K-neareast Neighbors


Show me your
friends and I'll show
you your future.


K-nearest neighbors
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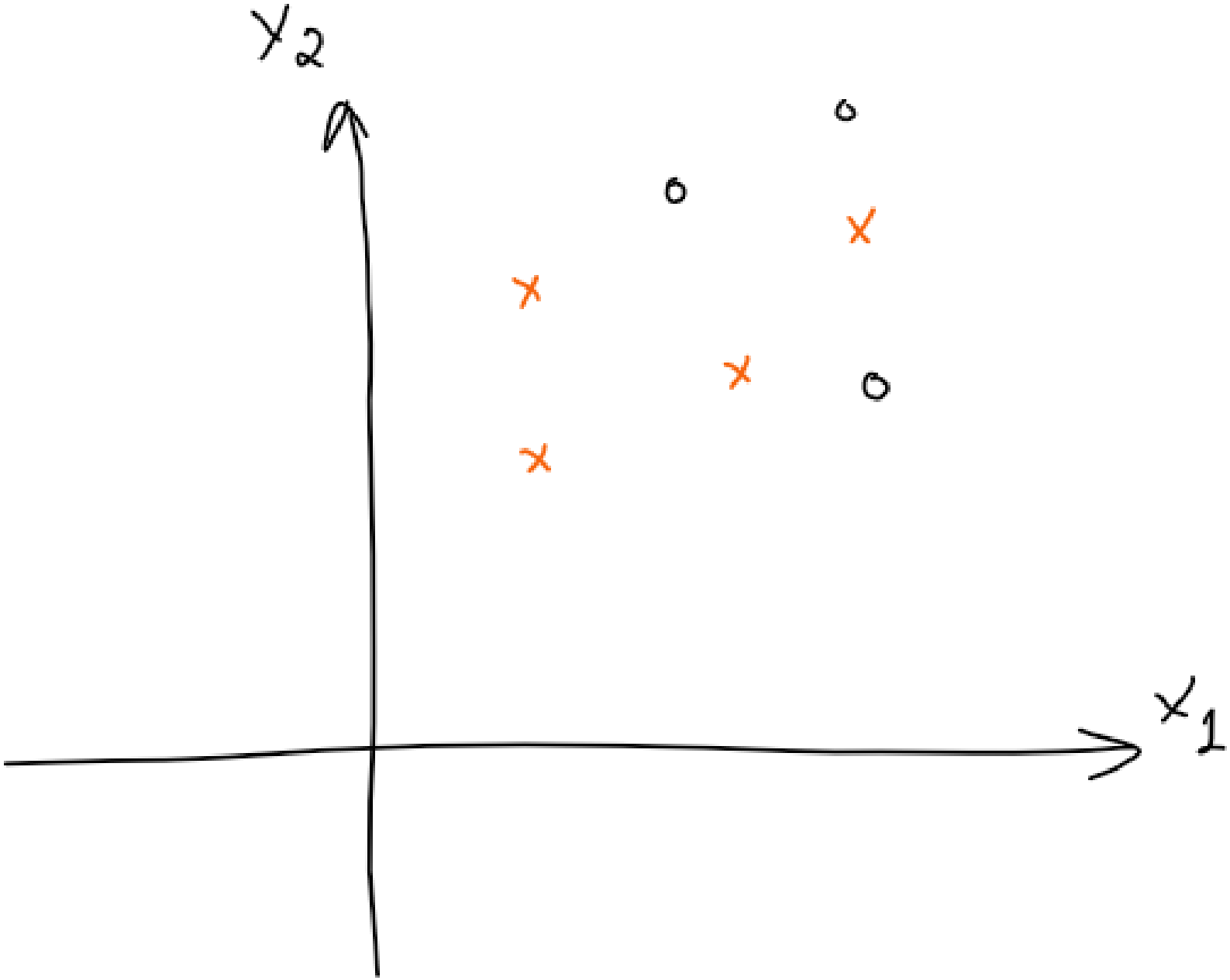
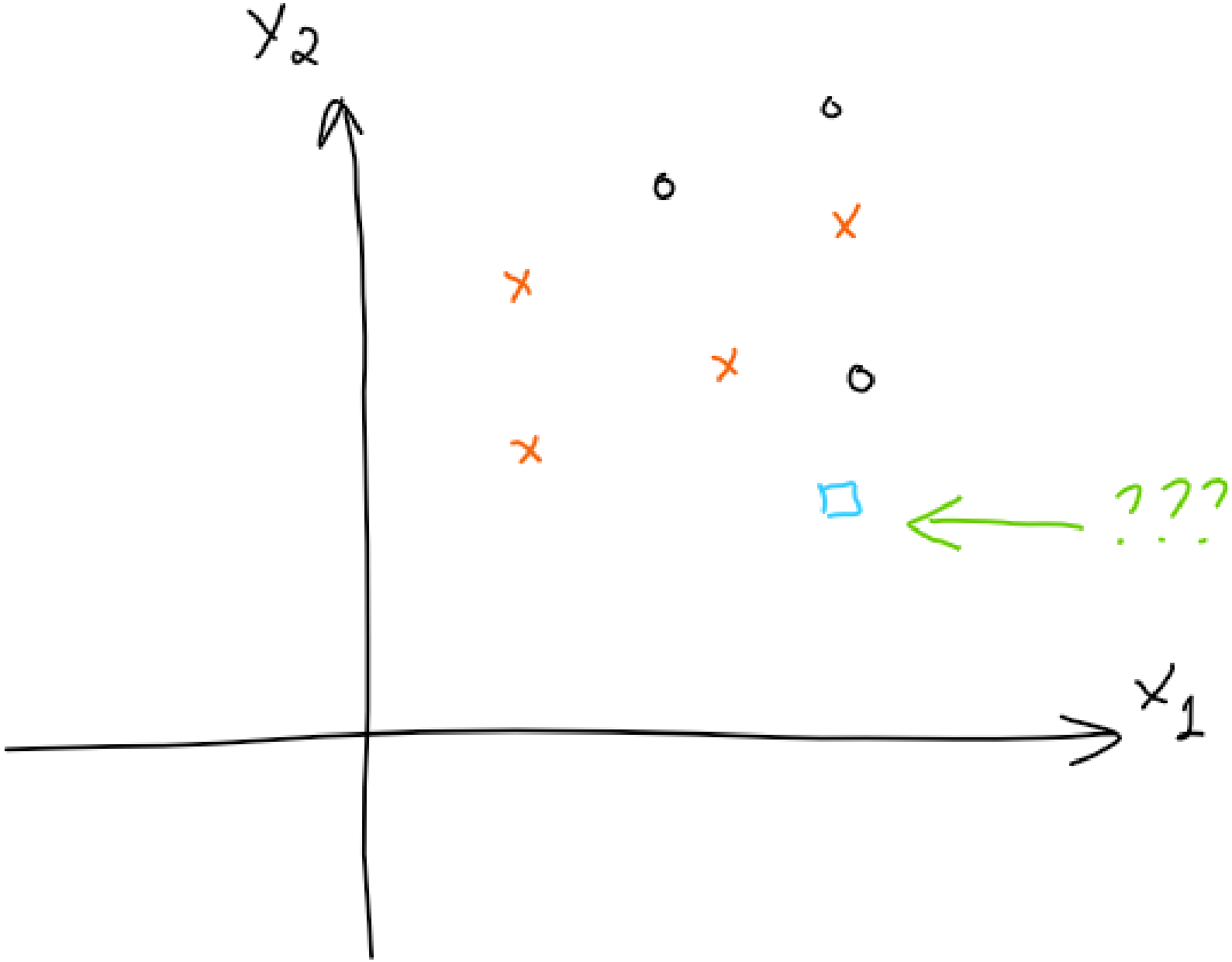
Example

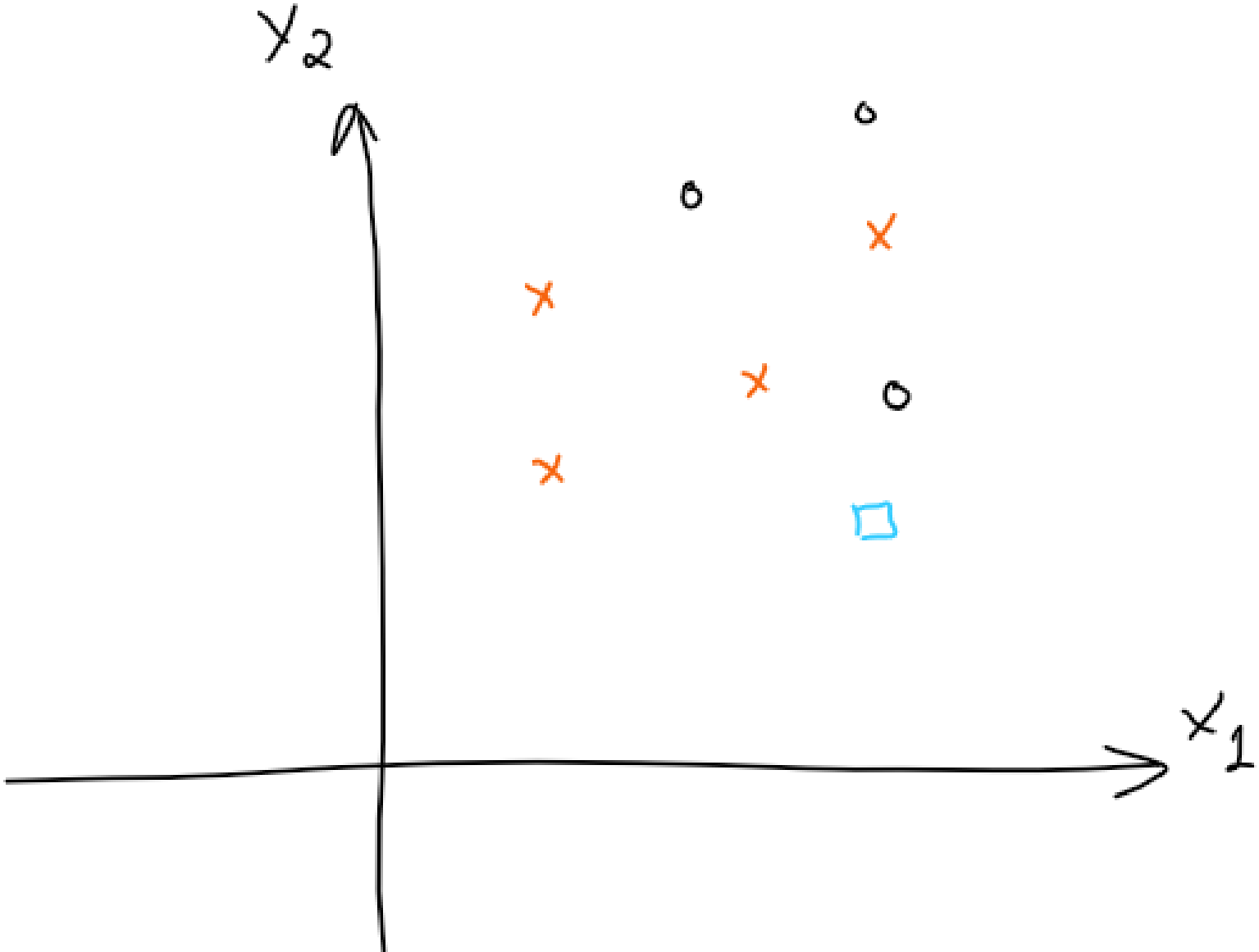


Example

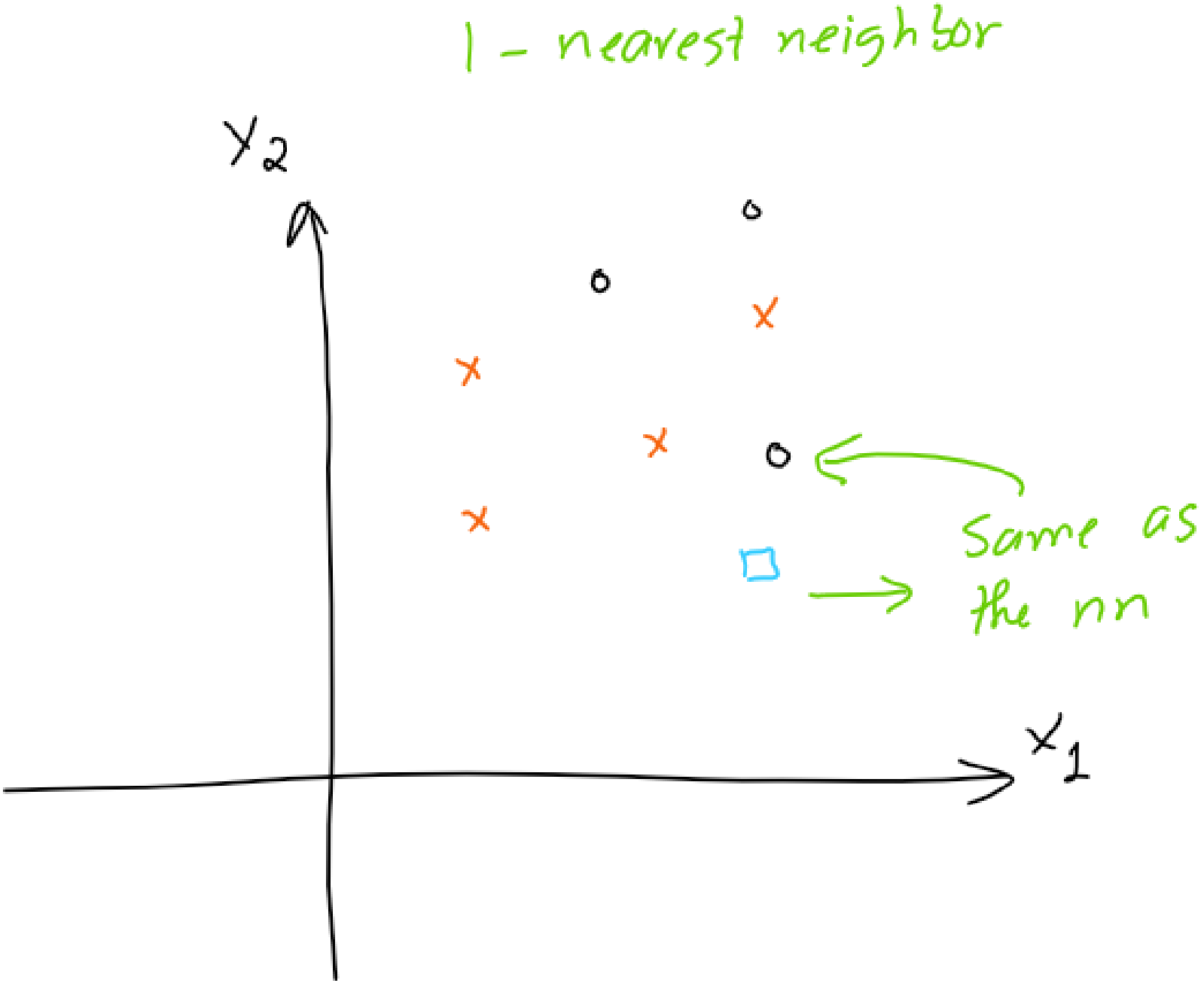


Example

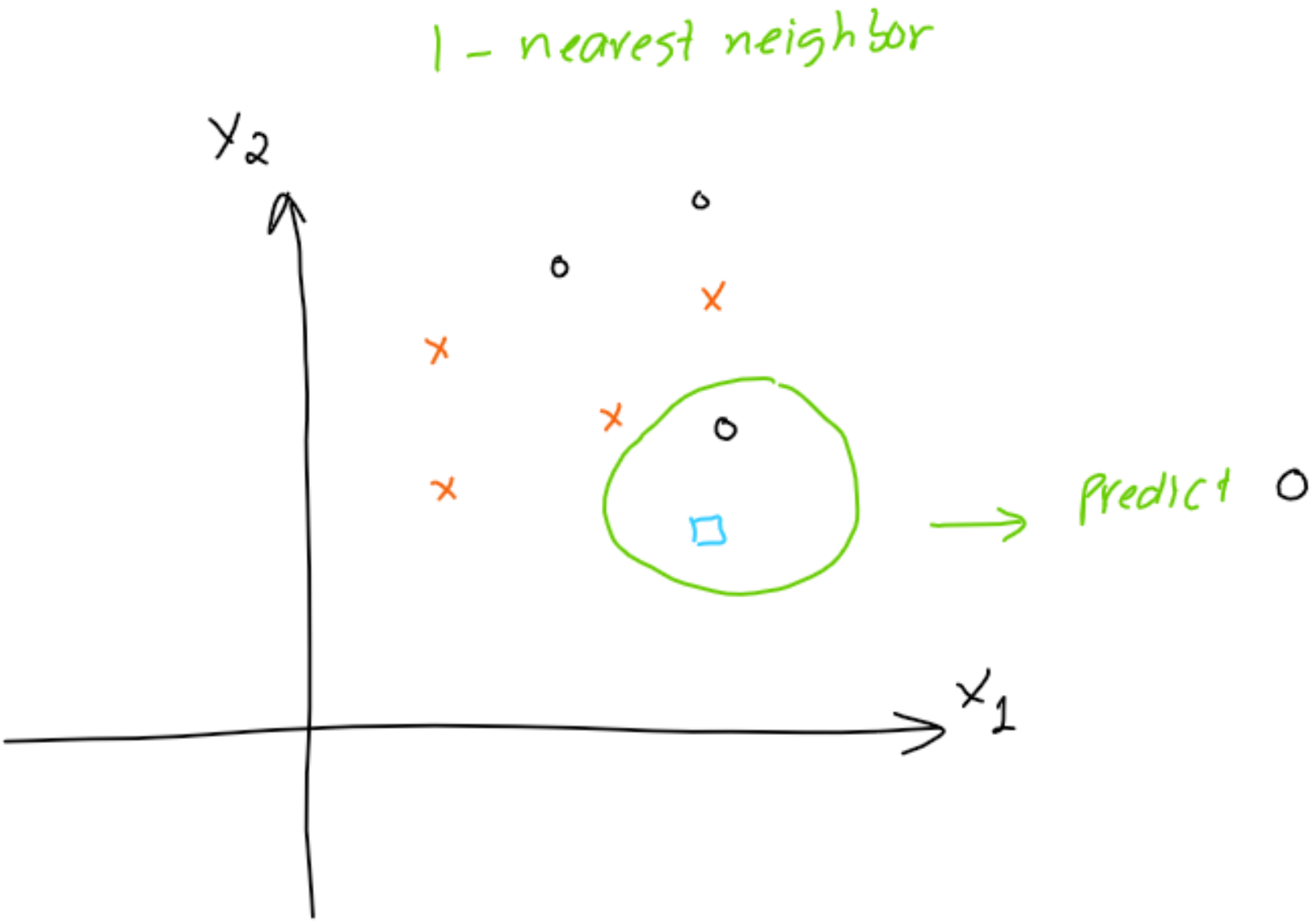
1 - nearest neighbor



Example



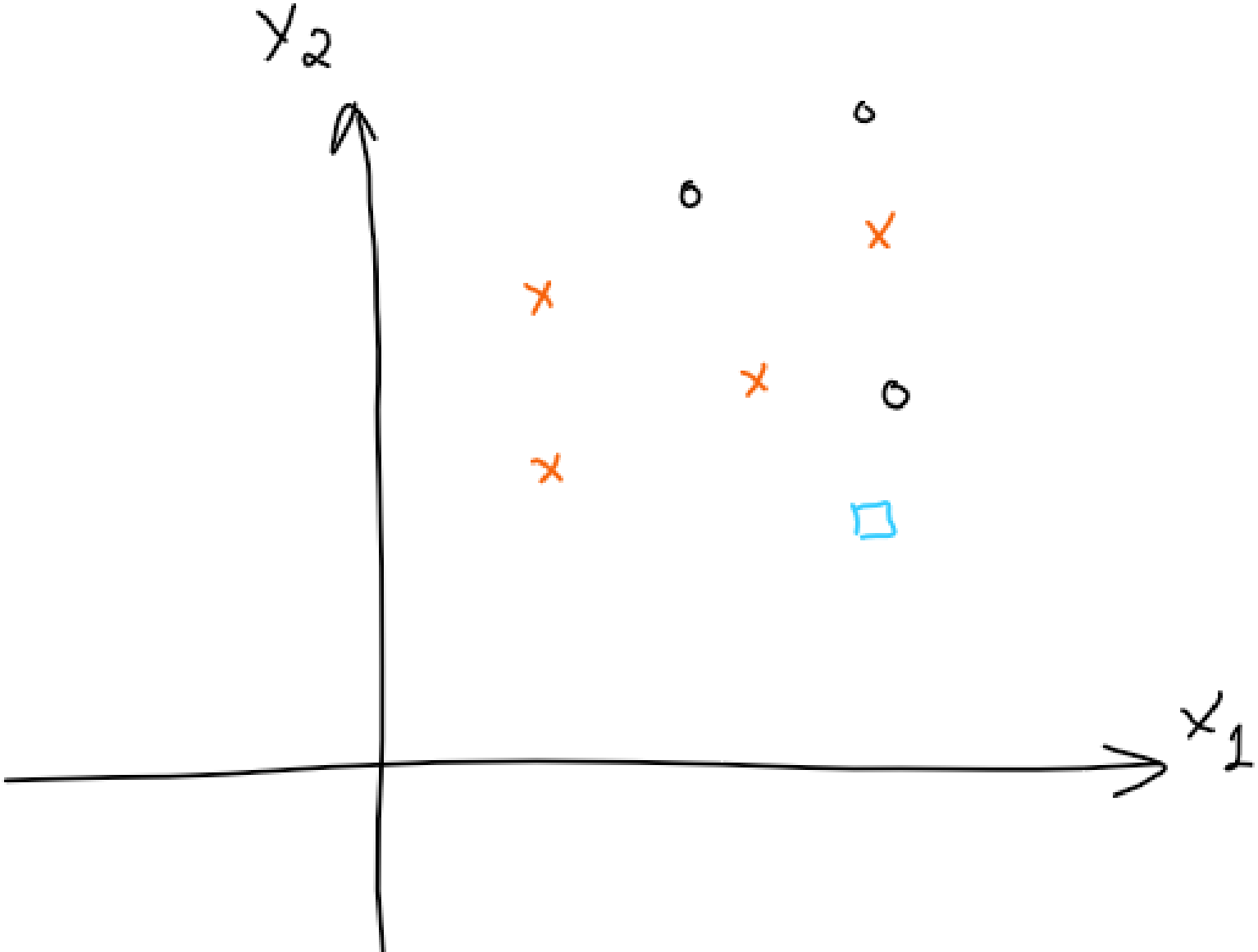
Example



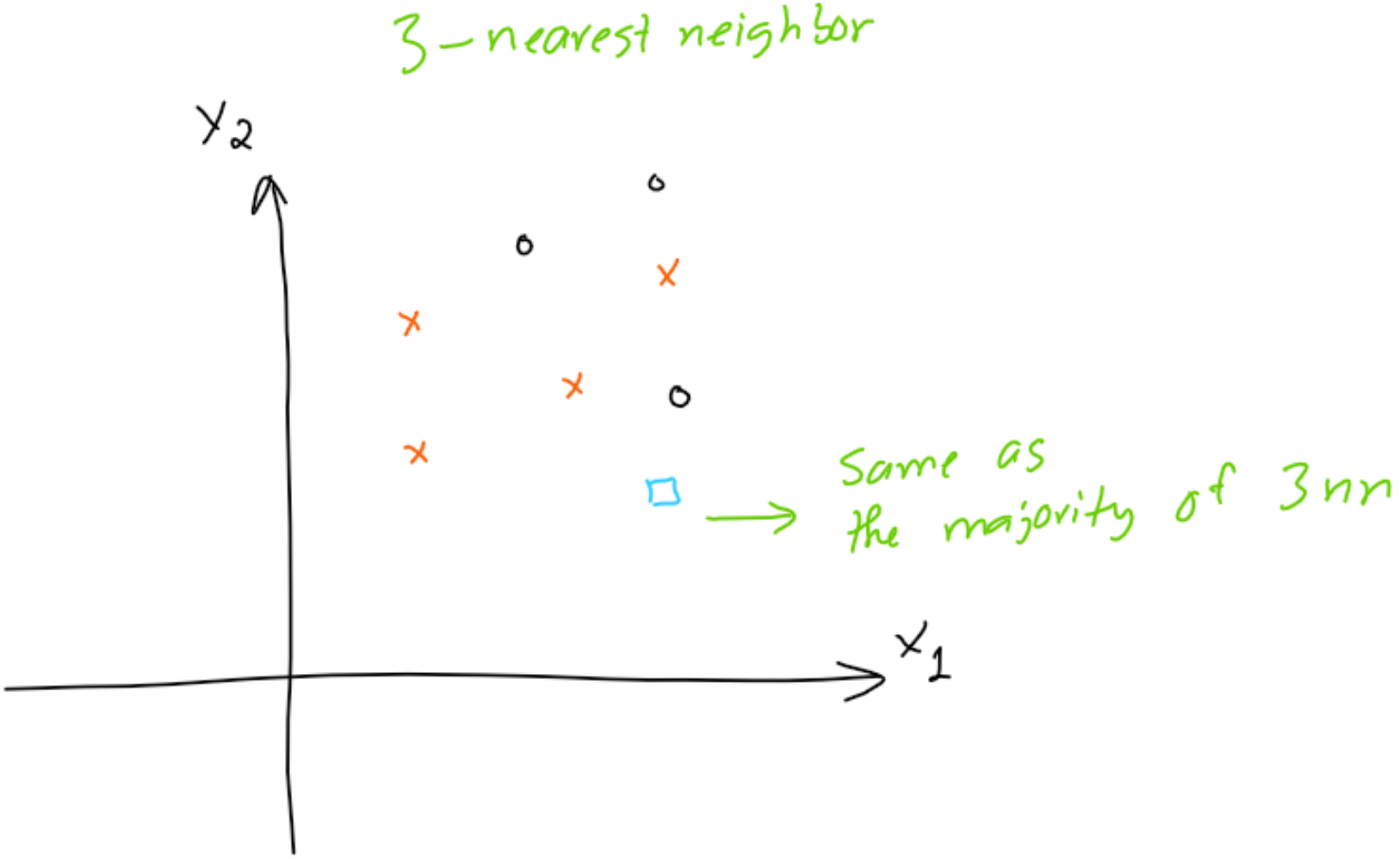
- 1NN model would classify the new sample as o

Example

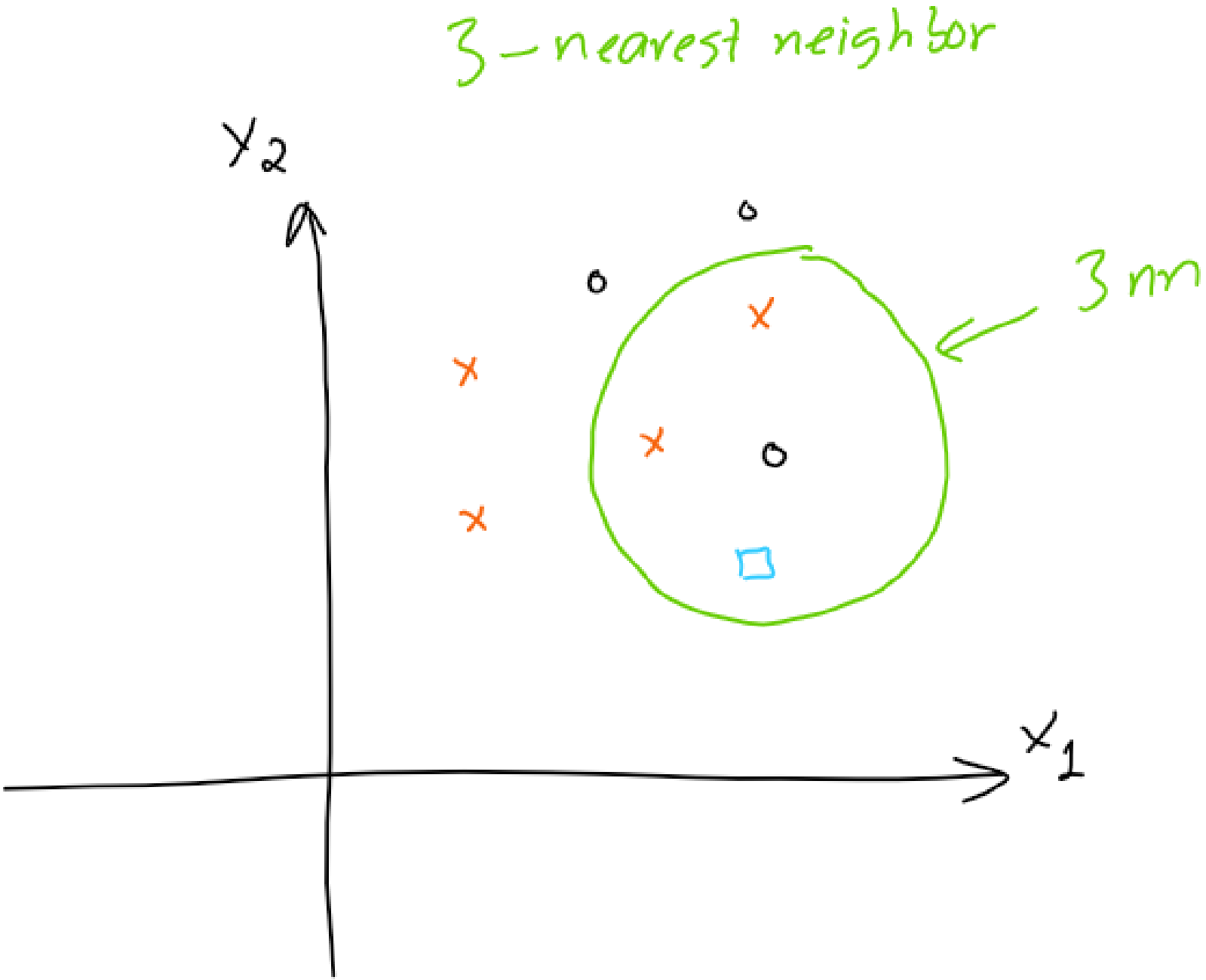
3-nearest neighbor



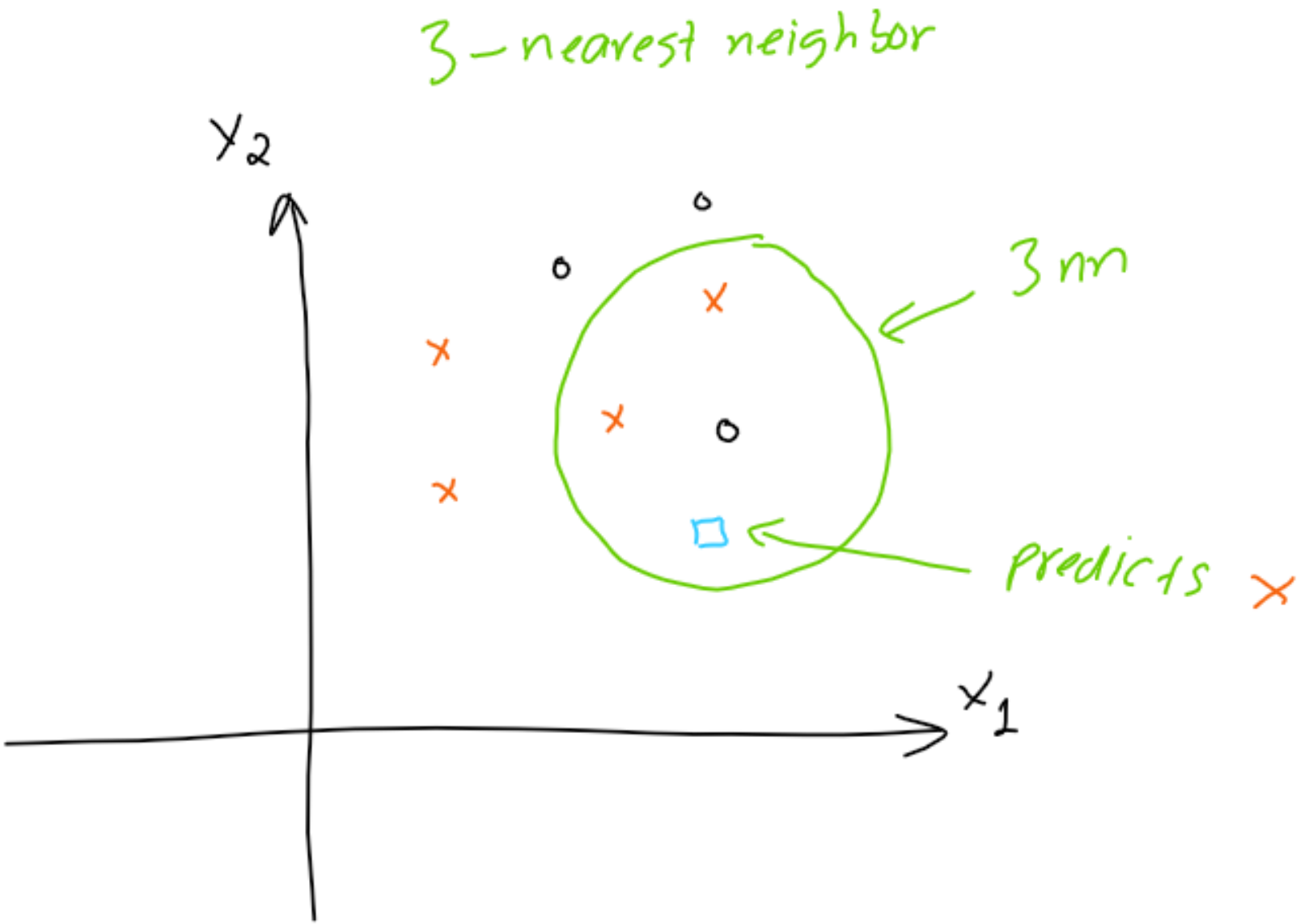
Example



Example



Example



- 3NN model would classify the new sample as x.

KNN Algorithm

- **Prediction Rule**: Look at the K most similar training examples
- For **classification**: assign the *majority* class label (majority voting)
- For **regression**: assign the *average* response

KNN Algorithm

- **Step 1**: Standardize the variables
- **Step 2**: Compute the test point's distance from each training point
- **Step 3**: Sort the distances in ascending (or descending) order
- **Step 4**: Use the sorted distances to select the K nearest neighbors
- **Step 5**: Use majority rule (for classification) or averaging (for regression)

Algorithm Requirements

- The algorithm requires:
  - **Tuning Parameter K**: number of nearest neighbors to look for
  - **Distance function**: To compute the similarities between examples

Distances

- The K-NN algorithm requires computing distances of the test example from each of the training examples
- Several ways to compute distances
- The choice depends on the type of the variables in the data

Distances

- **Euclidean distance** is commonly used when there are continious variables

$$d(u,v) = \sqrt{(u_1 - v_1)^2 + (u_1 - v_1)^2 + ... + (u_n - v_n)^2},$$

where

$$u = [u_1, u_2, ..., u_n]$$

and

$$v = [v_1, v_2, ..., v_n]$$

- **Hamming distance** is commonly used when there are categorical variables: $d(u,v) =$ Number of times u and v are different.

Distance Example

	Sex	Age	Class
u	Male	27	A
v	Famale	30	A
Difference	1	3	0

$$d(u, v) = \sqrt{1^2 + 3^2 + 0^2} = \sqrt{10}$$

- Notice: Usually the **Age** variable needs to be standardized to have the range from 0 to 1 before calculating the distance.

Why standardizing the variables?

- Considering the following data:

	Age	Salary ($1000)
A	15	90
B	30	80
C	80	87

We have

$$AB = d(A, B) = \sqrt{(30 - 15)^2 + (80 - 90)^2} = 18.03$$

$$AC = d(A, C) = \sqrt{(80 - 15)^2 + (87 - 90)^2} = 65.07$$

Thus,

$$AB < AC$$

However, with the **same** data

	Age	Salary ($)
A	15	90,000
B	30	89,000
C	80	87,000

We have

$$AB = d(A, B) = \sqrt{(30 - 15)^2 + (80,000 - 90,000)^2} = 10,000.01$$

$$AC = d(A, C) = \sqrt{(80 - 15)^2 + (87,000 - 90,000)^2} = 3000.70$$

Thus,

$$AB > AC$$

Not good!

Why standardizing the variables?

- Distances are affected by scaler-multiplication. Hence, the units of the variables will affect the distances.
- Standardizing variables will cancel this effect.

Why standardizing the variables?

- Common practice: Standardize variables to have the range from 0 to 1:

$$\text{Standardized}X = \frac{X - X_{min}}{X_{max} - X_{min}}$$

Standardize the previous data (in either unit for salary):

	Age	Salary ($1000)
A	0	1
B	0.23	0.7
C	1	0

We have

$$AB = d(A, B) = \sqrt{(0 - .23)^2 + (1 - .7)^2} = 0.38$$

$$AC = d(A, C) = \sqrt{(0 - 1)^2 + (1 - 0)^2} = 1.41$$

Choice of K - Neighborhood Size

- **Question**: Does larger or smaller K tend to overfit the model?

Choice of K - Neighborhood Size

- **Question**: Does larger or smaller K tend to overfit the model?
- **Hint**: Which one performs better on the training data?

Choice of K - Neighborhood Size

- Small K
  - Creates many small regions for each class
  - May lead to non-smooth decision boundaries and **overfit**
- Large K
  - Creates fewer larger regions
  - Usually leads to smoother decision boundaries (caution: too smooth decision boundary can **underfit**)

Weights in KNN

- If A, B, C are three nearest neighbors of D, then the predicted probability of the D by **3NN** is given by

$$\text{Predicted Probability of D} = \frac{w_A \cdot y_A + w_B \cdot y_B + w_C \cdot y_C}{w_A + w_B + w_c}$$

Weights in KNN

- **Uniform Weights**: All points in each neighborhood are weighted equally when predicting.
- If A, B, C are three nearest neighbors of D, then the predicted probability of the D by **3NN** with uniform **weights** becomes:

$$\text{Predicted Probability of D} = \frac{y_A + y_B + y_C}{3}$$

- Uniform weights are the default weights when using KNN

Weights in KNN

- **Distance Weights** weight points by the *inverse* of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- If A, B, C are three nearest neighbors of D, then the predicted probability of the D by **3NN** with **distance weights** is:

$$\text{Predicted Probability of D} = \frac{\frac{1}{DA} \cdot y_A + \frac{1}{DB} \cdot y_B + \frac{1}{DC} \cdot y_C}{\frac{1}{DA} + \frac{1}{DB} + \frac{1}{DC}}$$

Weights in KNN

- **Uniform Weights:** All the three neighbors are weighted the same, so the majority vote predicts x.
- For all neighbors:

$$Weight = 1$$

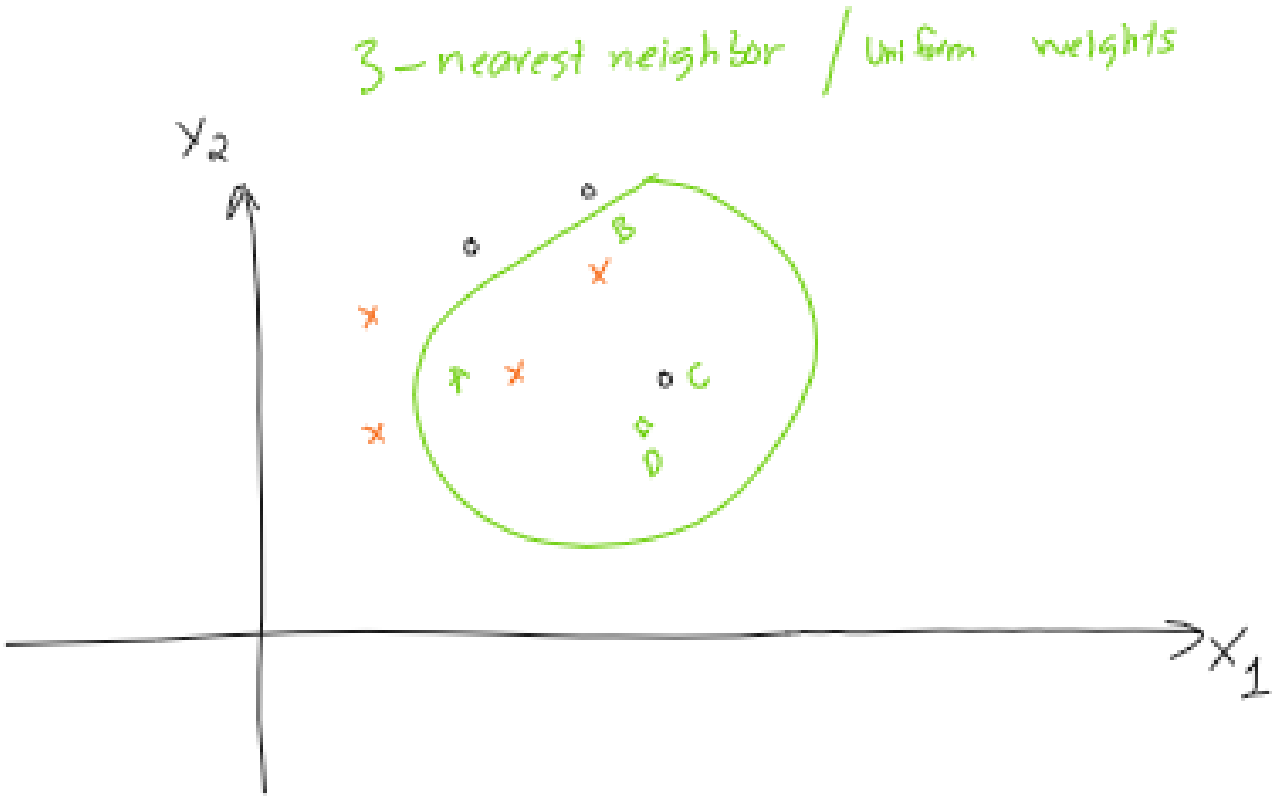
Weights in KNN

- **Distance Weights:** The closest neighbor (best friend!) is weighted more than the the two-further-away neighbors, so the weighted vote predicts o.

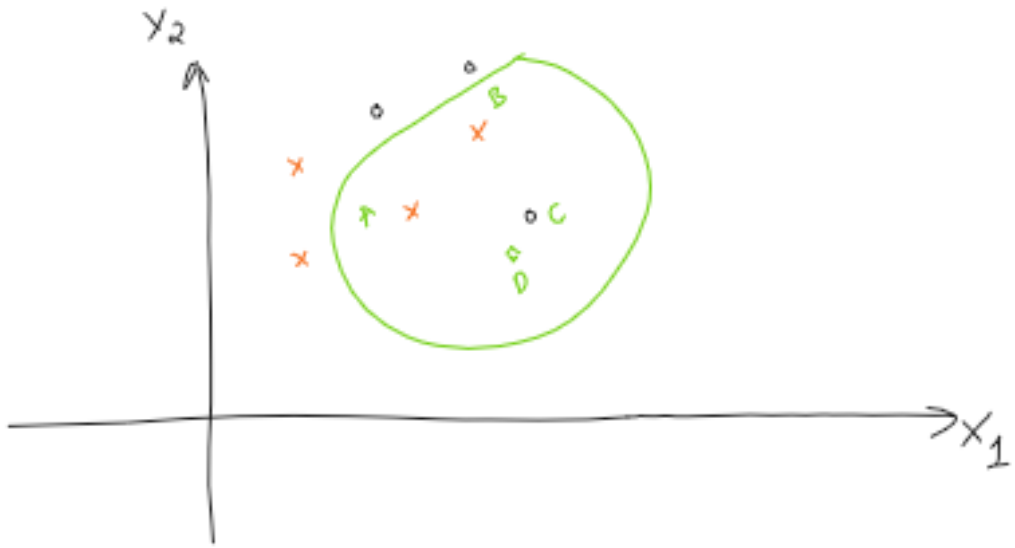
$$Weight = \frac{1}{Distance}$$

An Example of Unifom Weights

Use the uniform weights to calculate the predicted probability and the prediction of **3NN** for D. Consider x as 1 and o as 0.



3-nearest neighbor / uniform weights



weight = 1

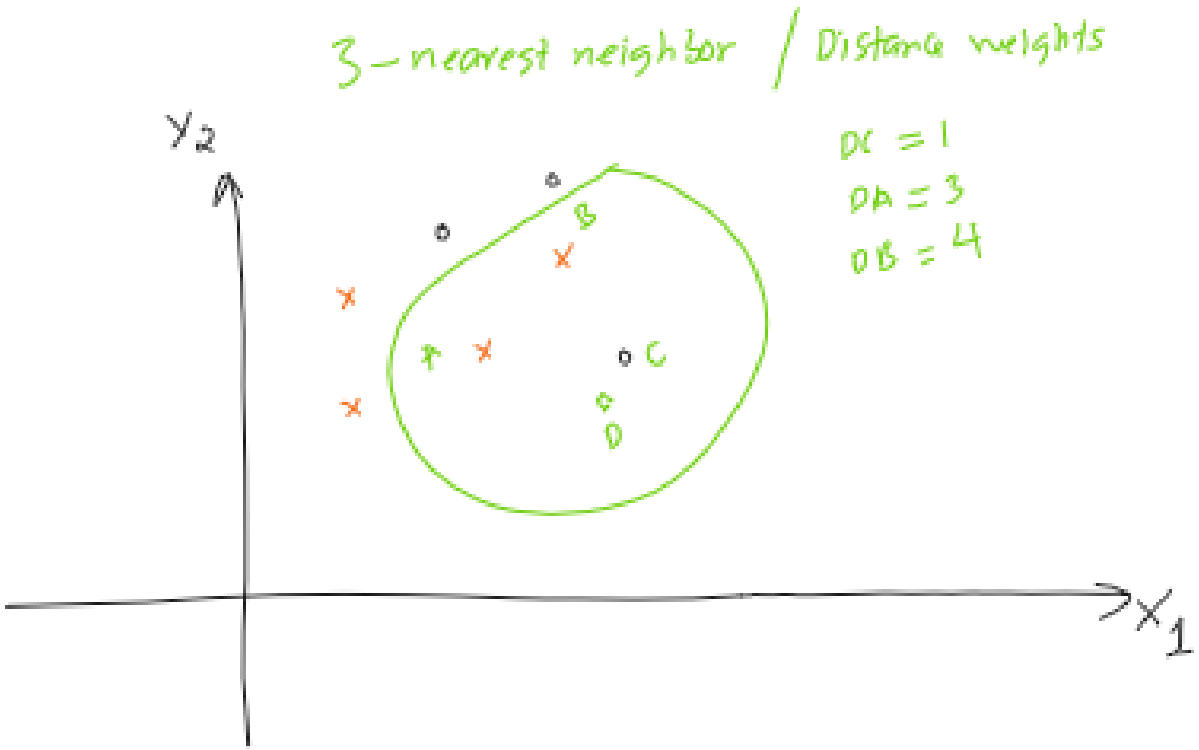
$$\text{predicted Prob. of } 0 = \frac{1 \cdot y_A + 1 \cdot y_B + 1 \cdot y_C}{3}$$

$$= \frac{0 + 1 + 1}{3} = \frac{2}{3} > \frac{1}{2}$$

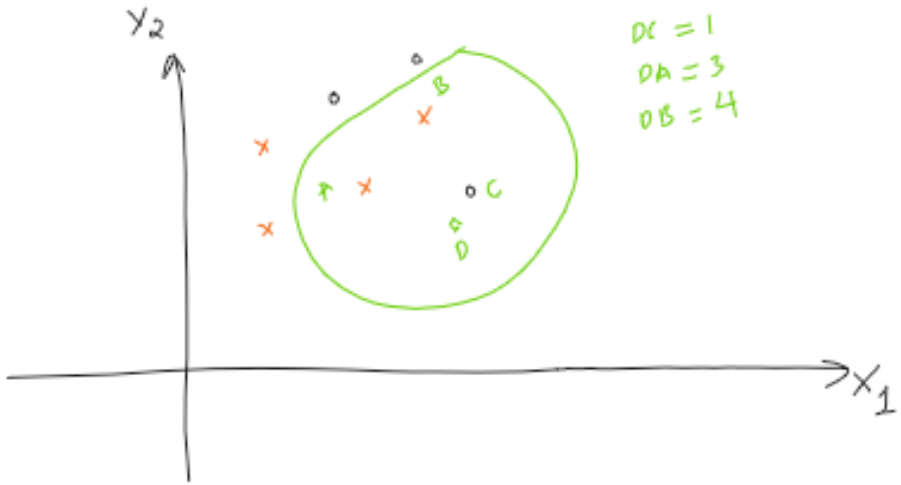
$\Rightarrow$ 3NN with distance weighted predict D ✗

An Example of Distance Weights

Use the distance weights to calculate the predicted probability and the prediction of **3NN** for D. Consider x as 1 and o as 0. Thus if a point A is x then $Y_A = 1$ and $Y_A = 0$ if A is an o.



3-nearest neighbor / Distance weights



$DC = 1$
$DA = 3$
$DB = 4$

$$\text{weight} = \frac{1}{\text{Distance}}$$

$$\text{predicted Prob. of } D = \frac{\frac{1}{DC} \cdot Y_D + \frac{1}{DA} \cdot Y_A + \frac{1}{DB} \cdot Y_B}{\frac{1}{DC} + \frac{1}{DA} + \frac{1}{DB}}$$

$$= \frac{1 \cdot 0 + \frac{1}{3} \cdot 1 + \frac{1}{4} \cdot 1}{1 + \frac{1}{3} + \frac{1}{4}}$$

$$= 0.368 < \frac{1}{2}$$

$\Rightarrow$ 3NN with distance weighted predict D as o

K-Nearest Neighbor: Properties

- What's nice: Simple and intuitive; easily implementable
- What's NOT nice:
  - Computationally expensive.
  - Perform not well in higher dimention data, i.e. data with many columns.