



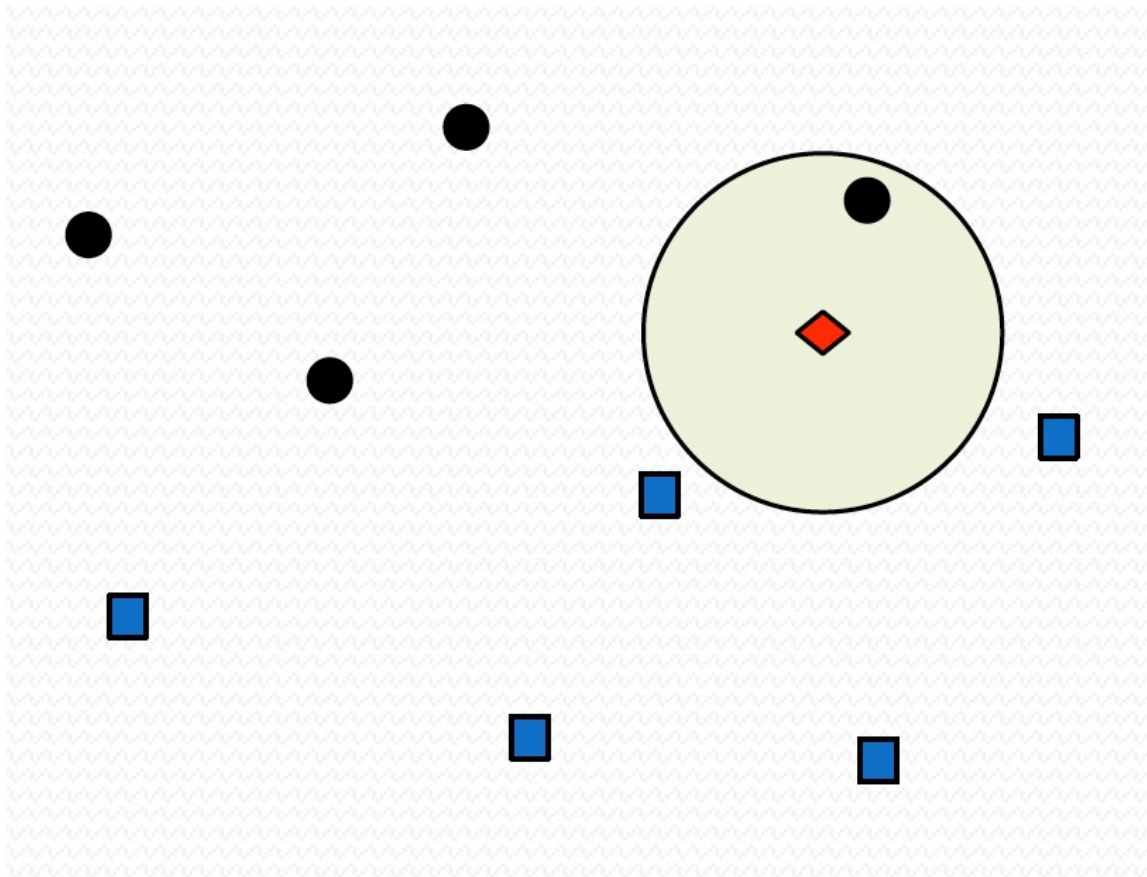
## ***$k$ -Nearest Neighbors ( $k$ -NN)***

# Instance-Based Learning

- ▶ Knn works like a classifier in supervised mode.
  - ▶ Have training examples:  $(x_i, y_i), i=1, \dots, N$ 
    - ▶  $x_i$  could have discrete or real value
  - ▶ Try to predict the class for new example  $x$ 
    - ▶  $y=f(x) \in \{C_1, \dots, C_c\}$
- ▶ 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 similarity?
  - ▶ How many similar training examples to consider?
  - ▶ How to resolve inconsistencies among the training examples?

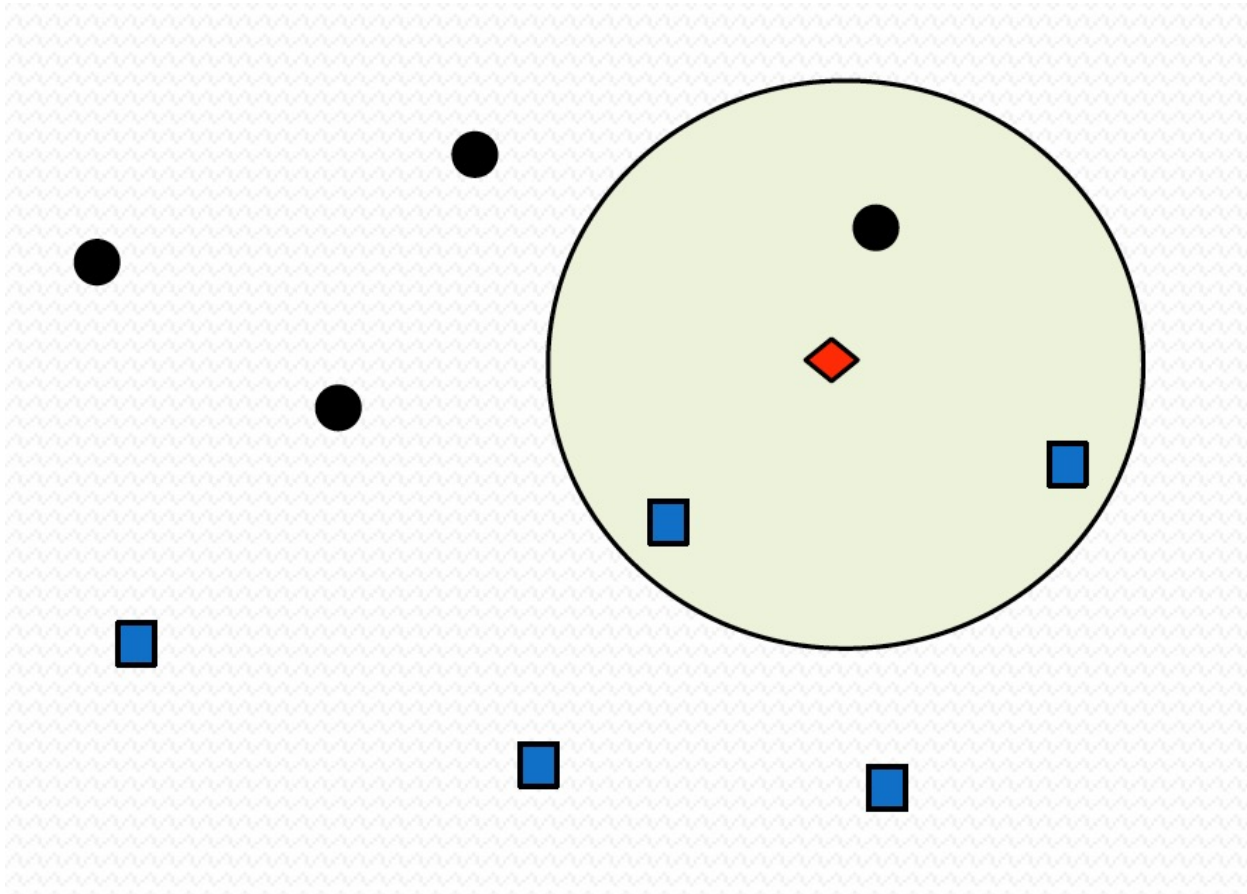
# 1-Nearest Neighbor

- ▶ 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  $k$  nearest neighbors



# K-Nearest Neighbors (KNN)

- ▶ K-Nearest neighbour:
  - ▶ Given a query instance  $x$ ,
  - ▶ First locate the  $k$  nearest training examples  $x_1, x_2, \dots, x_k$
- ▶ Classification:
  - ▶ Discrete values target function
  - ▶ Take vote among its  $k$  nearest neighbors
- ▶ Regression
  - ▶ Real valued target function
  - ▶ Take the mean of the  $f$  values of the  $k$  nearest neighbors
- ▶ Remember. We have to answer to:
  1. How to determine similarity?
  2. How many similar training examples to consider?
  3. How to resolve inconsistencies among the training examples?

# 1. How to determine similarity?

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

- ▶ It's from 'distance properties'
  - ▶ Non-negative:  $d(i, j) \geq 0$
  - ▶  $d(i, i) = 0$
  - ▶ Symmetry:  $d(i, j) = d(j, i)$
  - ▶ Triangle inequality:  $d(i, k) \leq d(i, j) + d(j, k)$
- ▶ Some distance
  - ▶ Euclidian distance:  $d(x, y) = \sqrt{\sum (x_i - y_i)^2}$
  - ▶ Manhattan distance ("city-block"):  $d(x, y) = \sum |x_i - y_i|$
  - ▶ Uniform or weighted distance
    - ▶ Weighted: assign weights to the neighbors based on their "distance" from the query point
      - Generally  $\text{weight} = 1/\text{distance}$

# 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.

- ▶  $d_{i,j} = \sqrt{\sum (x_i - x_j)^2}$

- ▶ An example

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

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

# 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)	<b>960</b>	<b>1</b>
d(Sam, Miranda)	1 141	2
d(Miranda, Carry)	2 101	3

**With normalized features**

	distance	rank
d(Carry, Sam)	1,1	<b>3</b>
d(Sam, Miranda)	<b>0,73</b>	<b>1</b>
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!

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

- ▶ Try to use more neighbours
- ▶ But give less weight to the far neighbours compared to the close neighbours
- ▶ Hard to tune to!

# K-Nearest Neighbors in python

- ▶ `from sklearn.neighbors import KNeighborsClassifier`
  - ▶ 3 main parameters
    - ▶ Choose the neighbors: `n_neighbors` (k)
    - ▶ Choose the distance: `p` (power):  $(\sum |a_i - b_i|^p)^{1/p}$  for Minkowski distance
      - `p==1`: Manhattan
      - `p==2`: Euclidian
    - ▶ Choose the proximity weight
      - with weight ('distance') or without ('uniform')
- ▶ `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)`

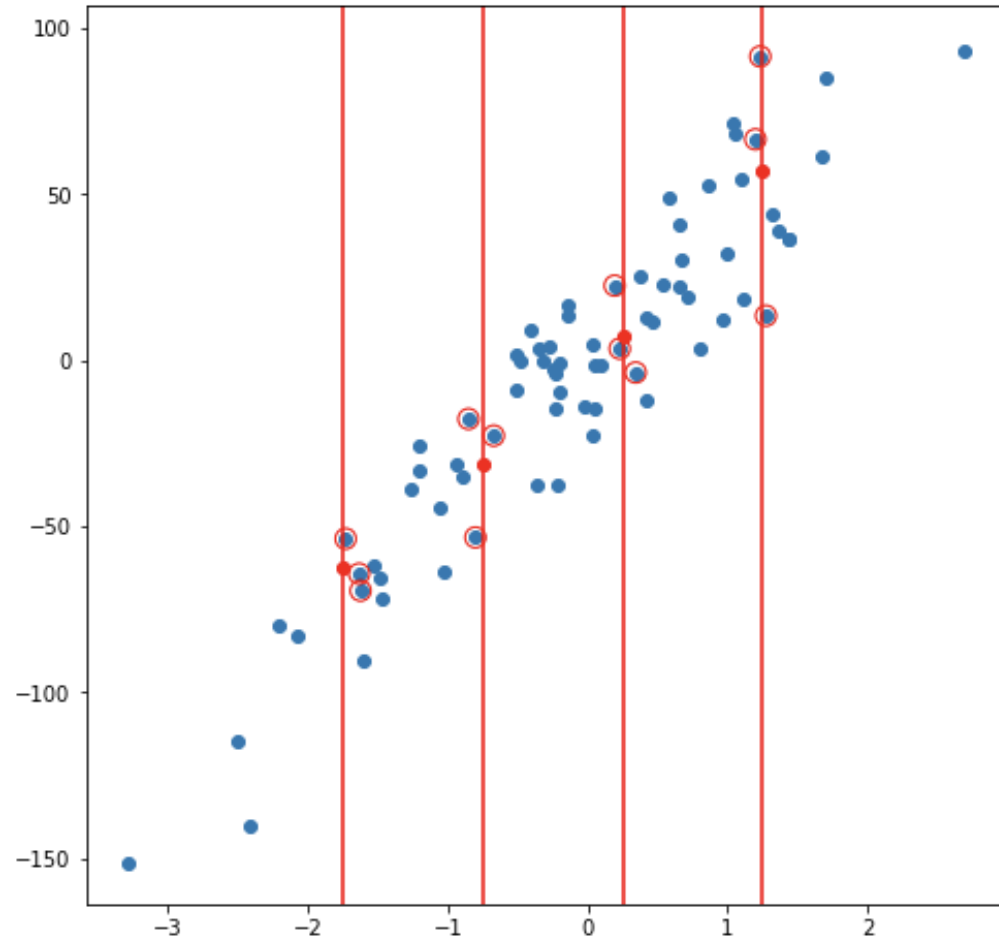
# K-Nearest Neighbors in python

## Other parameters

- ▶ **Weights** {'uniform', 'distance'} or callable, default='uniform'
  - ▶ weight function used in prediction.
- ▶ **Algorithm** {'auto', 'ball\_tree', 'kd\_tree', 'brute'}, default='auto'
  - ▶ Algorithm used to compute the nearest neighbors:
  - ▶ 'ball\_tree' will use [BallTree](#)
  - ▶ 'kd\_tree' will use [KDTree](#)
  - ▶ 'brute' will use a brute-force search.
  - ▶ 'auto' will attempt to decide the most appropriate algorithm based on the values passed to [fit](#) method.
- ▶ **leaf\_size**, default=30
  - ▶ Leaf size passed to BallTree or KDTree.
- ▶ **metric** {str or callable}, default='minkowski'
  - ▶ the distance metric to use for the tree. The default metric is minkowski, and with p=2 is equivalent to the standard Euclidean metric.
- ▶ **metric\_params**, default=None
  - ▶ Additional keyword arguments for the metric function.
- ▶ **n\_jobs**, default=None
  - ▶ The number of parallel jobs to run for neighbors search.

# Regression with k-NN

- ▶ Exactly the same approach
- ▶ use the neighbor label value to calculate the value of a new point



- ▶ `from sklearn.neighbors import KNeighborsRegressor`

# PRO of k-NN

- ▶ Highly efficient inductive inference method for noisy training data and complex target functions
- ▶ Learning is very simple
- ▶ 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 neighbours
- ▶ 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)
- ▶ **It's an excellent algorithm for replacing missing values...**

# CONS of k-NN

- ▶ Need a distance that "matches" the target function, possibly the distance depends on the feature
- ▶ k-NN must read the whole dataset for each prediction. Very expensive for large datasets
- ▶ **k-NN works well with a small number of features**
  - ▶ but the accuracy degrades as the number increases.
- ▶ **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.

# Today lab.

- ▶ Part I. K-nearest neighbors for classification
  - ▶ Part II. K-nearest neighbors for regression
  - ▶ Part III. K-nearest neighbors from scratch
  - ▶ Part IV. Your work
    - I. Impute missing and build knn model
      - ▶ Plot confusion matrix
      - ▶ Print classification report
      - ▶ find the previous values from the confusion matrix (put the formulas in a commented cell)
  - ▶ Part V. Papers reading
- Read and understand the code
- Read the code later
- Put comments on your notebook
- Lab part
- Read at least the first 2 papers before the next class