# K-nearest neighbours

## Advanced Topics in High-Performance Computing

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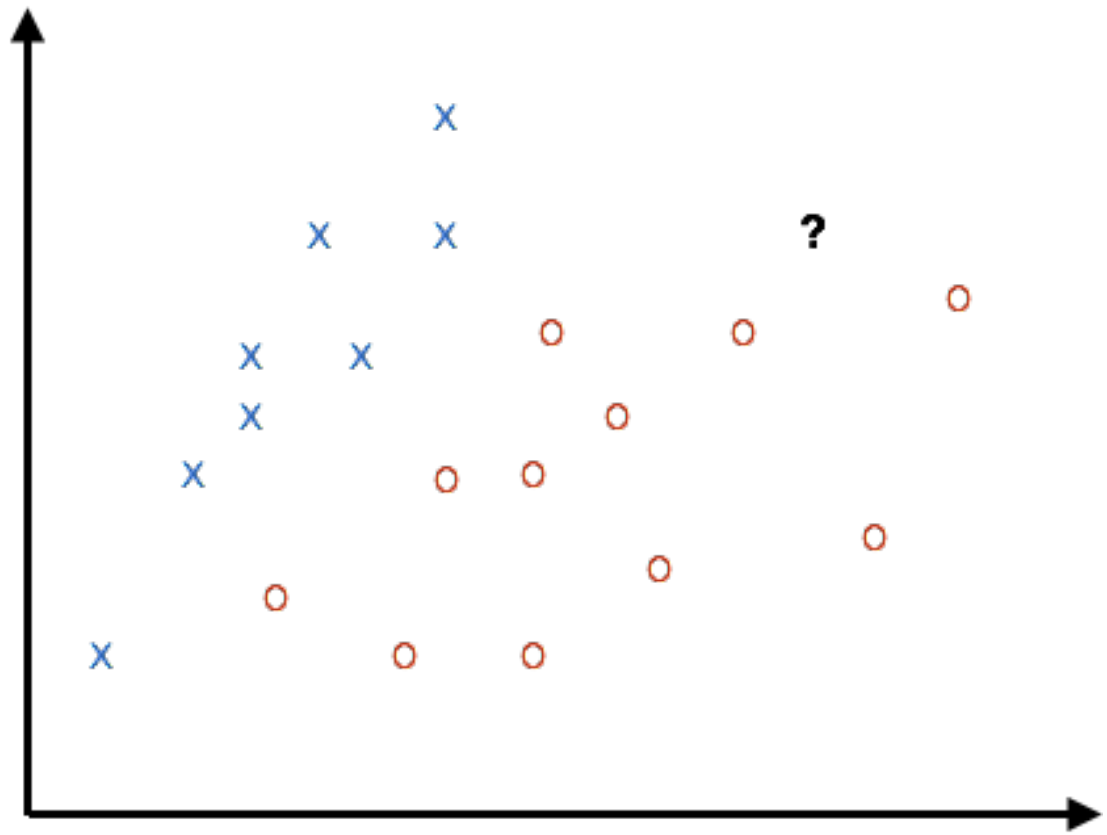
# Classification

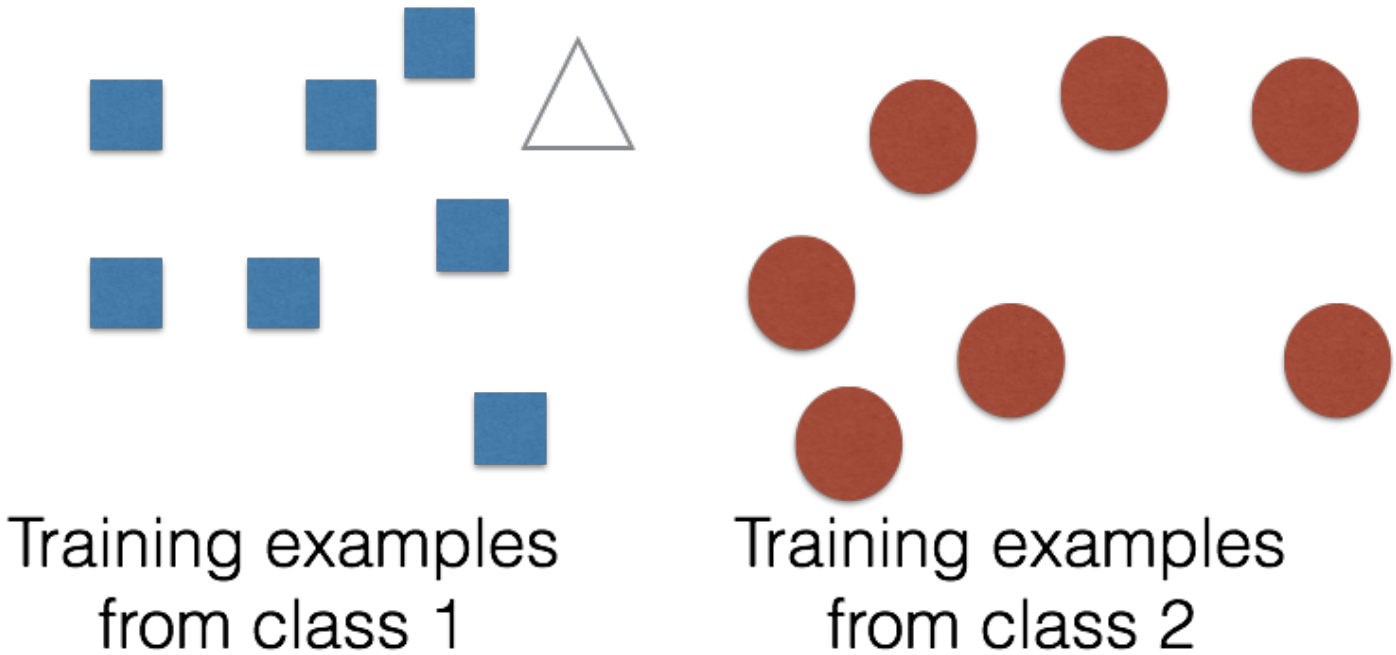
Given some data with corresponding labels, learn a function to predict a previously unseen data point.

Given data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)$, learn a function $y = f(\mathbf{x})$ that predicts the label $y$ for a previously unseen example $\mathbf{x}$. *For the following example,* $y_i \in \{0, 1\}$.



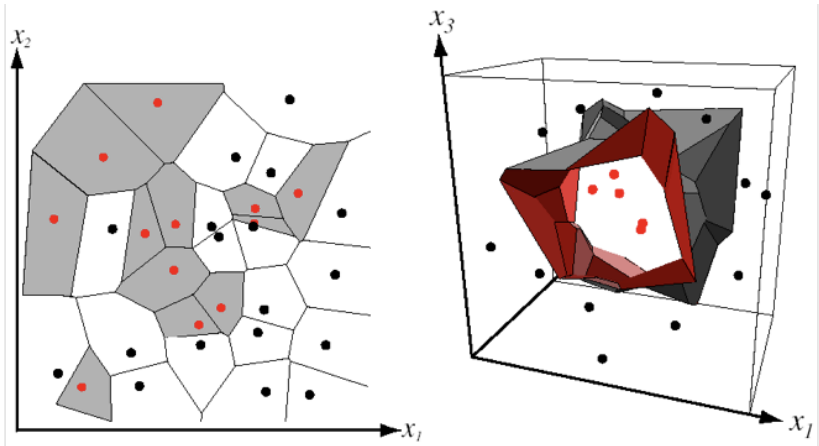
# K-nearest neighbour

Prediction function: label of the nearest training example.



# K-nearest neighbour

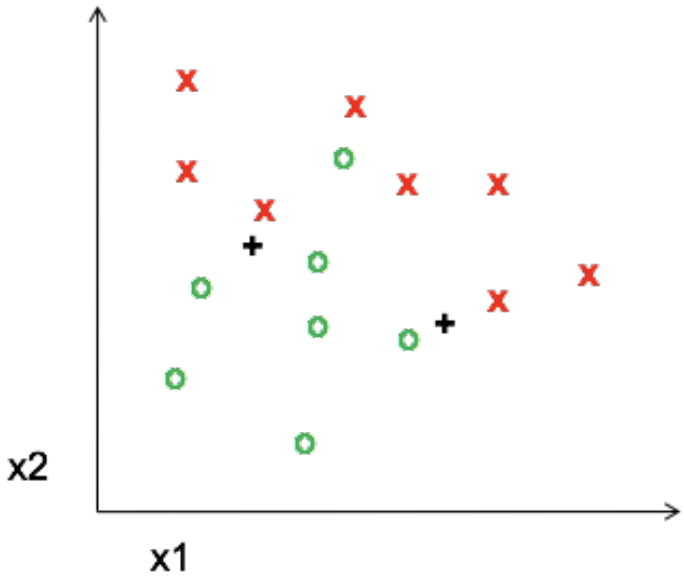
- No training needed
- Need to store the entire training set
- Need a distance function to compute the similarity between the new data point (the query) and those in training set

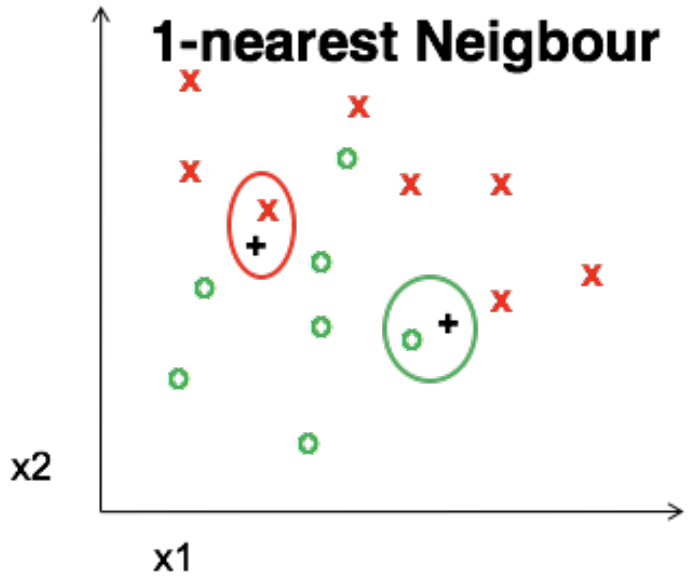


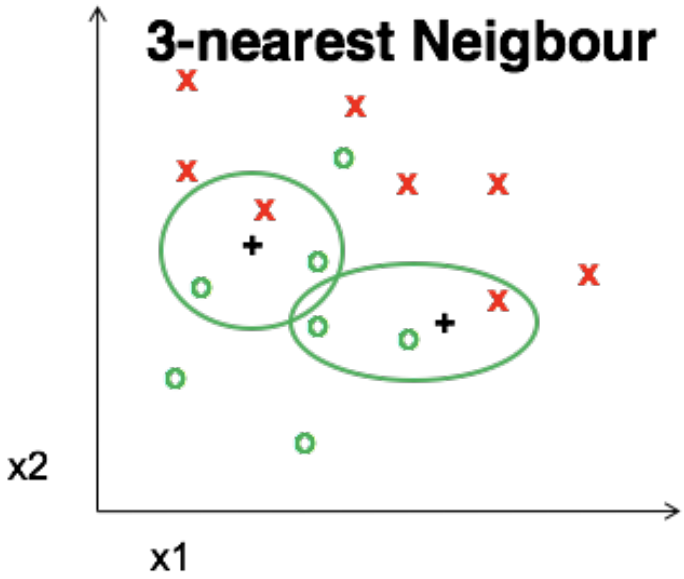

Voronoi partitioning of feature space for two-category 2D and 3D data

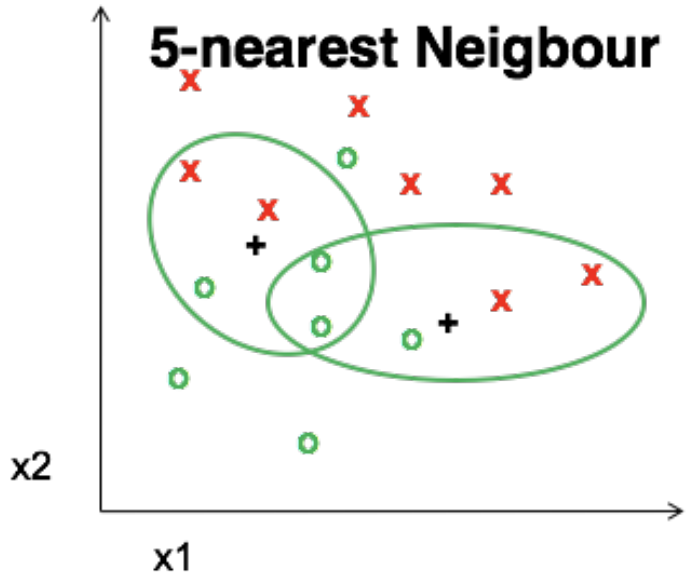
(Duda et al.)

# K-nearest neighbour



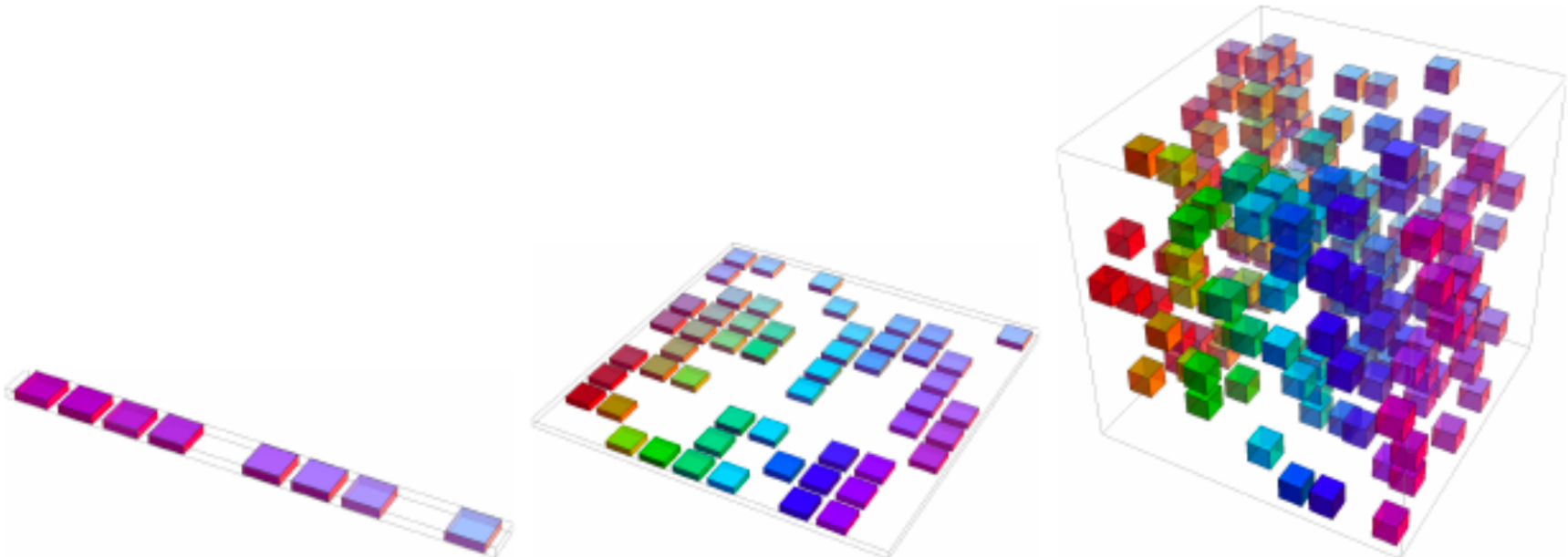



# K-nearest neighbour discussion

- K-nearest neighbour is a *non-parametric* learning algorithm that can be used for both classification and regression.
- K-nearest neighbour can achieve very high capacity
  - This implies that K-nearest neighbour can achieve very low training error, albeit at a very high computational cost
  - This also means that K-nearest neighbour may generalize very poorly
- K-nearest neighbour is also unable to learn if one feature is more discriminative than another feature.
- Reliance on local constancy
  - We shall see that many machine learning algorithms suffer from smoothness prior, and thus these fail on AI-level tasks, such as image recognition. Deep learing is in part motivated to relax local constancy and smoothness prior assumptions.

# Curse of dimensionality

- As the dimensions of the data increases, the number of configurations of interest often grows exponentially.



Curse of dimensionality (Goodfellow et al., 2017)

# Summary

We looked at K-nearest neighbour for classification and regression. K-nearest neighbour is a non-parametric learning algorithm with very high capacity, which leads to very low (zero, really) training error, but very high test errors. K-nearest neighbour suffers from the *curse of dimensionality*.

## Implementaion

Check out the Python Sklearn module, which implements k-nearest neighbour classification and regression:

- http://scikit-learn.org/stable/modules/neighbors.html

## Readings

- Sec. 5.7.3, Goodfellow, et. al., 2017