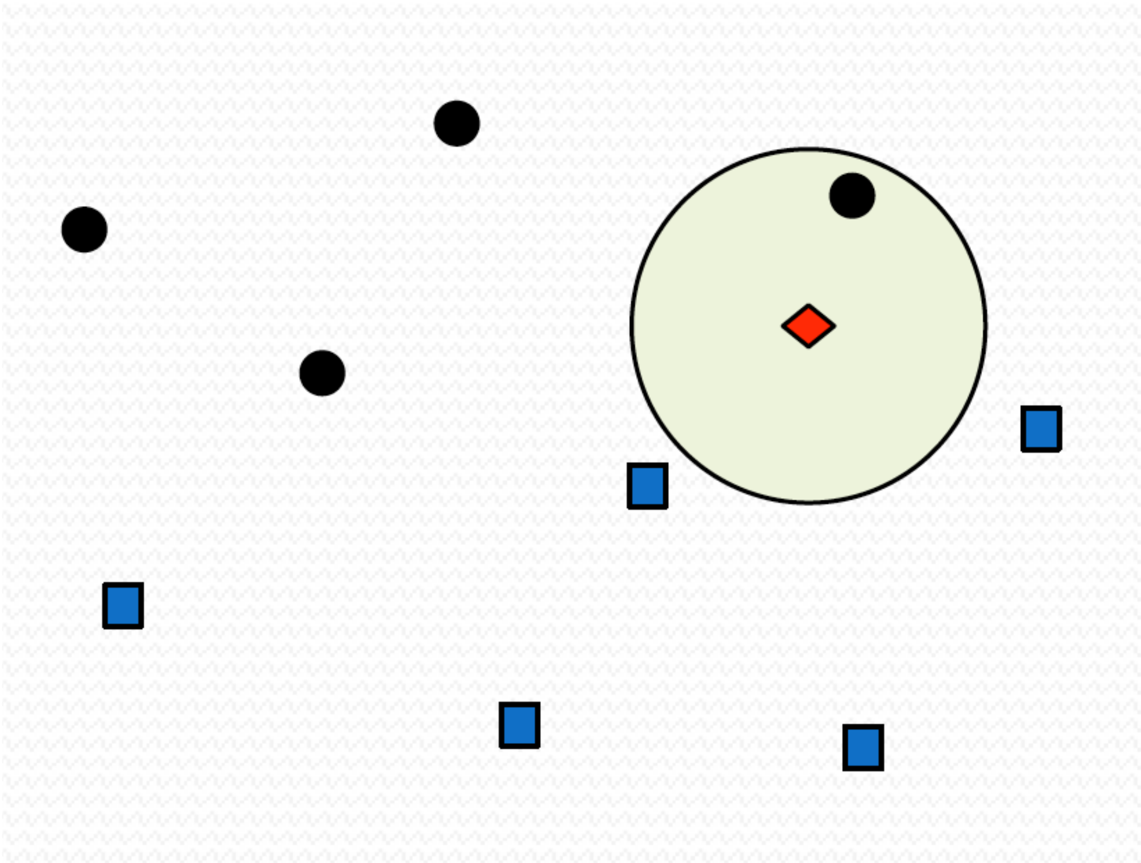
# *k-Nearest Neighbors (k-NN)*

# Instance-Based Learning

- Knn works like a classifier in supervised mode.
  - Have training examples: $(x_i, y_i)$, $i=1, \ldots, N$
    - $x_i$ could have discrete or real value
  - Try to predict the class for new example $x$
    - $y=f(x) \in \{C_1, \cdots, C_c\}$
- The main idea to determine the class
  - Similar examples have similar label
  - Algorithm:
    1. Find most similar training examples $x_n$
    2. Classify $x$ "like" these most similar examples
- Questions:
  - How to determine similar example?
  - How many similar training examples to consider?
  - How to resolve in consistencies among the training examples?

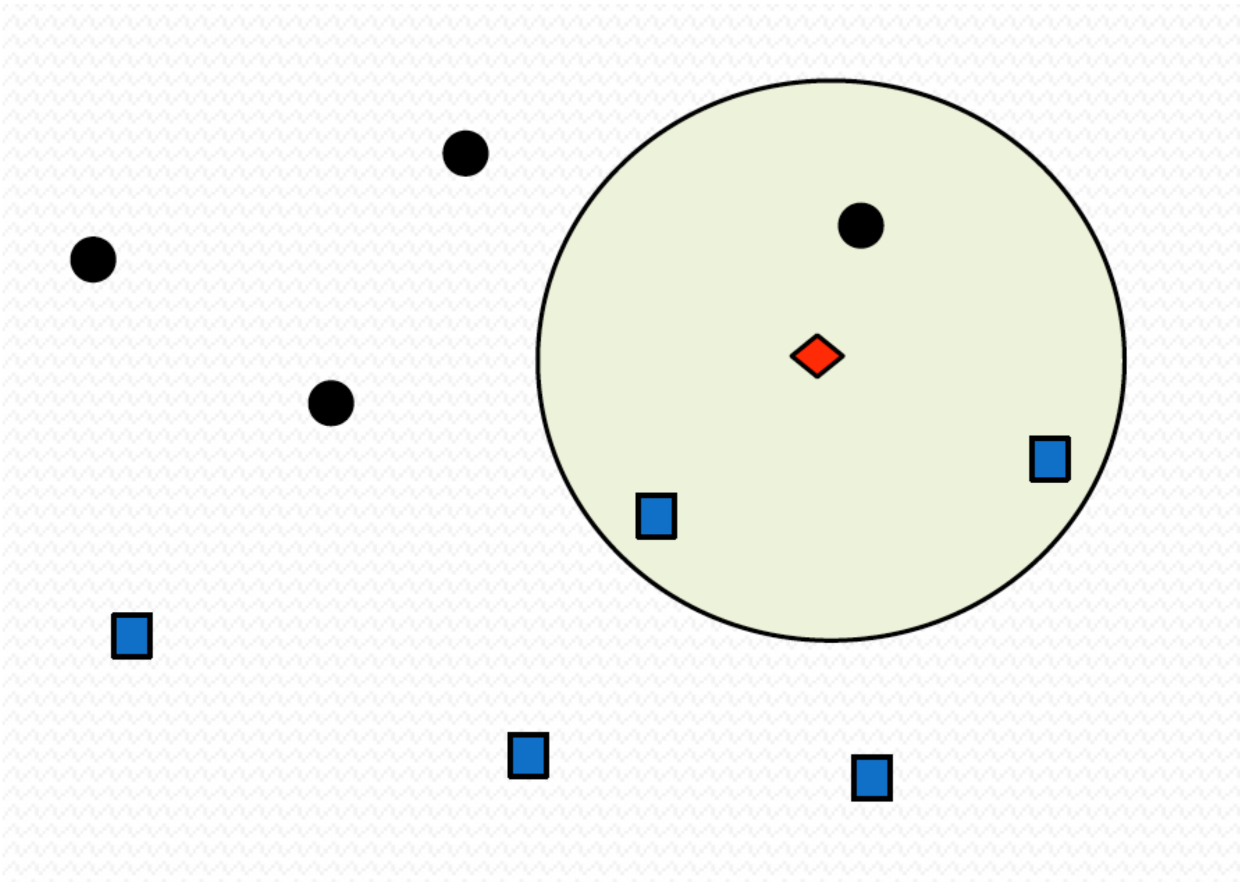
# 1-Nearest Neighbor

- One of the simplest of all machine learning classifiers
- **Simple idea:** label a new point the same as the closest known point



# 3-Nearest Neighbors

- Generalizes 1-NN to smooth away noise in the labels
- A new point is now assigned the most frequent label of its 3 nearest neighbors



# K-Nearest Neighbors (KNN)

- K-Nearest neighbors:
  - Given a query instance $x$,
  - First locate the k nearest training examples $x_1, x_2, \ldots, x_k$

  - Classification:
    - Discrete values target function
    - Take vote among its $k$ nearest neighbors
  - Extension for regression
    - Real valued target function
    - Take the mean of the values of the $k$ nearest neighbors

- Remember. We have to answer to:
  1. How to determine similar example?
  2. How many similar training examples to consider (value of k)?
  3. How to resolve in consistencies among the training examples (how to avoid noise)?

# 1. How to determine similarity?

It is possible to use any function that respects the following principles

- It's from 'distance properties'
  - Non-negative: $d(i, j) > 0$
  - $d(i, i) = 0$
  - Symmetry: $d(i, j) = d(j, i)$
  - Triangle inequality: $d(i, k) \leq d(i, j)+d(j, k)$
- Difference between distance and similarity
  - $d(i,i) = 0$ but $sim(i,i) = 1$
  - $d(i,j) \in [0, \ +\propto [$ but $sim(i,j) \in [-1, \ \ 1]$
  - From distance to similarity
    - Normalize : $d_{norm} = \frac{d}{\max(d)}$
    - Then : $sim = 1 - d_{norm}$
  - General approach : use a **strictly monotone decreasing** function f
    - Work in both sense
    - $d = f(sim)$ and $sim = f(d)$
    - Some example : $\frac{1}{a+x}$ or $e^{-x^a}$

# 1. How to determine similarity?

- Some distance
  - Manhattan distance ("city-block"): $d(\mathrm{x}, \mathrm{y}) = \sum |x_i - y_i|$
  - Euclidian distance: $d(\mathrm{x}, \mathrm{y}) = \sqrt{\sum (x_i - y_i)^2}$
  - Levenshtein distance: measure the difference between two sequences

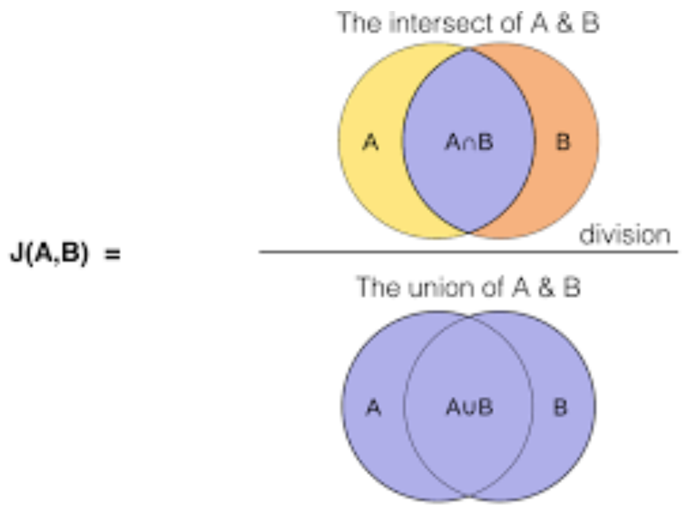
$$\operatorname{lev}(a, b) = \begin{cases} |a| & \text{if } |b| = 0, \\ |b| & \text{if } |a| = 0, \\ \operatorname{lev}\big(\operatorname{tail}(a), \operatorname{tail}(b)\big) & \text{if } a[0] = b[0], \\ 1 + \min \begin{cases} \operatorname{lev}\big(\operatorname{tail}(a), b\big) \\ \operatorname{lev}\big(a, \operatorname{tail}(b)\big) \\ \operatorname{lev}\big(\operatorname{tail}(a), \operatorname{tail}(b)\big) \end{cases} & \text{otherwise} \end{cases}$$

# 1. How to determine similarity?

- Some similarity
  - Cosine similarity (between vectors)

$$\text{cosine similarity} = S_C(A,B) := \cos(\theta) = \frac{\mathbf{A}\cdot\mathbf{B}}{\|\mathbf{A}\|\|\mathbf{B}\|} = \frac{\sum\limits_{i=1}^{n} A_i B_i}{\sqrt{\sum\limits_{i=1}^{n} A_i^2}\sqrt{\sum\limits_{i=1}^{n} B_i^2}},$$

  - Jaccard Index (between sets)



# Knn need to normalize each feature

- The distance measure is influenced by the units of the different variables, especially if there is a wide variation in units.
  - Variables with “larger” units will influence the distances more than others.
  - $di,j = \sqrt{\Sigma(x_i - x_j)^2}$
- An example

| | Income in $ | Age |
|---|---|---|
| Carry | $31 779 | 36 |
| Sam | $32 739 | 40 |
| Miranda | $33 880 | 38 |

- d(Carry, Sam) = $((31779 – 32739)^2 + (36 – 40)^2)^{1/2}$
  **= $((960)^2 + (4)^2)^{1/2}$ = $(921600 + 16)^{1/2}$ = 960,008**
  **± difference of income**
- In order to take into account all the features, the dataset must be normalized.

# Knn need to normalize each feature

| | Income in $ | Age | Normalized income | Normalized Age |
|---|---|---|---|---|
| Carry | $31 779 | 36 | 0 | 0 |
| Sam | $32 739 | 40 | 0,46 | 1 |
| Miranda | $33 880 | 38 | 1 | 0,5 |

**With un-normalized features**

| | distance | rank |
|---|---|---|
| d(Carry,Sam) | **960** | **1** |
| d(Sam,Miranda) | 1 141 | 2 |
| d(Miranda,Carry) | 2 101 | 3 |

**With normalized features**

| | distance | rank |
|---|---|---|
| d(Carry,Sam) | 1,1 | **3** |
| d(Sam,Miranda) | **0,73** | **1** |
| d(Miranda,Carry) | 1,12 | 2 |

# 2. How many similar training examples to consider?

Selecting the Number of Neighbors

- Increase $k$:
  - Makes KNN less sensitive to noise
- Decrease $k$:
  - Allows capturing finer structure of space
- Hard to tune!
- The main problem is to find the nearest neighbours efficiently
  - not covered in this course

# 3. How to resolve in consistencies among the training examples?

- Try to use more neighbors
- But give **less weight to the far neighbors** compared to the close neighbors

- Hard to tune to!

- Weigthed neighbors = soft voting
  - i.e. Weigthed contribution of each **neighbors**

# K-Nearest Neighbors with sklearn

- from sklearn.neighbors import KNeighborsClassifier
  - 3 main parameters
    - Choose the neighbors: n_neighbors (k)
    - Choose the distance: p (power): $(\sum|a_i - bi|^p)^{1/p}$ for Minskowski distance
      - p==1: Manhattan
      - p==2: Euclidian
      - Or your own distance
    - Choose the proximity weight
      - with weight ('distance') or without weight ('uniform') or you own function

- clf = KNeighborsClassifier(n_neighbors=5, weights='uniform', p=2)

- clf.fit(X_train, y_train)
- y_pred = clf.predict(X_test) or clf.predict_proba(X_test)

# PRO of k-NN

- Highly efficient inductive inference method for noisy training data and complex target functions
- k-NN is simple to understand and implement
- k-NN has no assumptions other than the need to standardize features.
- No training step: each new entry is labelled according to these neighbors
- It is possible to enrich the model with run-of-river data.
- No specific work to do to go from a problem with 2 classes, multiclass or regression
- A very wide variety of distances can be chosen (although we mainly looked at Minkowski)

# CONS of k-NN

- Need a distance that "matches" the target function
  - possibly the distance depends on the feature
- **k-NN works well with a properly balanced dataset**
  - Very expensive for large datasets
- **k-NN works well with a small number of features**
  - Need dimension reduction for high-dimensional data (more than 10) in order to avoid the effects of the curse of dimensionality.
  - Use PCA or LDA
- **k-NN works well with a properly balanced dataset**
- **Need to standardize the data to give equal weight to each feature**
- **k-NN doesn't work with missing value**
- **k-NN is very sensitive to outliers** because it simply chooses neighbors based on distance criteria.

- But one of the main problems with k-NN is to choose the optimal number of neighbors to be considered when classifying the new data entry.

# k-NN extension
# Approximate Nearest Neighbors

- KNN (K-Nearest Neighbors) is Dead!
  - https://pub.towardsai.net/knn-k-nearest-neighbors-is-dead-fc16507eb3e
- Comprehensive Guide To Approximate Nearest Neighbors Algorithms
  - https://towardsdatascience.com/comprehensive-guide-to-approximate-nearest-neighbors-algorithms-8b94f057d6b6
- Approximate Nearest Neighbor Search in High Dimensions
  - https://arxiv.org/abs/1806.09823

# k-NN extension
# Missing data inputation

- The KNN algorithm helps to impute missing data by finding the closest neighbors
  - Imputs missing data with non-missing values from neighbors.

- from sklearn.impute import KNNImputer
  - **n_neighbors:** Number of neighboring samples to use for imputation.
  - **Weights**: Weight function used in prediction.
    - 'uniform' : All points in each neighborhood are weighted equally.
    - 'distance' : weight points by the inverse of their distance.

# The lab of today
# → Short lecture… but long lab

- Part I. K-nearest neighbors for classification
- Part II. K-nearest neighbors for regression

Read, understand and complete the code

- Part III.
  - Step 1: Build a pipeline
    - Impute missing value
    - Normalize data
    - Predict with knn model
  - Evaluate your pipeline with default parameters
  - Search best hyper-parameters
    - Plot confusion matrix
    - Print classification report

Put comments on your notebook and submit it

Lab part

- Part IV. Read paper « KNN (K-Nearest Neighbors) is Dead! »
  - Try to understand ANN (Approximate Nearest Neighbors)

# Some complements to help you revise

# Exercise: data

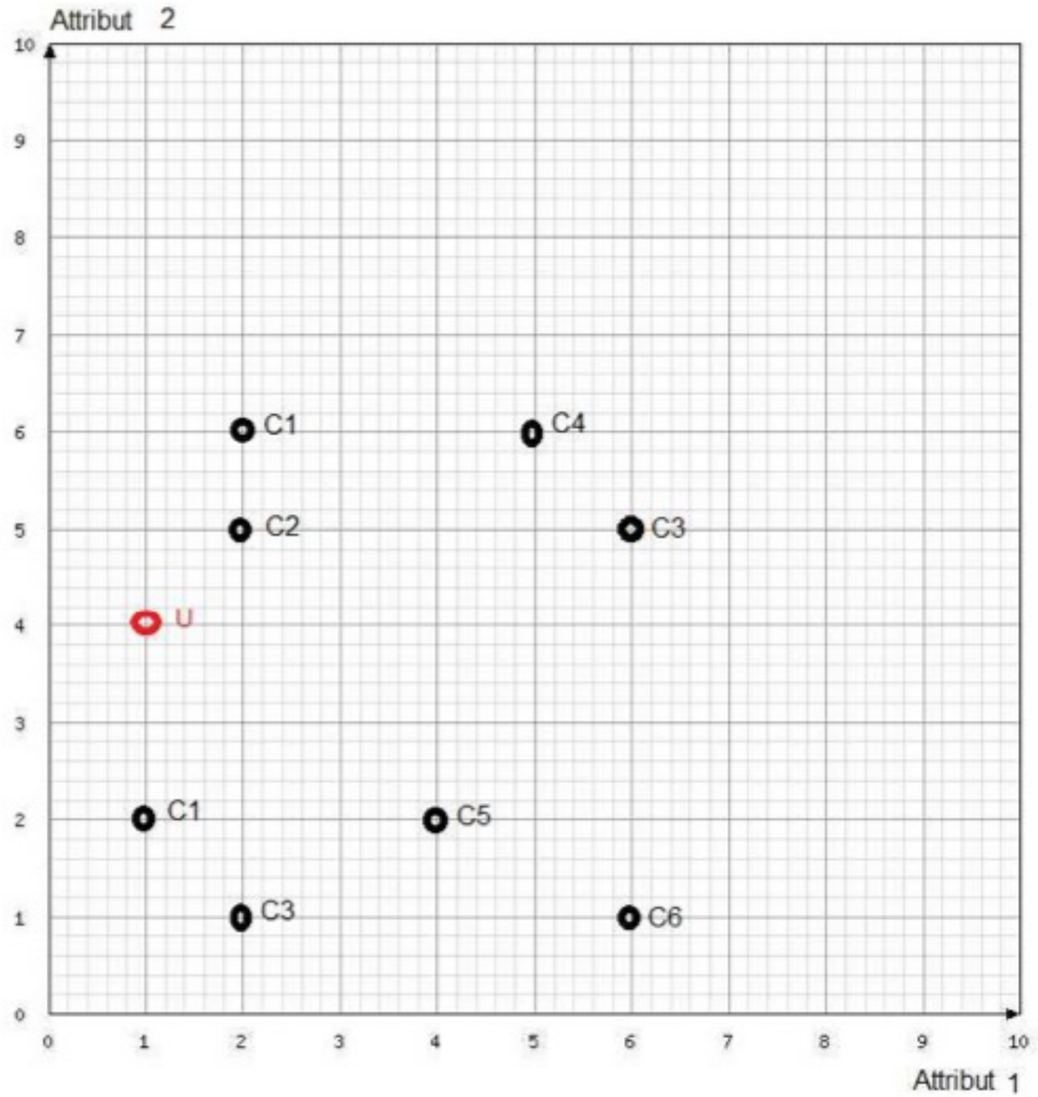
- The following table contains data on individuals in a population described by two attributes: attribute 1 and attribute 2. The class of an individual can be: C1, or C2, ... or C6.

| N° | Attribut 1 | Attribut 2 | Class |
|---|---|---|---|
| 1 | 1 | 2 | C1 |
| 2 | 2 | 6 | C1 |
| 3 | 2 | 5 | C2 |
| 4 | 2 | 1 | C3 |
| 5 | 4 | 2 | C5 |
| 6 | 5 | 6 | C4 |
| 7 | 6 | 5 | C3 |
| 8 | 6 | 1 | C6 |

# Exercise: questions

1. **Dataset**
   - Plot the data from the previous table.
2. **3-NN Manhattan**
   - We want to classify a new individual U with attributes (1, 4) using the KNN method. What will be the class of U if we choose k=3 and Manhattan distance. Justify.
3. **3-NN Euclidian**
   - We want to classify a new individual U with attributes (1, 4) using the KNN method. What will be the class of U if we choose k=3 and Euclidian distance. Justify.
4. **Weigted 3-NN**
   - We now use the variant of KNN which uses the distance 1/d2 (inverse of the distance squared) to calculate the neighbours. The distance is the Euclidian one. What will be the class of U with k=3? Justify.

# Exercise: solutions



# Exercise: solutions (cont')

- *Euclidian distance*
  - *Dist(U, P1) = 2*
  - *Dist(U, P2)= 2.24*
  - *Dist(U, P3) = 1.41*
  - *Dist(U, P4) = 3.16*
  - *Etc. The other points are further on.*

  - Point U is class C1 (2 votes for C1, against 1 vote for C2)

- Weigthed Euclidian distance
  - For class 1, the weights are 1/(2*2) and 1/(2.24*2.24) → 0.25+0.20 = 0.45
  - For class 2, the weight is 1/(1.41*1.41) = 0.5

  - The U-point will therefore be assigned to class C2