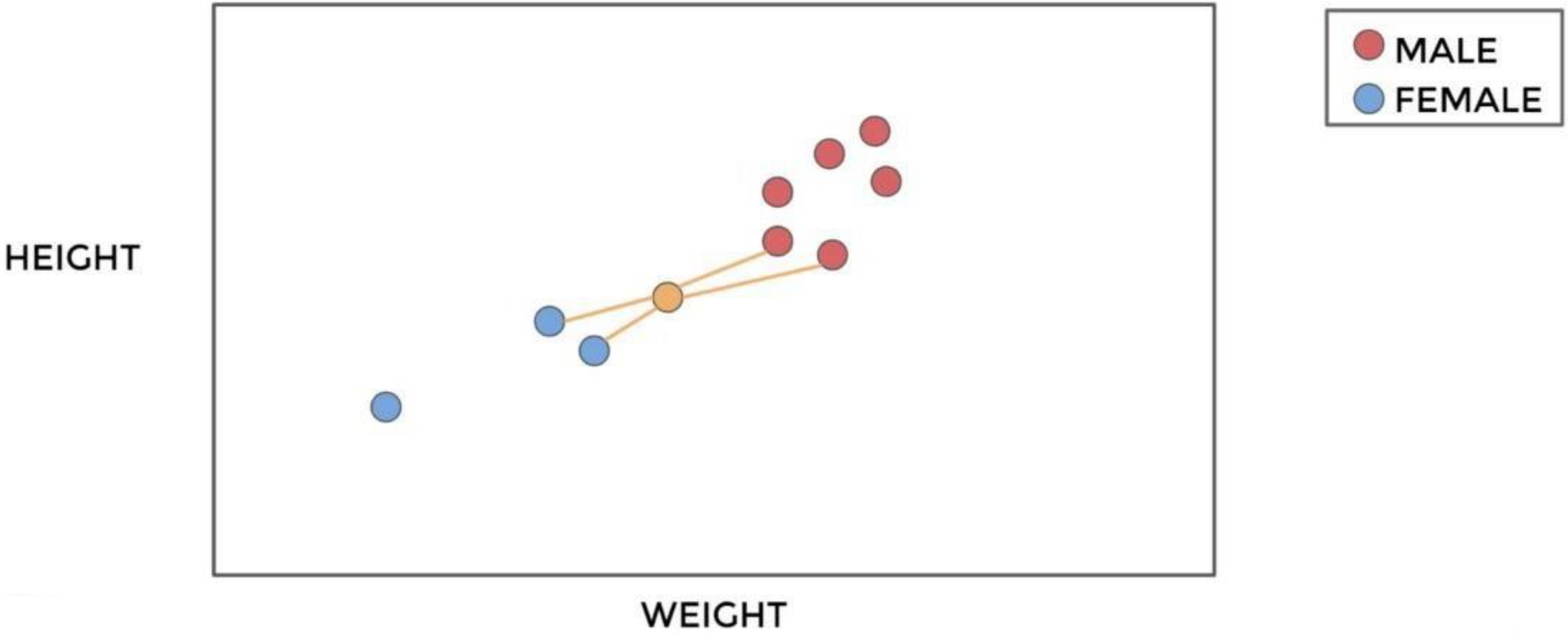
KNN

- **What does Scikit-Learn do in case of tie?**
  - *Warning: Regarding the Nearest Neighbors algorithms, if it is found that two neighbors, neighbor k+1 and k, have identical distances but different labels, the results will depend on the ordering of the training data.*

- **What does Scikit-Learn do in case of tie?**
  - *In the case of ties, the answer will be the class that happens to appear first in the set of neighbors.*
  - *Results are ordered by distance, so it chooses the class of the closest point.*

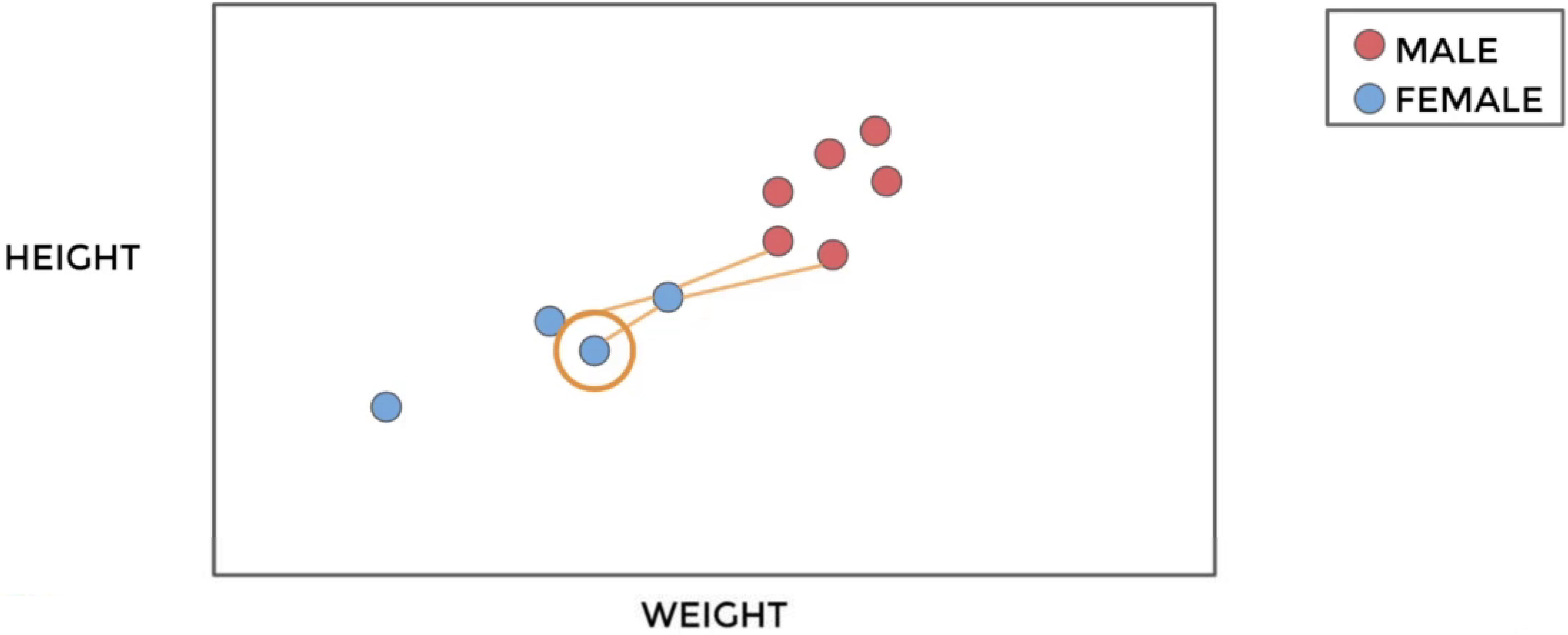
KNN

- K=4 leads to a tie!



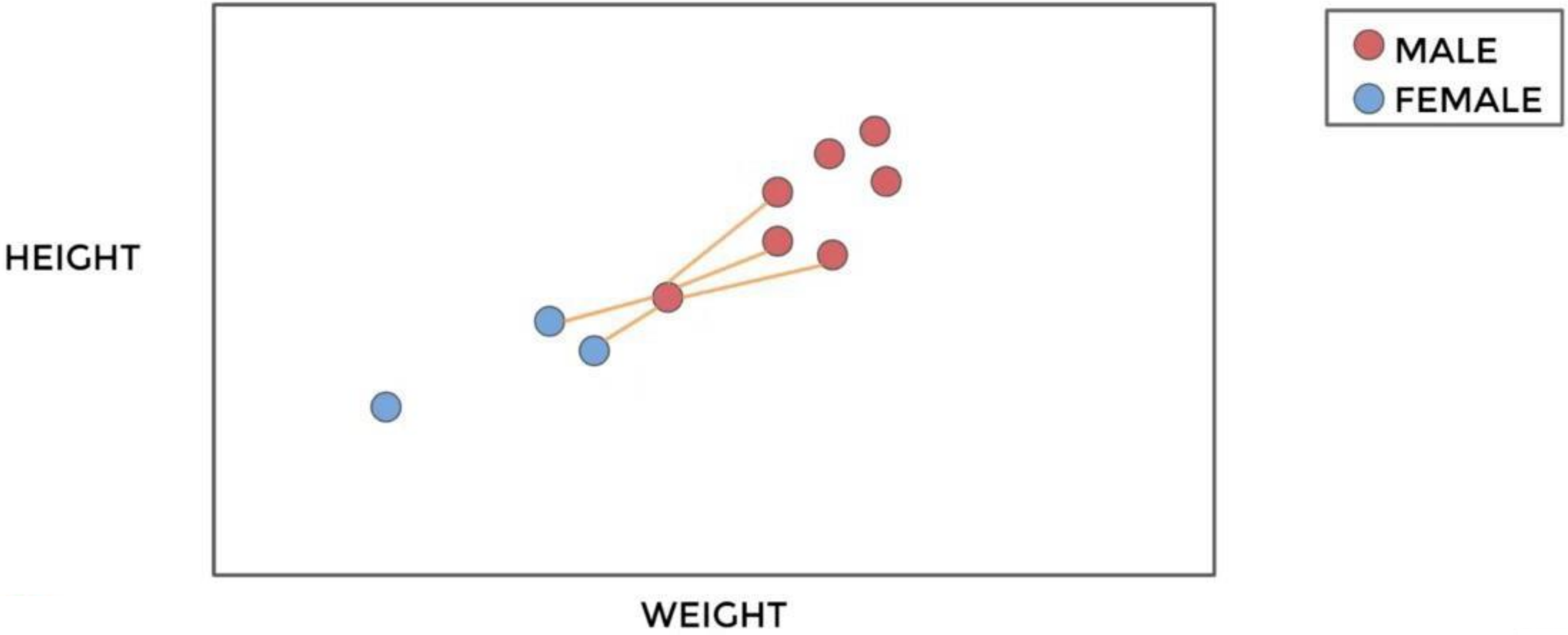
KNN

- Choose closest K



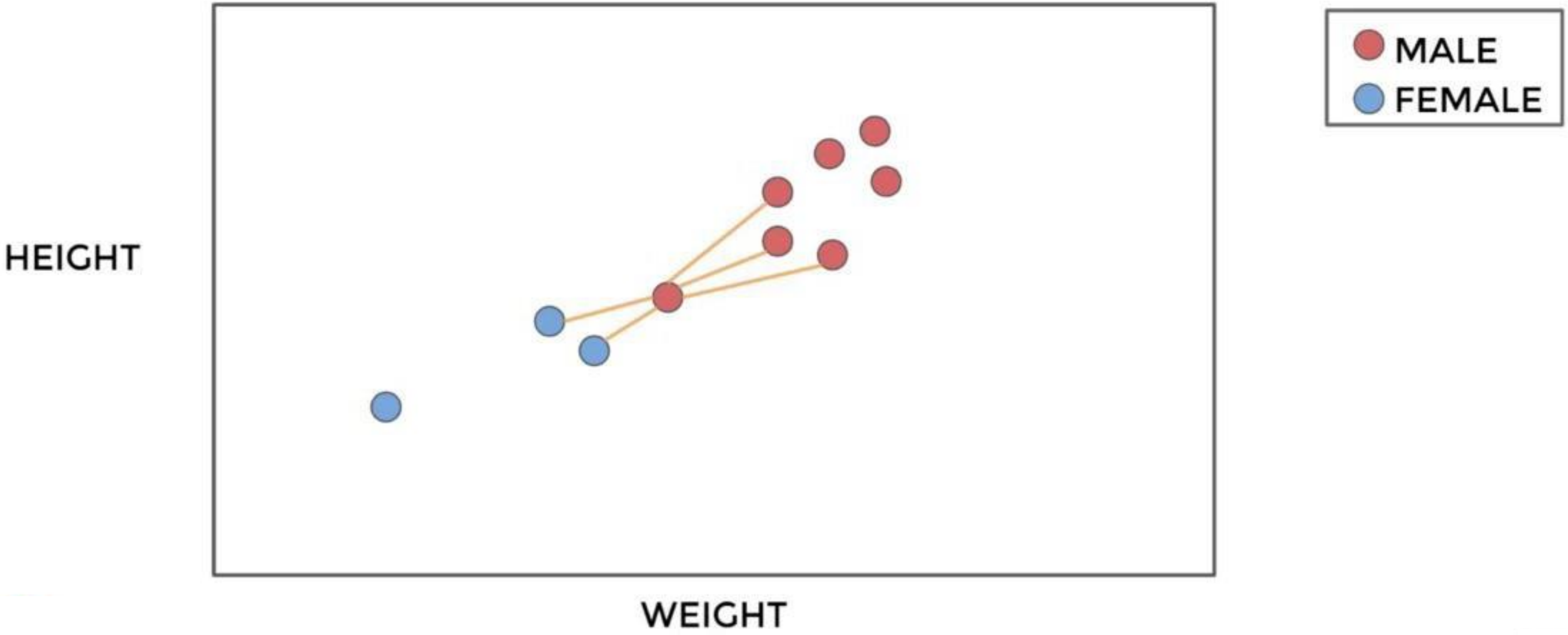
KNN

- K=5 causes a switch from previous K values.



KNN

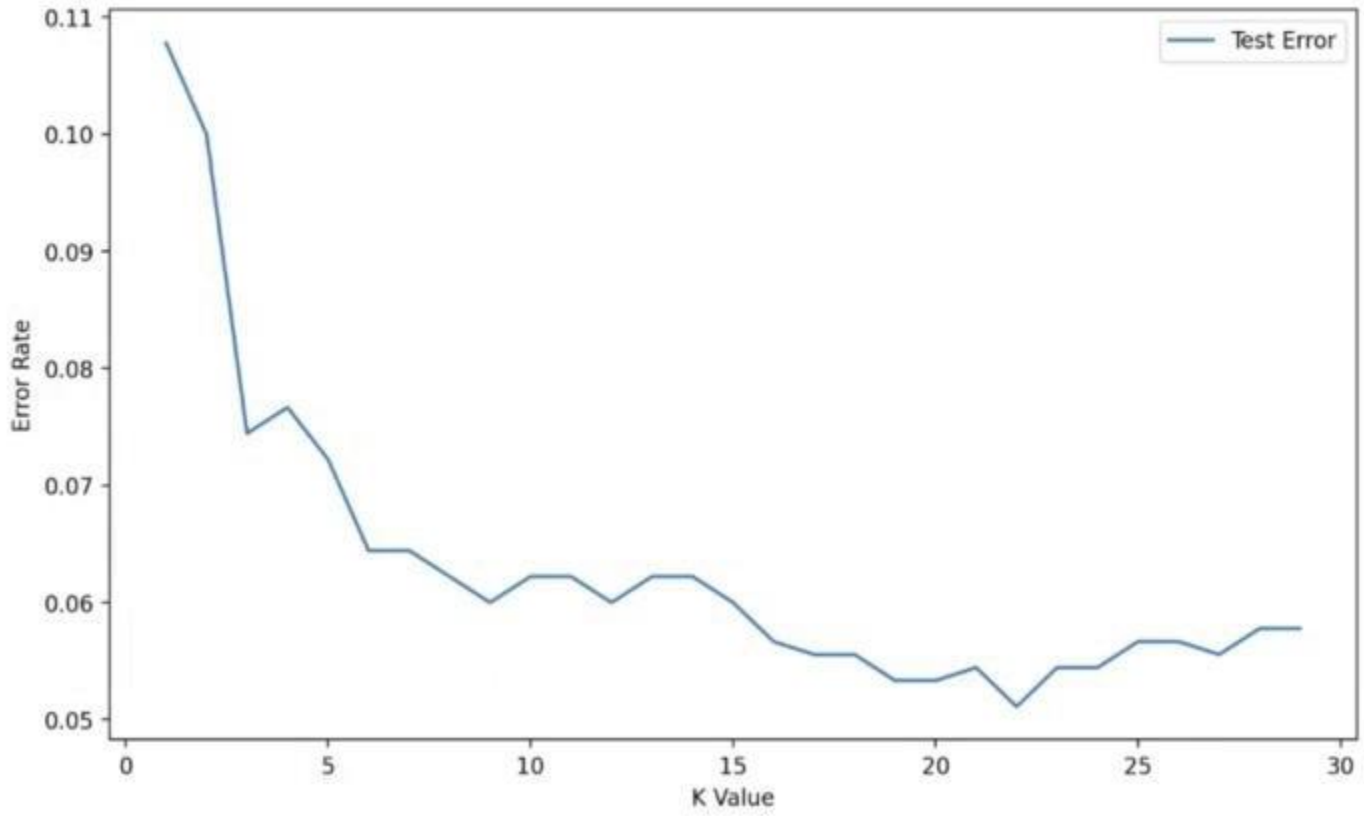
- How to choose best K value?



KNN

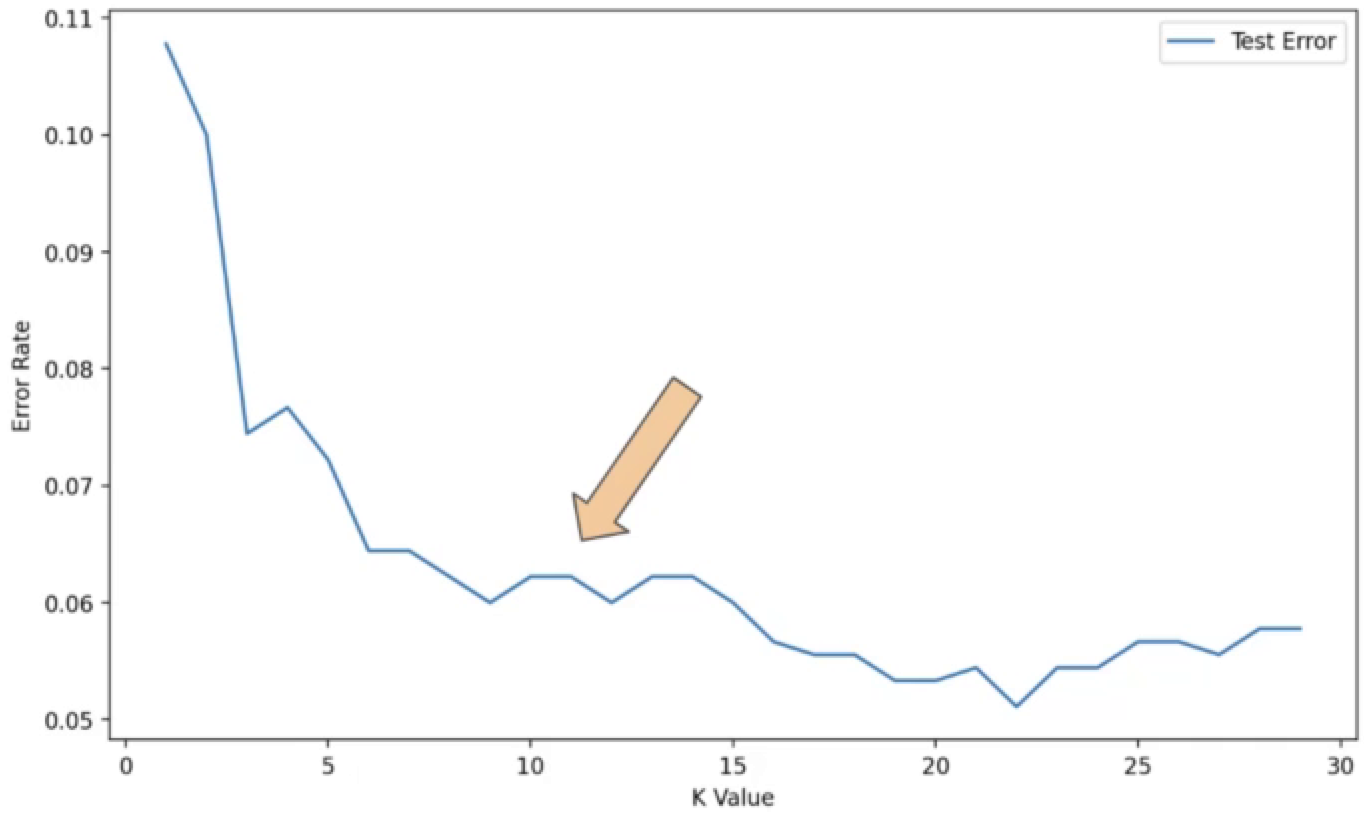
- We want a K value that **minimizes** error:
  - Error = 1 - Accuracy
- Two methods:
  - Elbow method.
  - Cross validate a grid search of multiple K values and choose K that results in lowest error or highest accuracy.

- ## Elbow method:

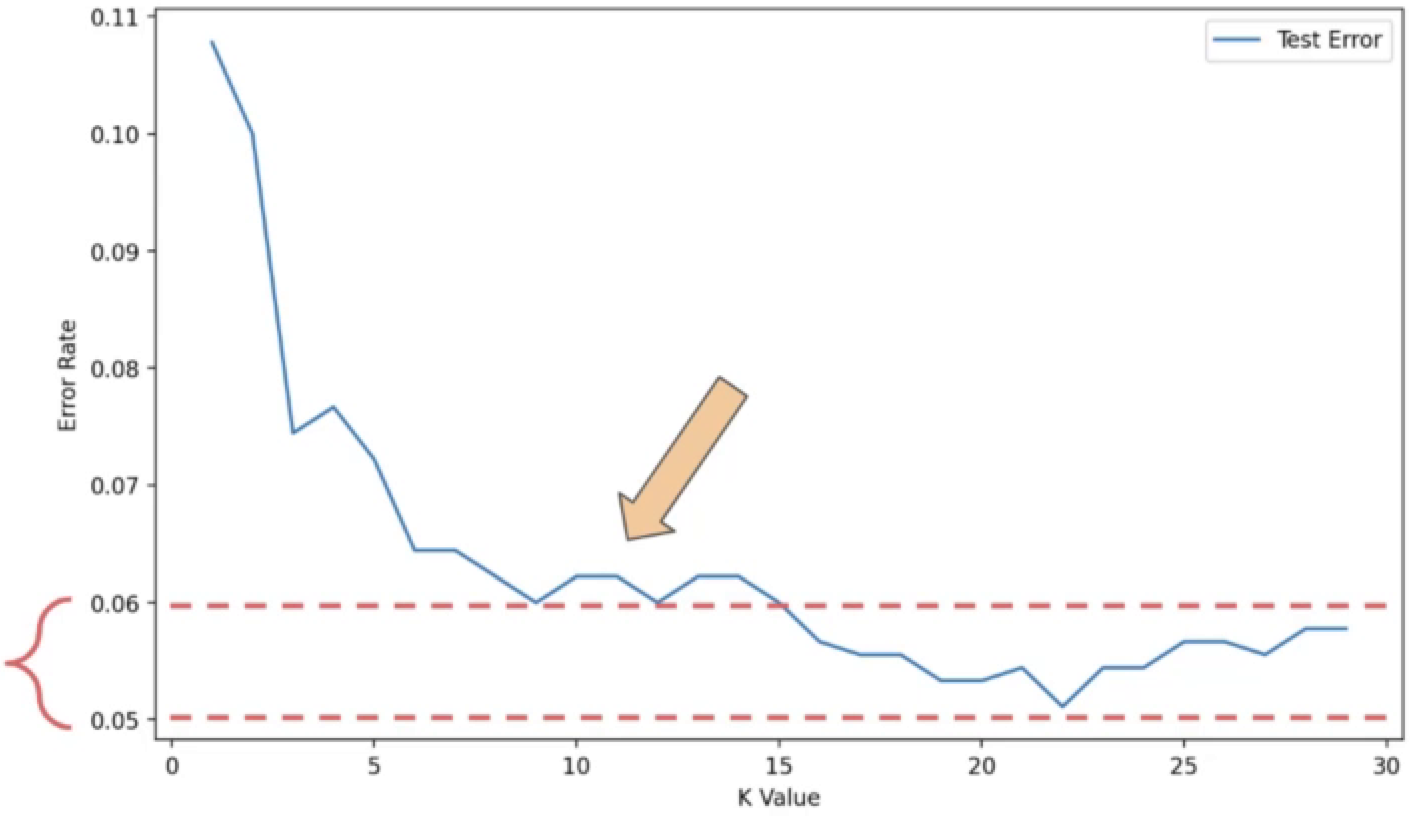


KNN

- Elbow method:



- Elbow method:



KNN

- Cross validation only takes into account the K value with the lowest error rate across multiple folds.
- This could result in a more complex model (higher value of K).
- Consider the context of the problem to decide if larger K values are an issue.

KNN

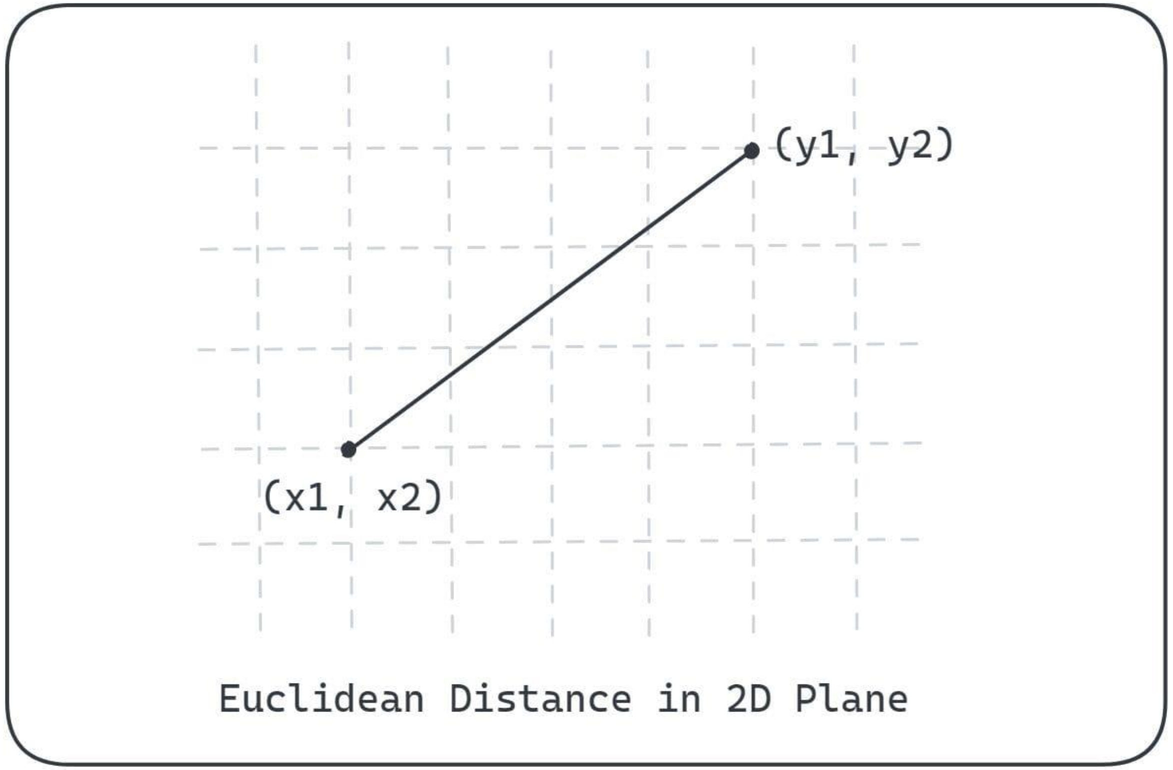
- KNN Algorithm
  - Choose K value.
  - Sort feature vectors (N dimensional space) by distance metric.
  - Choose class based on K nearest feature vectors.

KNN

- KNN Considerations:
  - Distance Metric
    - Many ways to measure distance:
      - Minkowski
      - Euclidean
      - Manhattan
      - Chebyshev

KNN

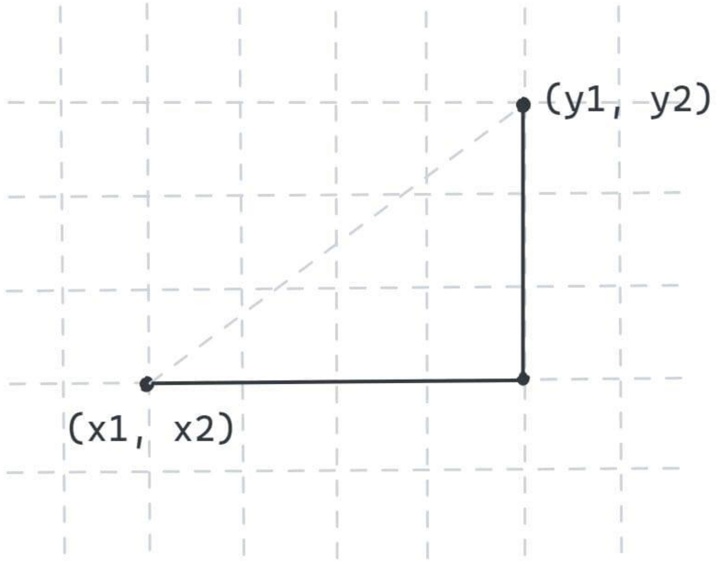
Euclidean Distance (in 2D)



$$d(\mathbf{x}, \mathbf{y}) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}$$

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

Manhattan Distance (in 2D)



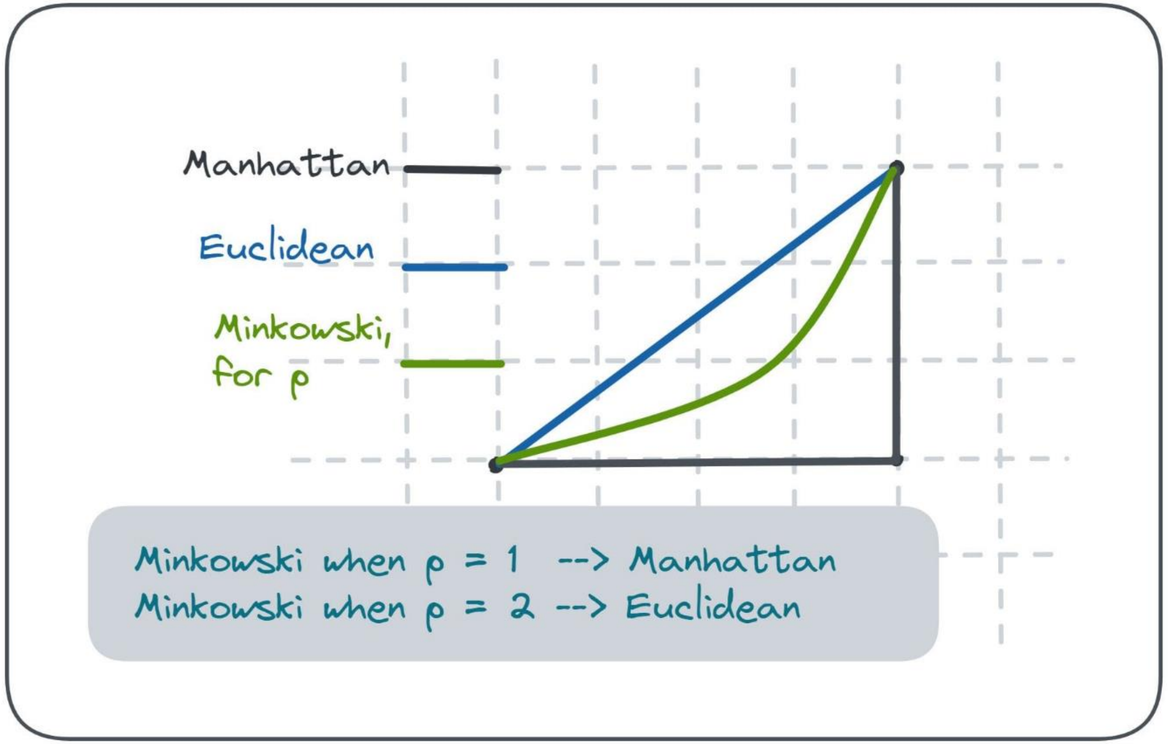
Manhattan Distance in 2D Plane
d(x,y) = |x1 - y1| + |x2 - y2|

$$d(\mathbf{x}, \mathbf{y}) = |x_1 - y_1| + |x_2 - y_2|$$

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} |x_i - y_i|$$

KNN

Minkowski Distance (in 2D)



$$d(\mathbf{x},\mathbf{y}) = \left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{1/p} \quad for\ p \geq 1$$

$p = 1$

$$d(\mathbf{x},\mathbf{y}) = \sum_{i=1}^{n} |x_i - y_i|$$

$p = 2$

$$d(\mathbf{x},\mathbf{y}) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

KNN

- KNN Considerations:
    - Scaling for Distance
        - Features could have vastly different value ranges!

KNN

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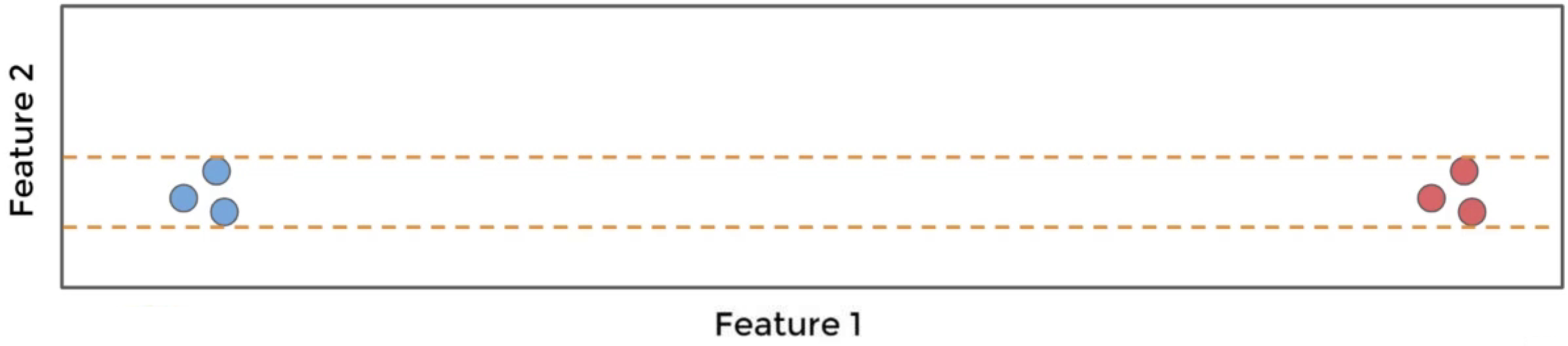
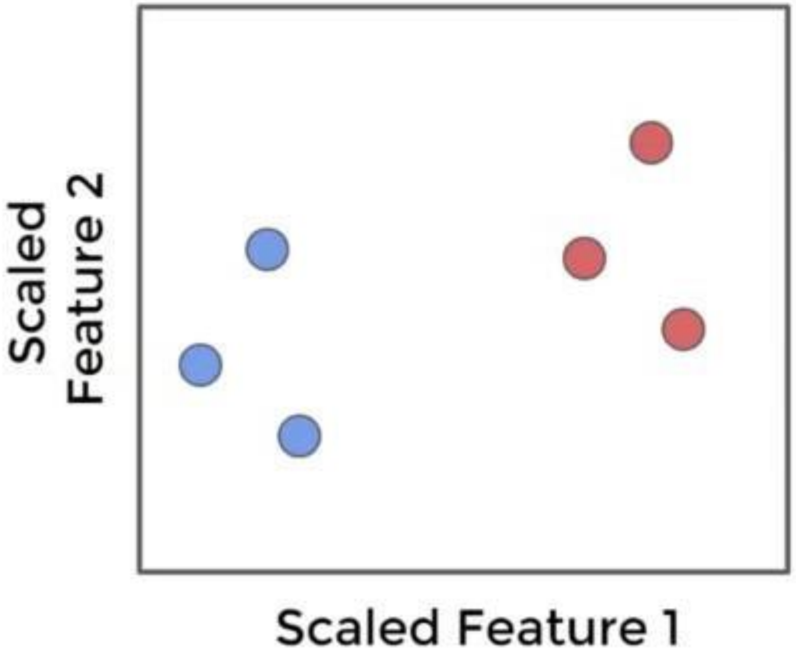


- KNN Considerations:
  - Scaling is necessary for KNN.



KNN

- While the KNN Algorithm is relatively simple, keep in mind the following considerations:
  - Choosing the optimal K value.
  - Scaling features.
- Let's continue to explore how to perform KNN for classification!

KNN Classification

Coding Part One: Data and Model

00-KNN-Classification.ipynb

KNN Classification

Coding Part Two: Choosing K

KNN

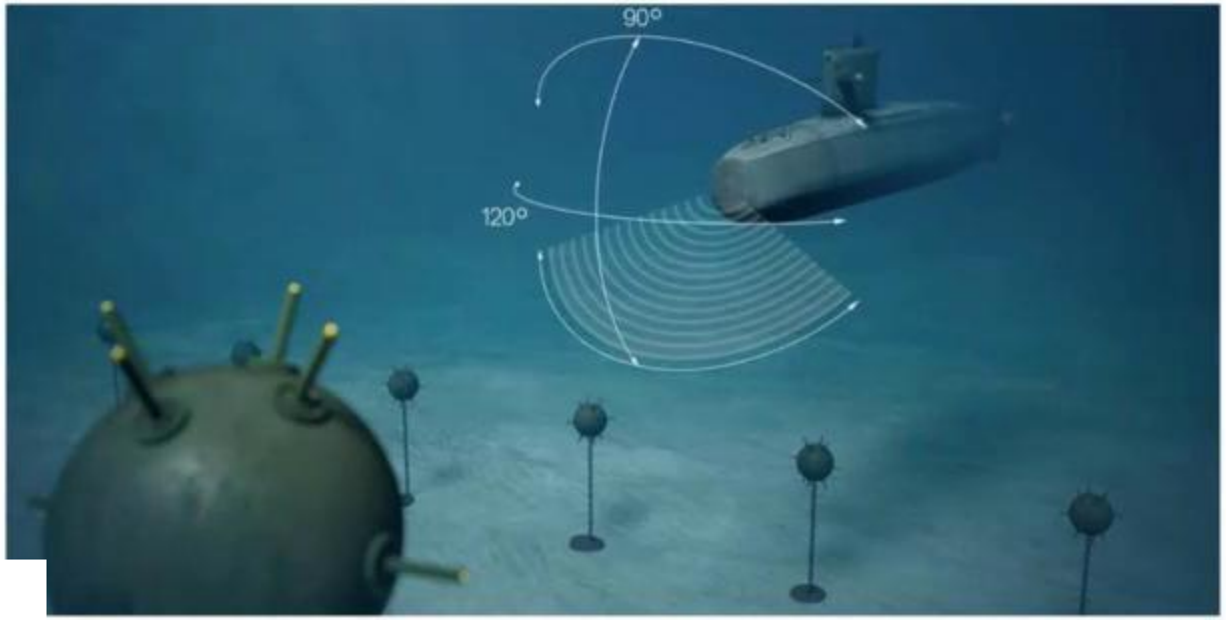
- A Pipeline object in Scikit-Learn can set up a sequence of repeated operations, such as a scaler and a model.
- This way only the pipeline needs to be called, instead of having to repeatedly call a scaler and a model.

00-KNN-Classification.ipynb

KNN Exercise Overview

KNN

- Let's test your new skills on a real data set.
- We'll be analyzing sonar frequencies to help distinguish between rocks or sea mines!



01-KNN-Exercise .ipynb