Machine learning: Knn approaches

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Selected algorithms

- The **clustering algorithms**
- **The knn approach**
- **The randomforest classifier**
- The **support vector machine**
- **Neural network and Deep Neural Networks**

Intuition Behind K-Nearest Neighbors (KNN)

"Birds of a feather flock together."

- KNN is a **simple, intuitive** classification algorithm.
- Given a new data point, it looks at the **k closest points** in the training set.
- The **majority class** among those neighbors is assigned to the new point.
- It relies on the idea that **similar data points tend to be near each other**.

Key Concepts:

- Distance = similarity
- Decision is based on local neighborhood
- No training phase (lazy learning)

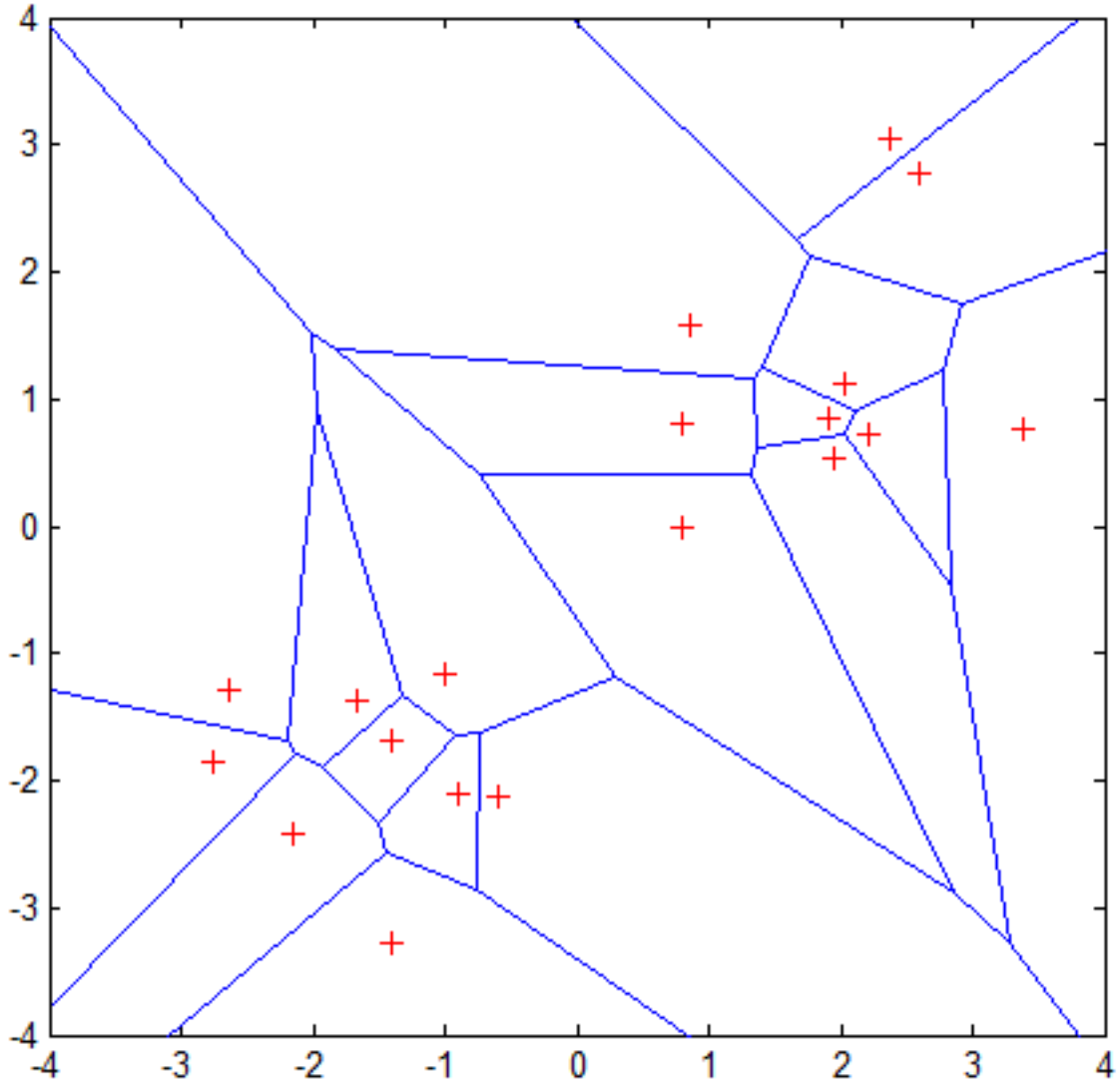
Instance based learning and knn

- Instance-based learning is often termed *lazy* learning, as there is typically no "transformation" of training instances into more general "statements"
- Instead, the presented training data is simply stored and, when a new query instance is encountered, a set of similar, related instances is retrieved from memory and used to classify the new query instance
- Hence, instance-based learners never form an explicit general hypothesis regarding the target function. They simply compute the classification of each new query instance as needed

k-NN Approach

- The simplest, most used instance-based learning algorithm is the *k*-NN algorithm
- *k*-NN assumes that all instances are points in some *n*-dimensional space and defines neighbors in terms of distance (usually Euclidean in R-space)
- *k* is the number of neighbors considered

Graphic Depiction



Properties:

1) All possible points within a sample's Voronoi cell are the nearest neighboring points for that sample

1) For any sample, the nearest sample is determined by the closest Voronoi cell edge

Basic Idea

- Using the second property, the *k*-NN classification rule is to assign to a test sample the majority category label of its *k* nearest training samples
- In practice, *k* is usually chosen to be odd, so as to avoid ties
- The *k* = 1 rule is generally called the nearest-neighbor classification rule

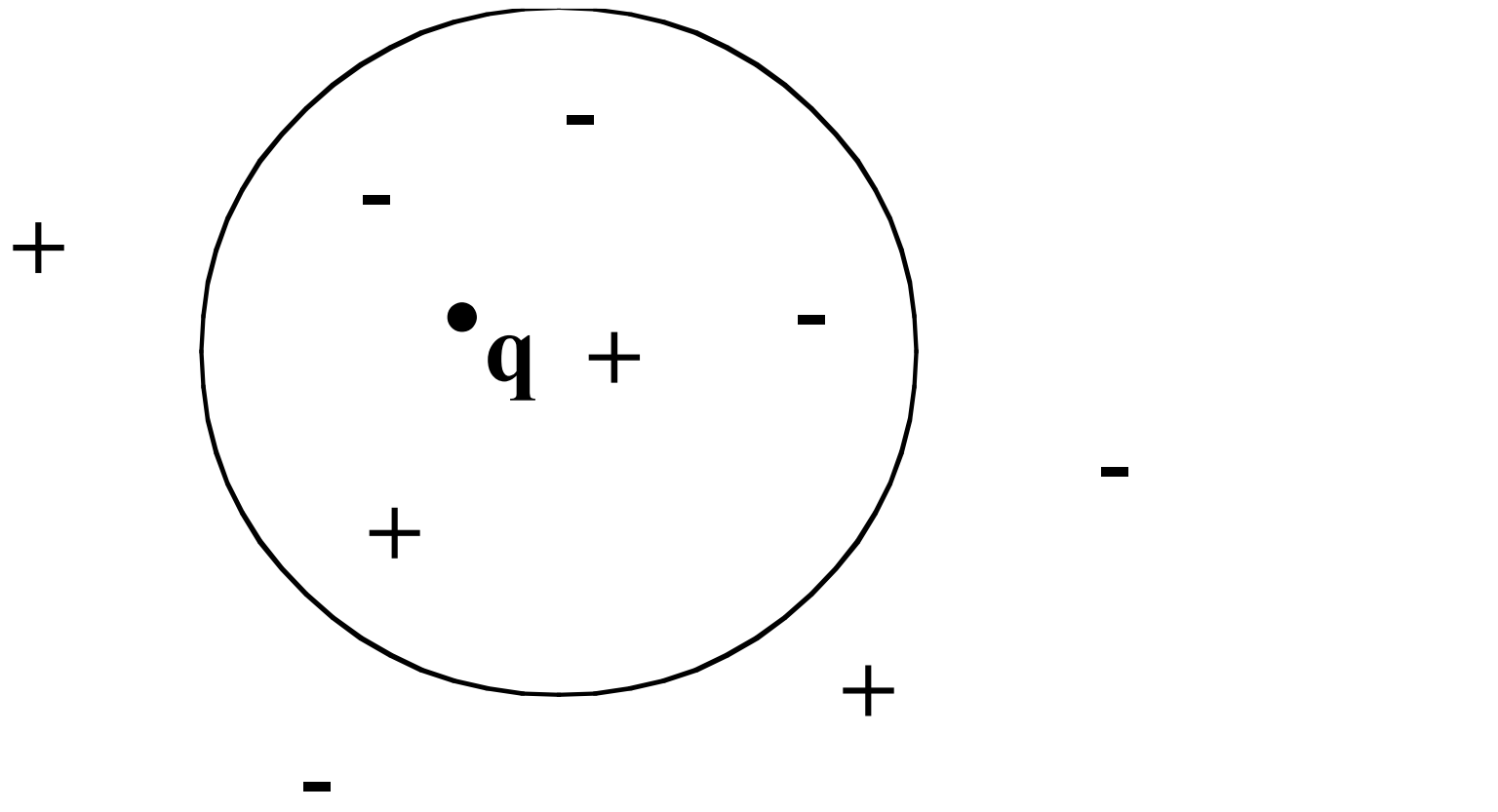
k-NN Algorithm

- For each training instance $t=(x, f(x))$
  - Add t to the set *Tr_instances*
- Given a query instance *q* to be classified
  - Let $x_1, \ldots, x_k$ be the *k* training instances in *Tr_instances* nearest to *q*
  - Return

$$\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} \delta(v, f(x_i))$$

- Where *V* is the finite set of target class values, and $\delta(a,b)=1$ if $a=b$, and 0 otherwise (Kronecker function)
- Intuitively, the *k*-NN algorithm assigns to each new query instance the **majority class among its *k* nearest neighbors**

Simple Illustration



q is + under 1-NN, but – under 5-NN

Distance-weighted *k*-NN

- Replace $\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} \delta(v, f(x_i))$ by:

$$\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} \frac{1}{d(x_i, x_q)^2} \delta(v, f(x_i))$$

Scale Effects

- Different features may have different measurement scales
  - E.g., patient weight in kg (range [50,200]) vs. blood protein values in ng/dL (range [-3,3])
- Consequences
  - Patient weight will have a much greater influence on the distance between samples
  - May bias the performance of the classifier

Standardization

- Transform raw feature values into z-scores

$$z_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j}$$

  - x_{ij} is the value for the i^{th} sample and j^{th} feature
  - μ_j is the average of all x_{ij} for feature j
  - σ_j is the standard deviation of all x_{ij} over all input samples
- Range and scale of z-scores should be similar (providing distributions of raw feature values are alike)

Distance Metrics

Minkowsky:

$$D(\boldsymbol{x},\boldsymbol{y}) = \left(\sum_{i=1}^{m} |x_i - y_i|^r \right)^{1/r}$$

Euclidean:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

Manhattan / city-block:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} |x_i - y_i|$$

Camberra:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{|x_i - y_i|}{|x_i + y_i|}$$

Chebychev:

$$D(\boldsymbol{x},\boldsymbol{y}) = \max_{i=1}^{m} |x_i - y_i|$$

Quadratic:

$$D(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x} - \boldsymbol{y})^T Q(\boldsymbol{x} - \boldsymbol{y}) = \sum_{j=1}^{m} \left(\sum_{i=1}^{m} (x_i - y_i) q_{ji} \right) (x_j - y_j)$$

Q is a problem-specific positive definite $m \times m$ weight matrix

Mahalanobis:

$$D(\boldsymbol{x},\boldsymbol{y}) = [\det V]^{1/m} (\boldsymbol{x} - \boldsymbol{y})^{\mathrm{T}} V^{-1} (\boldsymbol{x} - \boldsymbol{y})$$

V is the covariance matrix of $A_1..A_m$, and A_j is the vector of values for attribute j occuring in the training set instances $1..n$.

Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = \frac{\sum_{i=1}^{m} (x_i - \overline{x_i})(y_i - \overline{y_i})}{\sqrt{\sum_{i=1}^{m} (x_i - \overline{x_i})^2 \sum_{i=1}^{m} (y_i - \overline{y_i})^2}}$$

$\overline{x_i} = \overline{y_i}$ and is the average value for attribute i occuring in the training set.

Chi-square:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{1}{sum_i} \left(\frac{x_i}{size_{\boldsymbol{x}}} - \frac{y_i}{size_{\boldsymbol{y}}} \right)^2$$

sum_i is the sum of all values for attribute i occuring in the training set, and $size_{\boldsymbol{x}}$ is the sum of all values in the vector $\boldsymbol{x}$.

Kendall's Rank Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = 1 - \frac{2}{n(n-1)} \sum_{i=1}^{m} \sum_{j=1}^{i-1} \mathrm{sign}(x_i - x_j)\,\mathrm{sign}(y_i - y_j)$$

sign(x)=-1, 0 or 1 if $x < 0$, $x = 0$, or $x > 0$, respectively.

Figure 1. Equations of selected distance functions. ($\boldsymbol{x}$ and $\boldsymbol{y}$ are vectors of m attribute values).

Issues with Distance Metrics

- Most distance measures were designed for linear/real-valued attributes

- Two important questions in the context of machine learning:
  - How best to handle nominal attributes
  - What to do when attribute types are mixed

Some Remarks

- *k*-NN works well on many practical problems and is fairly noise tolerant (depending on the value of *k*)
- *k*-NN is subject to the curse of dimensionality (i.e., presence of many irrelevant attributes)
- *k*-NN needs adequate distance measure
- *k*-NN relies on efficient indexing

How is kNN Incremental?

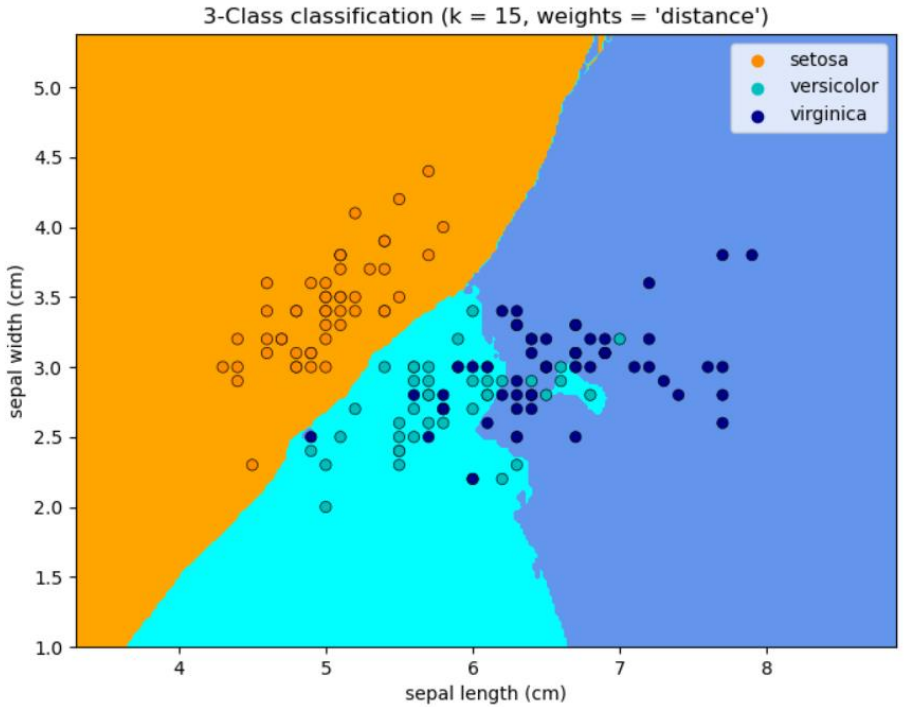
- All training instances are stored
- Model consists of the set of training instances
- Adding a new training instance only affects the computation of neighbors, which is done at execution time (i.e., lazily)
  - Note that the storing of training instances is a violation of the strict definition of incremental learning.

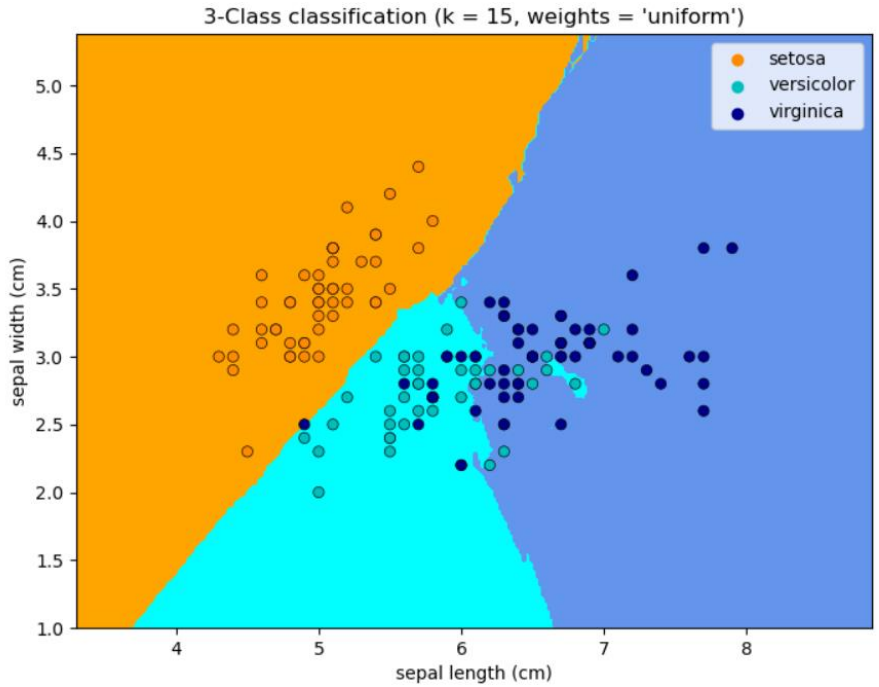
Predicting Continuous Values

- Replace $\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} w_i \delta(v, f(x_i))$

- Note: unweighted corresponds to $w_i=1$ for all i

$$\hat{f}(q) = \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$





Example of k nearest classification with the iris database

KNN (example in python)

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

# Load data
X, y = load_iris(return_X_y=True)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3)

# Train model
knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(X_train, y_train)

# Predict
y_pred = knn.predict(X_test)

# Evaluate
print("Accuracy:", accuracy_score(y_test, y_pred))
```