

# Generic Machine Learning

Clustering and Classification

*TCTI-VKAAI-17: Applied Artificial Intelligence*

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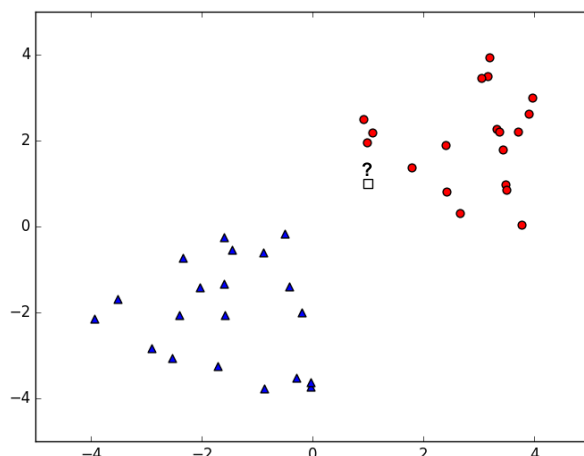
## Classification

- The problem of identifying to which set of categories a new observation belongs
  - On the basis of a training data set containing observations whose category is known
- Examples:
  - Spam filtering, Optical Character Recognition (OCR), Search Engines, Computer Vision

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## Intuition of Classification



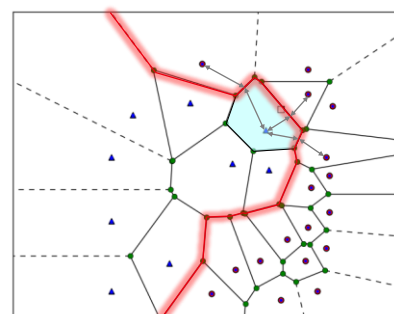
- Set of points  $(x,y)$ 
  - Two classes (red / blue)
- Is the box red or blue?
- How did you do it?
  - Calculate prior?
  - Gaussian probability?
- Nearby points are red
  - Use as basis for learning algorithm

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## Nearest Neighbor Classification

- Use the intuition to classify new point  $x$ :
  - Find the most similar training example  $x'$
  - Predict its class  $y'$
- Voronoi tessellation
  - Partitions in space into regions
  - Boundary: points at same distance from two different training examples
- Classification boundary
  - Non-linear, reflects classes well
  - Impressive for simple method

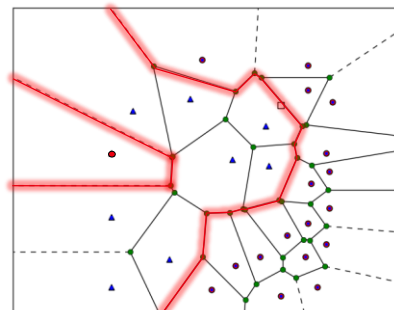


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## Nearest Neighbor: Outliers

- Algorithm sensitive to outliers
  - Single mislabeled example dramatically changes boundary
- Overfitting
  - Boundary exactly follows your training data
- Idea:
  - Use more than one nearest neighbor to make decision
  - Count class labels in  $k$  most similar training examples
    - Many “triangles” will outweigh single “circular” outlier



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## kNN Classification Algorithm

- Given:
  - Training examples  $\{x_i, y_i\}$ 
    - $x_i$  ... attribute-value representation of examples
    - $y_i$  ... class labels: {ham, spam}, digit {0, 1, ..9} etc.
  - Testing point  $x$  that we want to classify
- Algorithm:
  - Compute distance  $D(x, x_i)$  to every training example  $x_i$
  - Select  $k$  closest instances  $x_{i_1}, \dots, x_{i_k}$  and their labels  $y_{i_1}, \dots, y_{i_k}$
  - Output the class  $y^*$  which is most frequent in  $y_{i_1}, \dots, y_{i_k}$

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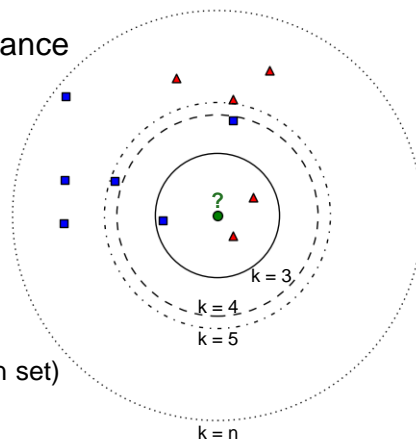
## Choosing value of k

- Value of k has strong effect on kNN performance

- Large value  $\rightarrow$  everything classified as most frequent class in training set
- Small value  $\rightarrow$  highly variable, unstable decision boundaries
  - Small changes to training set  $\rightarrow$  large changes in classification
  - Affects 'smoothness' of the boundary

- Selecting the value of k

- Set aside a portion of the training data (validation set)
- Vary k, observe training  $\rightarrow$  validation error
- Pick k that gives best generalisation performance



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## Training & Validation Data

- A common method to validate the performance of machine learning algorithms

- Split available set of data into
  1. Training Data
  2. Validation Data
- Train algorithm on Training Data
- Use Validation Data to see how well the algorithm performs on 'new' cases.

- Why should you never validate on training data?

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## Practical Issues of kNN

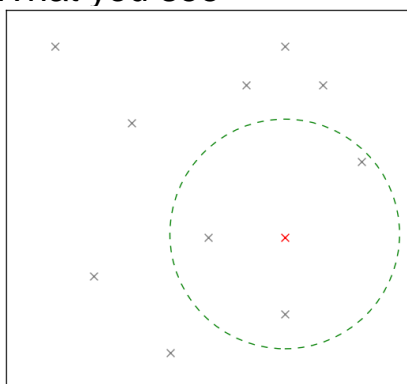
- Resolving ties:
  - Equal number of positive/negative neighbors
  - Use odd k (does not solve multi-class)
  - Breaking ties:
    - Random: flip a coin
    - Prior: pick the most common class
    - Nearest: use 1-nn classifier to decide
- K-Nearest Neighbors is a **slow** mechanism!

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## Why is kNN slow?

- What you see



Find nearest neighbors  
of testing point (red)

- What the algorithm sees

```
data = np.array([
    (1, 9), (2, 3), (4, 1), (3, 7),
    (5, 4), (6, 8), (7, 2), (8, 8),
    (7, 9), (9, 6)
])
testPoint = (7, 4)
```

- Nearest neighbors?
  - Compare one-by-one to each training instance
- n comparisons
- Each takes d operations

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## Making kNN fast

- Reduce dimensions
  - Simple feature selection (throw away attributes that do not look promising)
- Reduce number of examples
  - Idea: quickly identify  $m \ll n$  potential near neighbors
  - Compare only to those neighbors