Scikit-learn and Tour of Classifiers

K-Nearest Neighbors

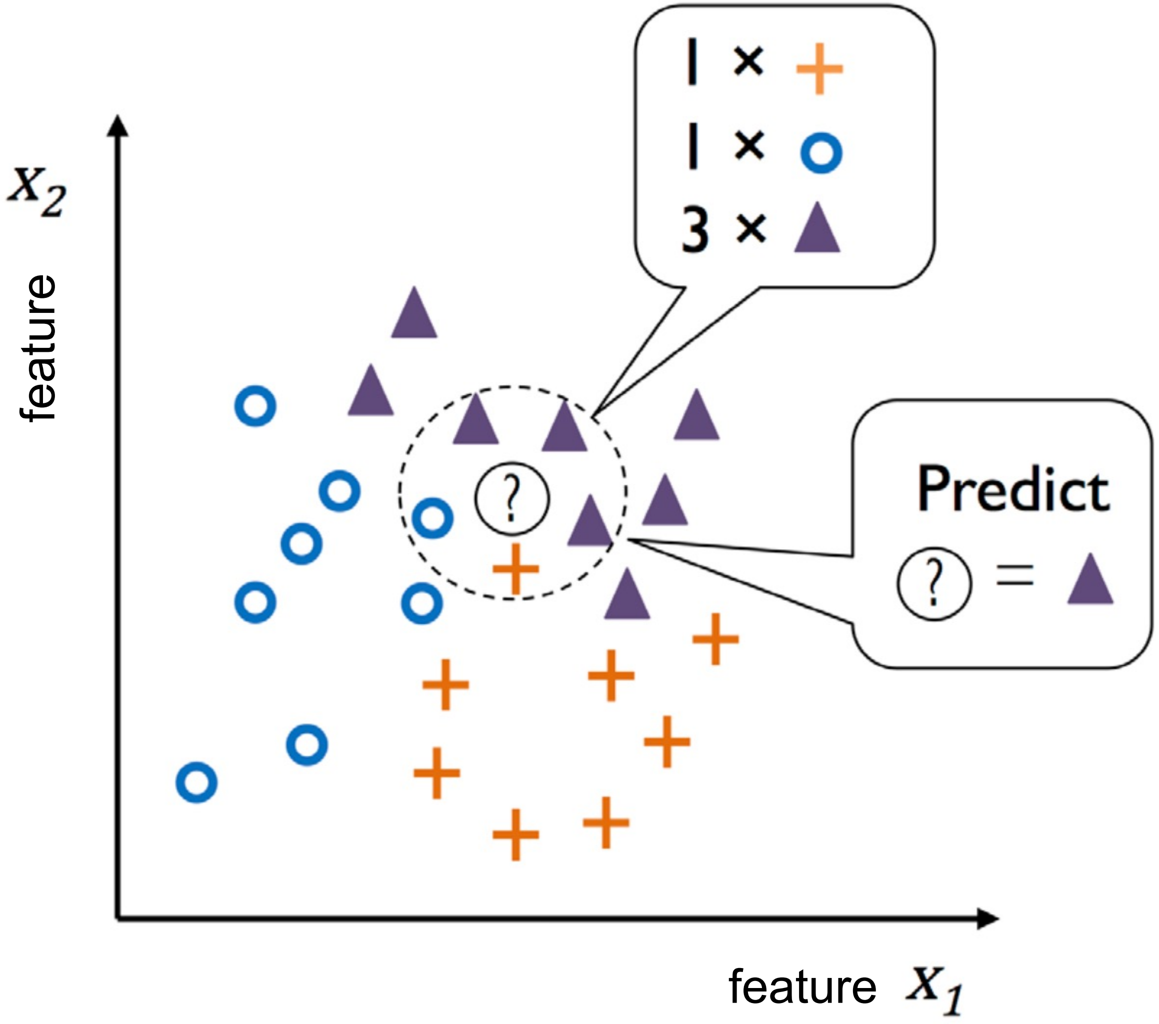
K-Nearest Neighbors

- Fundamentally different algorithm from what we learned so far
- Does not learn a discriminative function
- Memorizes the training data set and makes prediction based on that

K-Nearest Neighbors – Algorithm

1. Choose parameter ”**k**” and a **distance metric**
2. Find the k-nearest neighbors of a data record that we want to classify
3. Assign the class label by majority vote
   - *Tie break*: take the class of the closest neigbor and if still tied use lowest label

K-Nearest Neighbors – Algorithm



Example: 5-nearest neighbors of a new data record *(?)* that we want to classify

Figure from Python Machine Learning (Raschka & Mirjalili)

K-Nearest Neighbors – Distance metric

- A **distance metric** measures **distance** between two samples
- **Should fit the type of data**
- Common for real numbers: Euclidean distance

$$d\left(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}\right) = \sqrt[p]{\sum_k \left|x_k^{(i)} - x_k^{(j)}\right|^p}$$

Minkowski distance (used in scikit-learn K-NN)

p = 1

p = 2

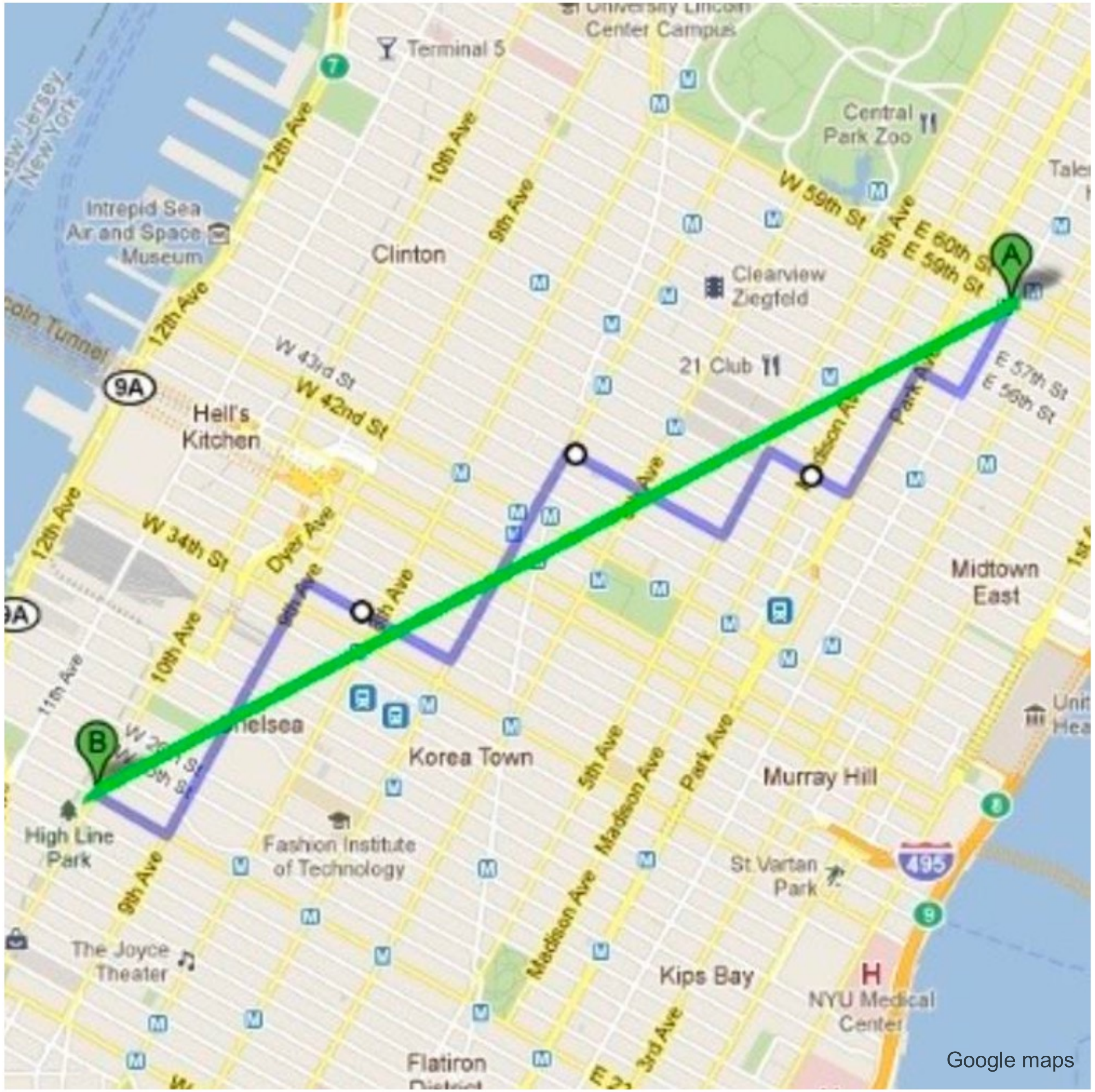
$$\sum_k \left|x_k^{(i)} - x_k^{(j)}\right|$$

Manhattan distance

$$d\left(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}\right) = \sqrt{\sum_k \left|x_k^{(i)} - x_k^{(j)}\right|^2}$$

Euclidean distance

- Euclidean distance
- Manhattan distance



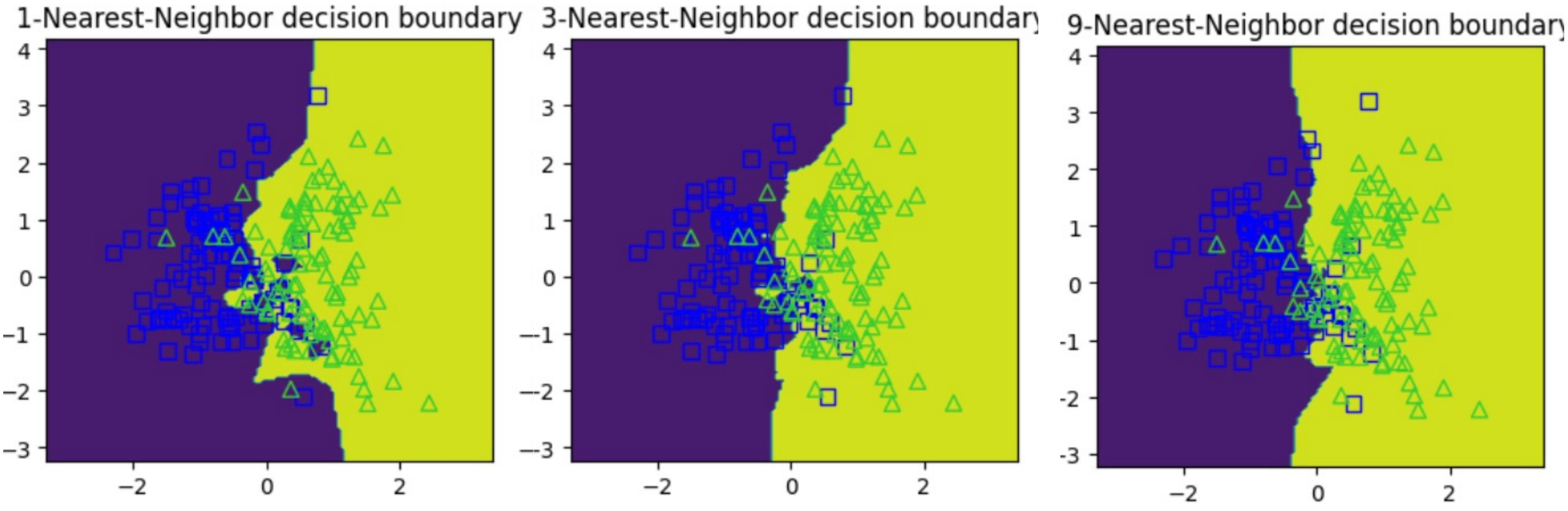
K-Nearest Neighbors

- Tuning **k** (and distance metric) is crucial to find a good balance between overfitting and underfitting
  - Lower **k** means that the model is more complex and has higher variance
  - Higher **k** means less variance (consulting more neighbors) but higher bias (far away neighbors might be consulted)
  - Higher **k** means that prediction becomes more costly

K-Nearest Neighbors

`03_knn.ipynb`

- Code example, testing accuracy on test/train set for different **k**



Parametric versus non-parametric models

Parametric versus non-parametric models

- **Parametric models**
  - Learn **parametrized** discriminative functional (fixed set of parameters)
  - Predict/classify new points **without need for** the training data
  - Examples: Perceptron, Adaline, Linear Regression, Logistic Regression, (*linear* SVM)
- **Non-parametric models**
  - No fixed set of params, no. of parameter **changes with amount of training data**
  - Training data (at least a subset) is needed for prediction
  - Examples: Decision trees, most kernel machines (Kernel-SVM, Kernel-Perceptron, …)

Some advantages and disadvantages of a memory-based non-parametric approach like K-NN

- Advantages:
  - Low (or zero) cost adaption to new training samples
  - Good predictive vs computational performance for small to medium-sized data sets
- Disadvantages:
  - Storage and prediction cost grows with the number of samples (prediction cost can be lowered by using efficient data structures, e.g. k-d trees for K-NN)
  - **Curse of dimensionality** → for a high number of features, prone to overfitting, no other training sample may be informative due to increasingly sparse feature space population with increasing dimension (number of features)

Concluding tour of classifiers

Tour of classifiers

- Learned about a number of popular classifiers for tackling linear and nonlinear classification problems; some insights into the corresponding algorithms; how to use them in sci-kit learn
- **Logistic regression:** allows for predict the probability of a particular event
- **Support vector machines:** powerful linear models; extended to non-linear problems using the kernel trick; several parameters need to be tuned to make good predictions
- **Decision trees:** easy to interpret, implicitly select features
- **Random forest:** Ensemble method; little parameter tuning; Doesn’t overfit as easily as decision trees; attractive and performant (easy parallelization) for many practical problems
- **K-NN:** Lazy learner; predictions can be expensive; good in low dimensions; susceptible to overfitting in high dimensions

Tour of classifiers (sci-kit learn)

- Scit-kit learn has an overview on **supervised learning and classification**
- **Perceptron:** `from sklearn.linear_model import Perceptron`
- **Logistic regression:** `from sklearn.linear_model import LogisticRegression`
- **Support vector machines:** `from sklearn.svm import SVC`
- **Decision trees:** `from sklearn.tree import DecisionTreeClassifier`
- **Random forest:** `from sklearn.ensemble import RandomForestClassifier`
- **K-NN:** `from sklearn.neighbors import KNeighborsClassifier`

Tour of classifiers

- Apply **several** classifiers to problem at hand – **no classifier is superior** in **all** situations for **all types** of data (*no-free-lunch theorem*)
- Importance of **training data** → **no algorithm** will be able to make **good predictions without informative** and **discriminatory features**

→ Next topic in class: Building a good dataset – Pre-processing and Feature selection