Machine Learning

Non-parametric Classification: k-NN Method and its variants. Common Metrics. Classification Mean Error.

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1. Classification Mean Error
2. Euclidean and Manhattan Distance
3. 1-NN

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6. Template Selection

Mean error

- X – set of objects descriptions, Y – set of objects labels
- Unknown target dependency: mapping $y : X \to Y$
- Finite training set: $X^m = \{(x_1, y_1), \ldots, (x_m, y_m)\}$, so as $y_i = y(x_i)$
- Finite test set: $X_t^q = \{(x_1, y_1), \ldots, (x_q, y_q)\}$, so as $y_i = y(x_i)$

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Mean error for classification

The main goal is to train an algorithm $a : X \to Y$ on the train set X^m so as the **mean error** on the test set is minimal: $R(a, X_t^q) = \frac{1}{q}\sum_{i=1}^{q}[a(x_i) \neq y(x_i)] \to min_a$

Common metrics

- Object $x \in X$ is represented in the R^n space: $x = (x^1, \dots, x^n)$ — n-dimensional vector
  - E.g., points on the XY-plane are from R^2: $x = (x_1, x_2)$

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Euclidean metric

Euclidean, or L_2-distance, between 2 points x and y from R^n is:
$d_2(x, y) = ||x - y||_2 = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$

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Manhattan metric

Manhattan, or L_1-distance, between 2 points x and y from R^n is:
$d_1(x, y) = ||x - y||_1 = \sum_{i=1}^n |x_i - y_i|$

Parametric and non-parametric machine learning methods

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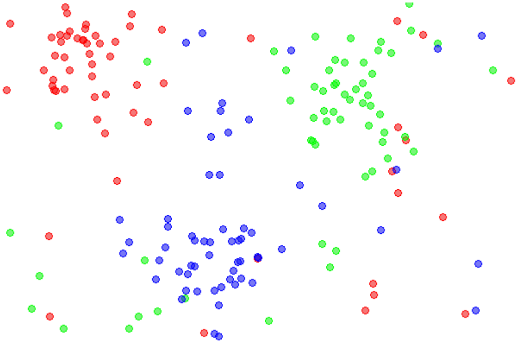
Non-parametric methods

Nonparametric methods are methods that are not parametric methods.

- Examples: Metric algorithms, kernel methods

Basic Assumption

- "Close" objects *usually* lie in the same class
- Proximity is specified by the metric
- Typical example [1]



[1] https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

Nearest neighbor (1-NN, NN) method

- Method parameter: metric
- Algorithm: using a given metric, we look for the nearest object in the training set and classify the object with the same class as the found nearest neighbor

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Disadvantages

- Instability to outliers
- Ambiguity of classification at equal distances to two objects
- The need to store the entire training set
- The search algorithm is computationally complex (if the training sample is quite large)
- Distance value is not taken into account

k-nearest neighbors (k-NN, kNN) method

- Method parameter: metric, **k**
- Algorithm: using a given metric, we search for the **k** closest objects in the training set and classify the object as the **majority class** of the **k** objects

Advantages

- Ease of implementation
- Good interpretability
- Parameter **k** can be optimized using cross-validation

Disadvantages

- ~~Instability to outliers~~
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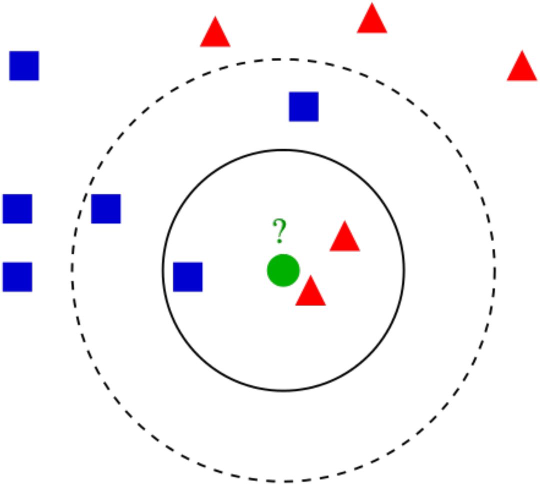
k-NN method



Weighted k-NN method

- Method parameters: metric, k, **weights**
- Algorithm: using a given metric, we look for the k closest objects in the training set and classify the object by weighted voting

Advantages

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- Parameter k can be optimized using cross-validation

Disadvantages

- ~~Instability to outliers~~
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- Fixed object weights

Weighted k-NN among a set of templates

- Method parameters: metric, k, weights, **template selection method**
- Algorithm: using a given metric, we look for the k closest objects among the templates selected from the training set and classify the object by weighted voting

Advantages

- Ease of implementation
- Good interpretability
- Parameter k can be optimized using cross-validation

Disadvantages

- ~~Instability to outliers~~
- ~~Classification ambiguity at equal distances to two objects~~
- ~~Need to store the entire training set~~
- ~~The search algorithm is computationally complex~~
- ~~Distance value is not taken into account~~

Template selection

Task

Get approximately the same quality of the algorithm with less stored data.
It is even possible to obtain an improvement in quality because outliers will be removed during the template selection process.

Ideas

- Object clustering
- Greedy algorithm

Template selection by k-means clustering method

Task

$$V = \sum_{i=1}^{k} \sum_{x \in S_i} (x - \mu_i)^2 \to \min_{S_i},$$

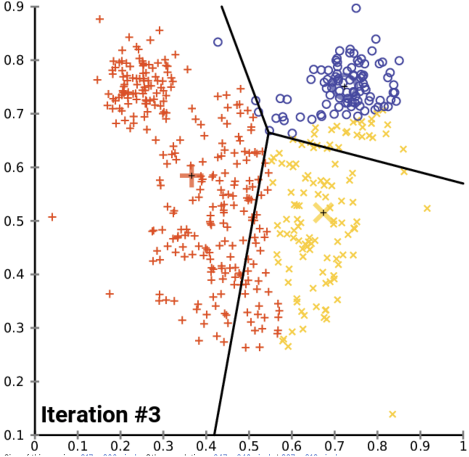
where k is the number of clusters, S_i is the resulting clusters, μ_i is the center of mass of the S_i cluster.

Algorithm

1. k elements are randomly selected from the sample and declared as centroids
2. For fixed **centroids**, each sample element belongs to one of the clusters
3. For fixed **clusters**, centroids are calculated
4. Steps 2 and 3 are repeated until convergence (or exhausting the computation/time budget)

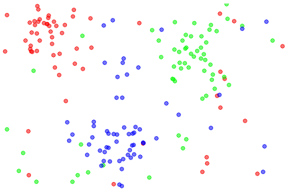
Visualization of k-means

Click to see the gif:



Examples of 1-NN w/o and w/ template selection

- 1st image: dataset
- 2nd image: 1-NN w/o template selection
- 3rd image: templates
- 4th image: 1-NN w/ template selection



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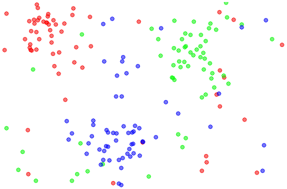
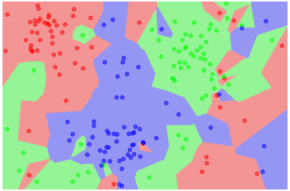

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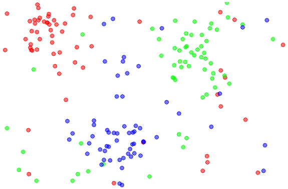

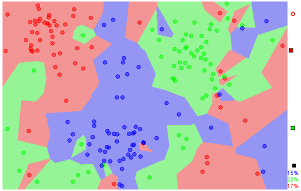

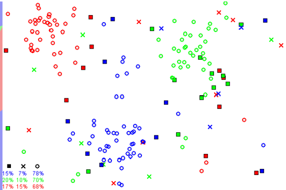

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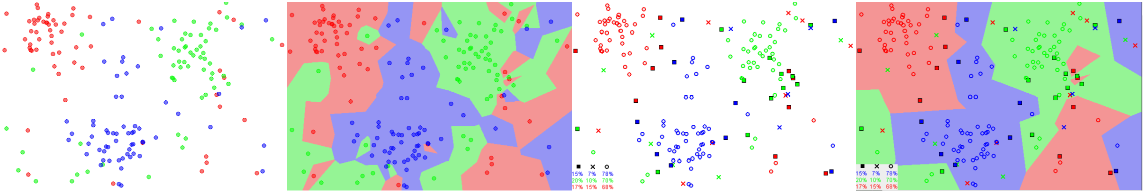

Additional modification: RadiusNN

Idea

Sometimes it makes sense to look for neighbors at a distance no greater than some radius r

Parameter r

Instead of the input parameter for the number of neighbors, the radius is used

Mandatory external links to read

1. Read the Introduction to K-Nearest Neighbor (kNN)
   - Main source ("*K Nearest Neighbor (KNN) in R*"section is fully optional)
   - Additional one (mostly section "*The KNN Algorithm*"), including the section 3.5 from **"The Hundred-Page Machine Learning Book"**(see "*References*" course page).

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- The method has a large number of variations for customization
  - Selection of metrics (metric learning)
  - Number of nearest neighbors
  - Weights in the weighted version of the method
  - Algorithm for selecting templates

Thank you!