Nearest centroids, K-NN

Victor Kitov
v.v.kitov@yandex.ru

Yandex School of Data Analysis

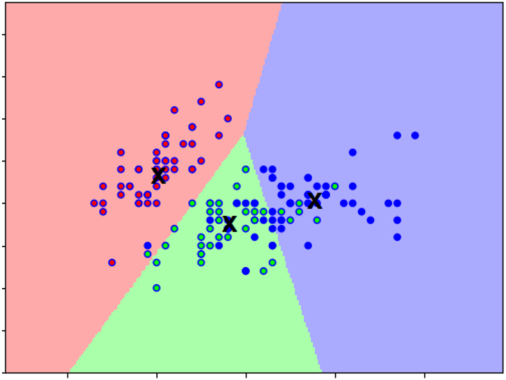
Table of Contents

Nearest centroids algorithm

- Consider training sample $(x_1, y_1), \dots (x_N, y_N)$ with
  - N_1 representatives of 1st class
  - N_2 representatives of 2nd class
  - etc.
- **Training:**
  Calculate centroids for each class $c = 1, 2, \dots C$:
  $$\mu_c = \frac{1}{N_1} \sum_{n=1}^{N} x_n \mathbb{I}[y_n = c]$$
- **Classification:**
  1. For object x find most close centroid:
     $$c = \arg\min_i \rho(x, \mu_i)$$
  2. Associate x the class of the most close centroid:
     $$\widehat{y}(x) = c$$

Illustration

Decision boundaries for 3-class nearest centroids



Questions

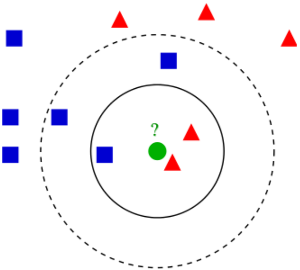
- What are discriminant functions $g_c(x)$ for nearest centroid?
- What is the complexity for:
  - training?
  - prediction?
- What would be the shape of class separating boundary?
- Can we use similar ideas for regression? Consider clustering.
- Is this method prone to the curse of dimensionality?

Table of Contents

K-nearest neighbours algorithm

Classification:

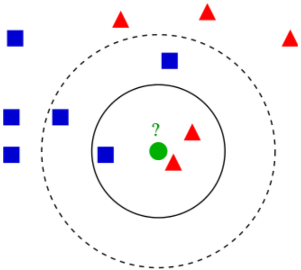
1. Find k closest objects to the predicted object x in the training set.
2. Associate x the most frequent class among its k neighbours.



K-nearest neighbours algorithm

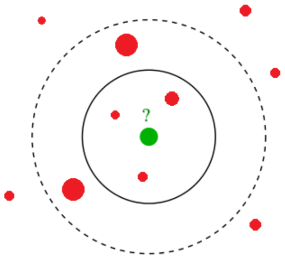
Classification:

1. Find k closest objects to the predicted object x in the training set.
2. Associate x the most frequent class among its k neighbours.



Regression:

1. Find k closest objects to the predicted object x in the training set.
2. Associate x average output of its k neighbours.

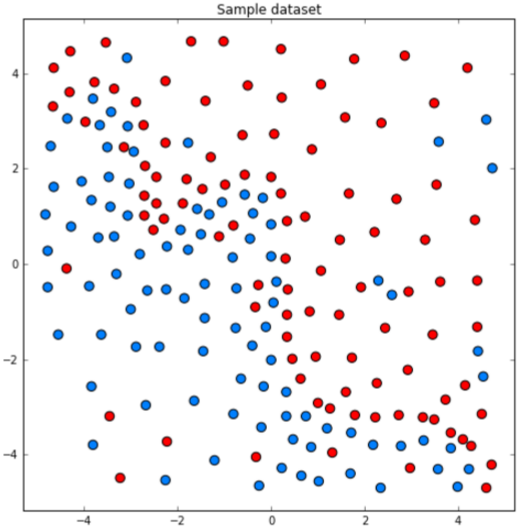


Comments

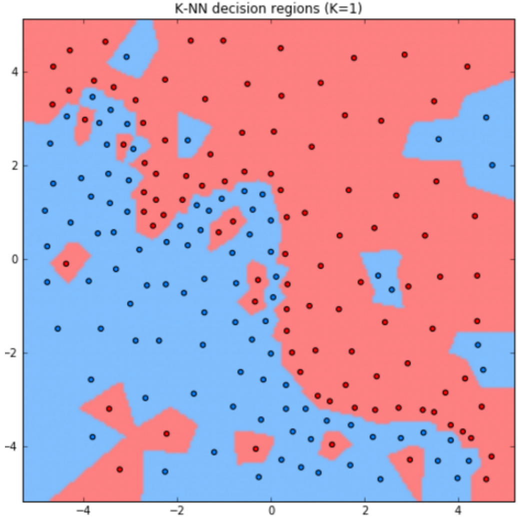
- K nearest neighbours algorithm is abbreviated as K-NN.
- $k = 1$: nearest neighbour algorithm[1]
- Base assumption of the method[2]:
  - similar objects yield similar outputs

[1] what will happen for $K = N$?
[2] what is simpler - to train K-NN model or to apply it?

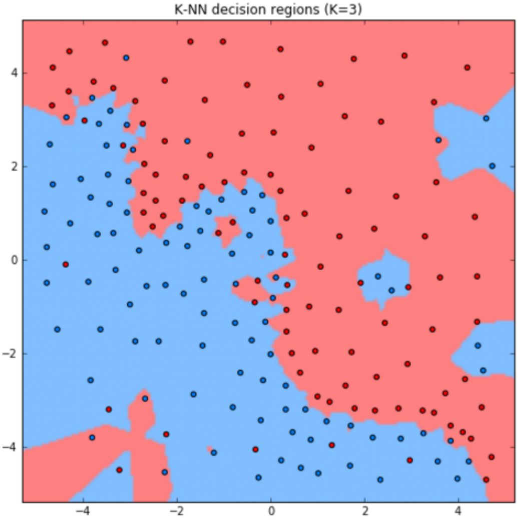
Sample dataset



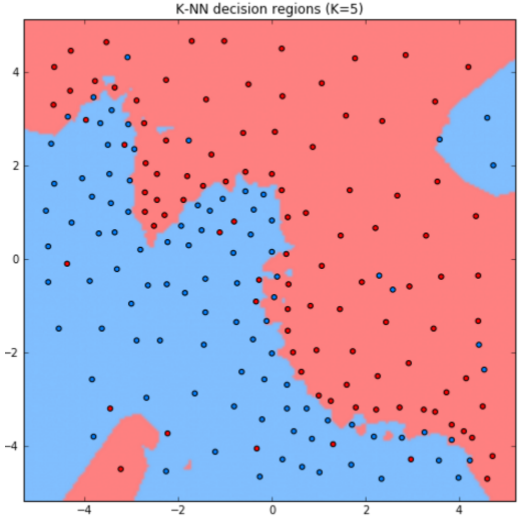
Example: K-NN classification



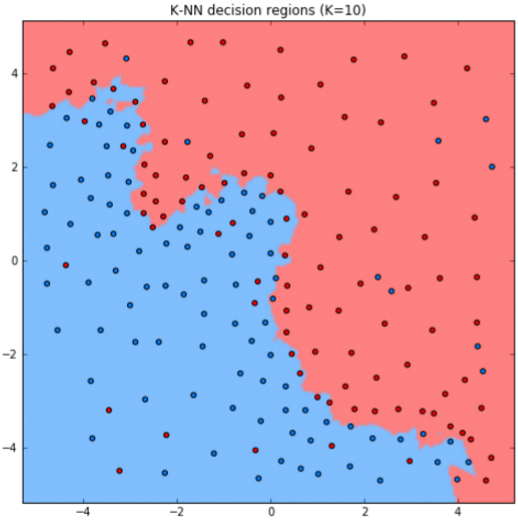
Example: K-NN classification



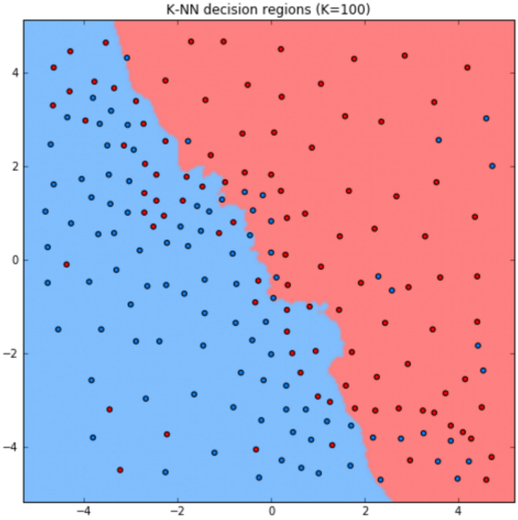
Example: K-NN classification



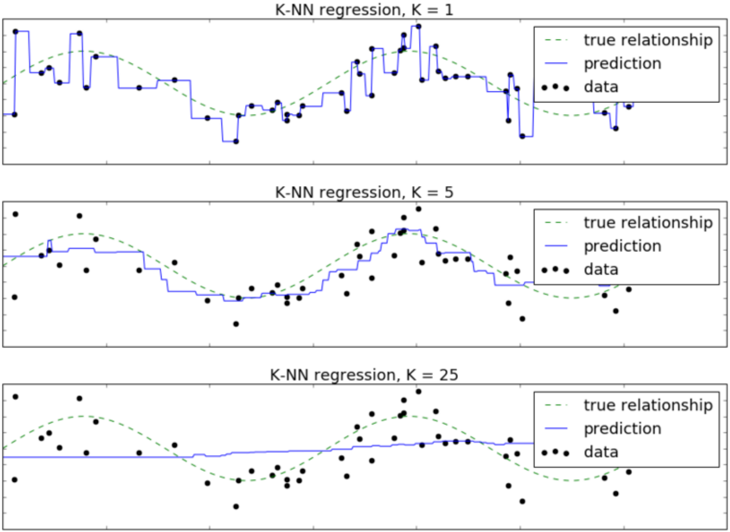
Example: K-NN classification



Example: K-NN classification



Example: K-NN regression



Dealing with similar rank

When several classes get the same rank, we can assign to class:

Dealing with similar rank

When several classes get the same rank, we can assign to class:

- with higher prior probability
- having closest representative
- having closest mean of representatives (among nearest neighbours)
- which is more compact, having nearest most distant representative

Parameters of the method

- Parameters:
    - the number of nearest neighbours K
    - distance metric $\rho(x, x')$
- Modifications:
    - forecast rejection option[3]
    - variable K[4]

[3] Propose a rule, under what conditions to apply rejection in a) classification b) regression

[4] Propose a method of K-NN with adaptive variable K in different parts of the feature space

Properties

- **Advantages:**
  - only similarity between objects is needed, not exact feature values.
    - so it may be applied to objects with arbitrary complex feature description
  - simple to implement
  - interpretable (case based reasoning)
  - does not need training
    - may be applied in online scenarios
    - Cross-validation may be replaced with LOO.
- **Disadvantages:**
  - slow classification with complexity $O(N)$
  - accuracy deteriorates with the increase of feature space dimensionality

Table of Contents

Normalization of features

- Feature scaling affects predictions of K-NN?

Normalization of features

- Feature scaling affects predictions of K-NN?
    - yes, so normalize them
- Equal scaling - equal impact of features
- Non-equal scaling - non-equal impact of features
- Typical normalizations:

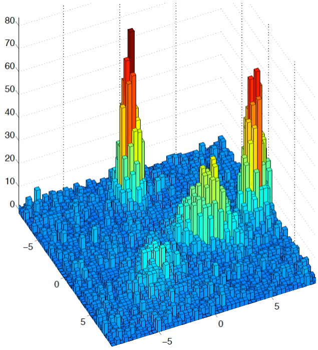
Name	Transformation	Properties of resulting feature
Autoscaling	$x_j' = \frac{x_j - \mu_j}{\sigma_j}$	zero mean and unit variance.
Range scaling	$x_j' = \frac{x_j - L_j}{U_j - L_j}$	belongs to $[0, 1]$ interval.

where μ_j, σ_j, L_j, U_j are mean value, standard deviation, minimum and maximum value of the j-th feature.

- for non-negative features range scaling does not affect feature sparsity: 0->0.

The curse of dimensionality

- The curse of dimensionality: with growing D data distribution becomes sparse and insufficient.
- Example: histogram estimation requires exponentially more data with increasing data dimensionality.



Curse of dimensionality

- Case of K-nearest neighbours:
  - assumption: objects are distributed uniformly in feature space
  - ball of radius R has volume $V(R) = CR^D$, where $C = \frac{\pi^{D/2}}{\Gamma(D/2+1)}$.
  - ratio of volumes of balls with radius $R-\varepsilon$ and R:

$$\frac{V(R-\varepsilon)}{V(R)} = \left(\frac{R-\varepsilon}{R}\right)^D \xrightarrow{D\to\infty} 0$$

  - most of volume concentrates on the border of the ball, so there lie the nearest neighbours.
  - nearest neighbours stop being close by distance
- Good news: in real tasks the true dimensionality of the data is often less than D and objects belong to the manifold with smaller dimensionality.

Table of Contents

Equal voting

- Consider for object x: x_{i_1} most close neigbour, x_{i_2} - second most close neighbour, etc.

$$\rho(x, x_{i_1}) \le \rho(x, x_{i_2}) \le ... \le \rho(x, x_{i_N})$$

- Classification:

$$g_c(x) = \sum_{k=1}^{K} \mathbb{I}[y_{i_k} = c], \quad c = 1, 2, ... C.$$

$$\widehat{y}(x) = \arg\max_c g_c(x)$$

- Regression:

$$\widehat{y}(x) = \frac{1}{K} \sum_{k=1}^{K} y_{i_k}$$

Weighted voting

- Weighted classification:

$$g_c(x) = \sum_{k=1}^{K} w(k,\ \rho(x, x_{i_k}))\mathbb{I}[y_{i_k} = c], \quad c = 1, 2, \dots C.$$

$$\widehat{y}(x) = \arg\max_c g_c(x)$$

Weighted voting

- Weighted classification:

$$g_c(x) = \sum_{k=1}^{K} w(k,\ \rho(x, x_{i_k}))\mathbb{I}[y_{i_k} = c], \quad c = 1, 2, \dots C.$$

$$\widehat{y}(x) = \arg\max_c g_c(x)$$

- Weighted regression:

$$\widehat{y}(x) = \frac{\sum_{k=1}^{K} w(k,\ \rho(x, x_{i_k}))y_{i_k}}{\sum_{k=1}^{K} w(k,\ \rho(x, x_{i_k}))}$$

Commonly chosen weights

Index dependent weights:

$$w_k = \alpha^k, \quad \alpha \in (0,1)$$

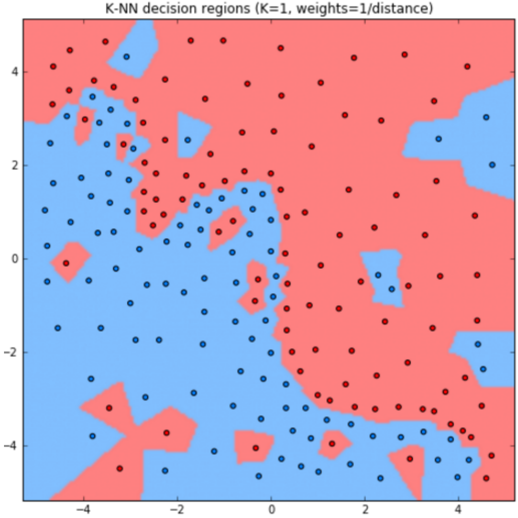
$$w_k = \frac{K+1-k}{K}$$

Distance dependent weights:

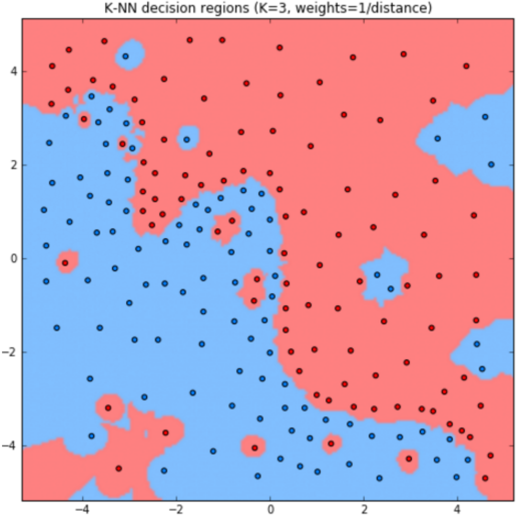
$$w_k = \begin{cases} \frac{\rho(z_K,x)-\rho(z_k,x)}{\rho(z_K,x)-\rho(z_1,x)}, & \rho(z_K,x) \neq \rho(z_1,x) \\ 1 & \rho(z_K,x) = \rho(z_1,x) \end{cases}$$

$$w_k = \frac{1}{\rho(z_k,x)}$$

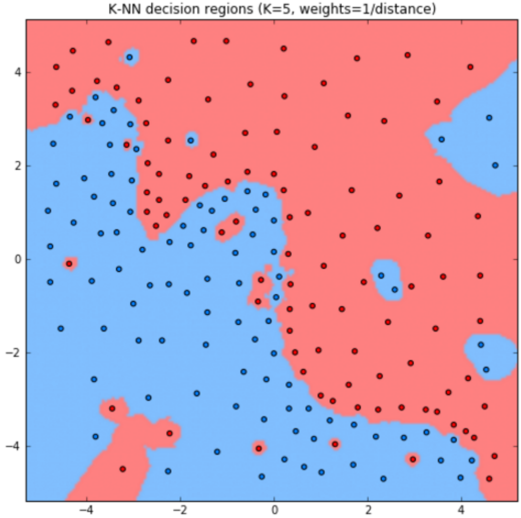
Example: K-NN classification with weights



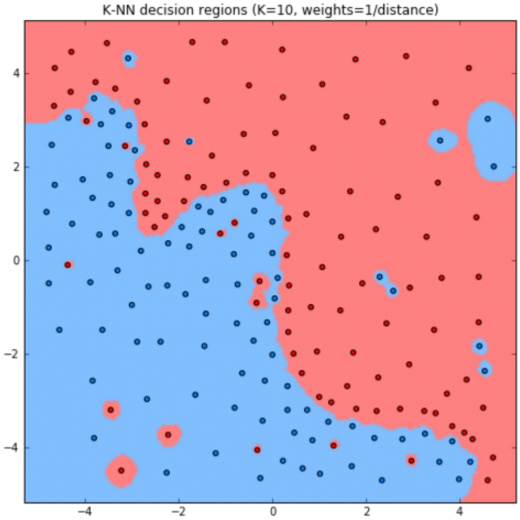
Example: K-NN classification with weights



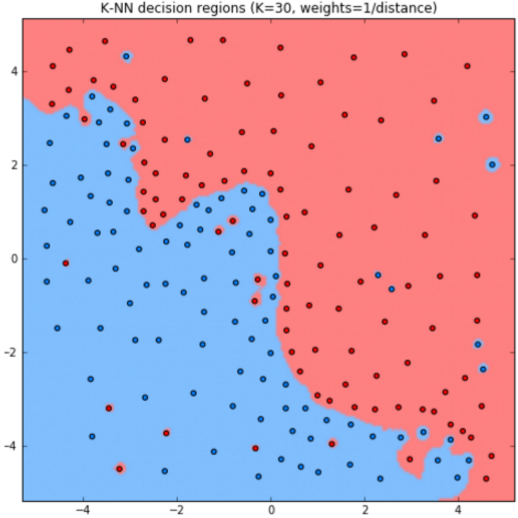
Example: K-NN classification with weights



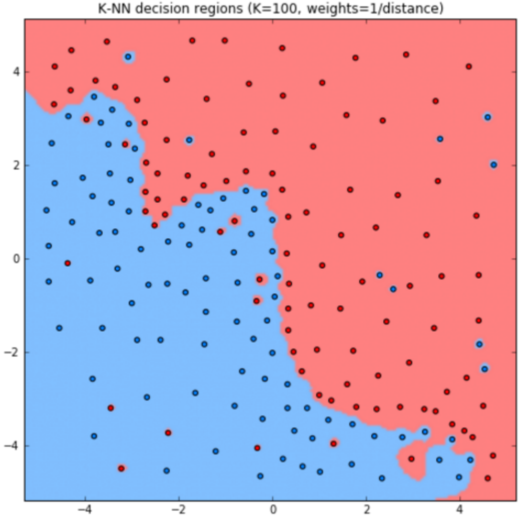
Example: K-NN classification with weights



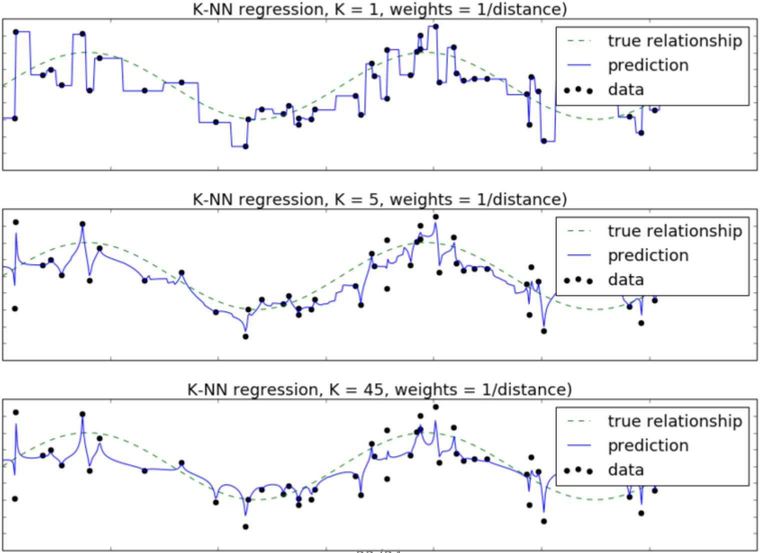
Example: K-NN classification with weights



Example: K-NN classification with weights



Example: K-NN regression with weights



Summary

- Important parameters of K-NN:
  - K: controls model complexity
  - $\rho(x, x')$
- Output depends on feature scaling.
  - scaling to equal / non-equal scatter possible.
- Prone to curse of dimensionality.
- Fast training but long prediction.
  - some efficiency improvements are possible though
- Weighted account for objects possible.
- Nearest centroid has different properties.