X/HEC Datascience for Business Master
2020/2021 **Alexandre Gramfort, Joseph Salmon, Mathurin Massias**

Lab n° 2 : k-nearest neighbor

The file `tp_knn_source.py` is on Moodle. It contains functions needed for this Lab.

- Reminder on classification -

Definitions and notation

We remind the setup of multiclass supervised classification.

— $\mathcal{Y}$ is the set of labels. Here we consider L classes, and we choose $\mathcal{Y} = \{1, \dots, L\}$ to represent the L possible labels. Binary classification corresponds to $L = 2$.

— $\mathbf{x} = (x_1, \dots, x_p)^\top \in \mathcal{X} \subset \mathbb{R}^p$ is one observation, one example, one point, one sample.

— $\mathcal{D}_n = \{(\mathbf{x}_i, y_i), i = 1, \dots n\}$ is the full dataset with the samples and their labels.

— We consider a probabilistic model governing random variables X and $Y : \forall i \in \{1, \dots, n\}, (\mathbf{x}_i, y_i) \overset{i.i.d}{\sim} (X, Y)$.

— We seek to construct from $\mathcal{D}_n$ a function, named classifier, $\hat{f} : \mathcal{X} \to \mathcal{Y}$ which to a new point $\mathbf{x}_{\text{new}}$ gives a label $\hat{f}(\mathbf{x}_{\text{new}})$.

Artificial data generation

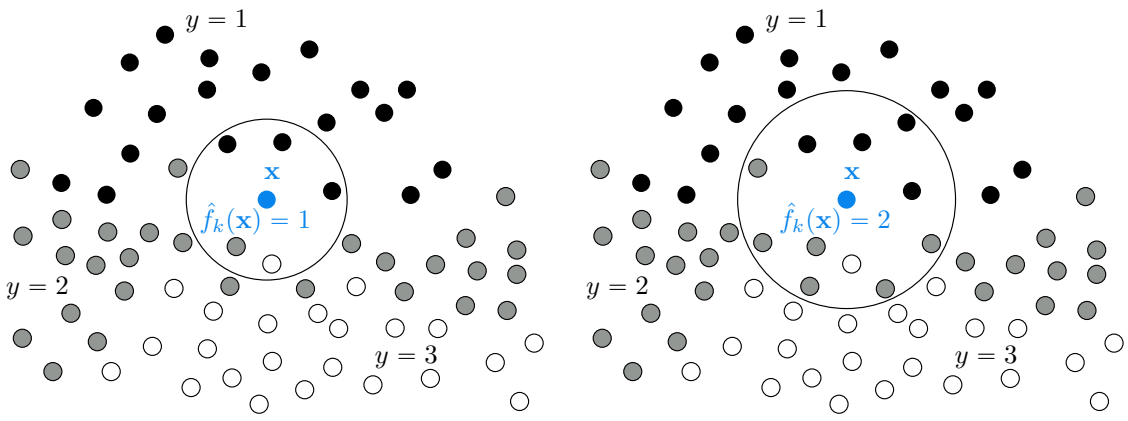
We consider two-dimensional samples, so that we can visualize them ($p = 2$).

1) Study the functions `rand_bi_gauss`, `rand_tri_gauss`, `rand_clown` and `rand_checkers` defined in `tp_knn_source.py`. What do they yield ? What is the last column ? Generate 4 datasets with these functions, and use `plot_2d` to plot them.

Intuitive approach

k-nn is an intuitive algorithm. Its principle is as follows : for each new point, $\mathbf{x}$ we first find its k-nearest neighbors in the training dataset, denoted $V_k(\mathbf{x})$ The class given to the new point is then the class which is the most represented in $V_k(\mathbf{x})$. An illustration is given in Figure 1 for $L = 3$ classes.

2) propose an adaptation of this algorithm to regression, that is, the case where $\mathcal{Y} = \mathbb{R}$.



(a) $k = 5$ (b) $k = 11$

FIGURE 1 – Exemple of k-nn for $k = 5$ and $k = 11$, with $L = 3$ classes represented in black ($y = 1$), grey ($y = 2$) and white ($y = 3$). For $k = 5$ (left) we predict black at the new point $\mathbf{x}$ (in blue), while for $k = 11$ (right) we predict grey.

Formal approach

We first choose a distance $d : \mathbb{R}^p \times \mathbb{R}^p \mapsto \mathbb{R}$. For a new point $\mathbf{x}$, we define the k-nearest neighbors $V_k(\mathbf{x})$ in the sense of this distance. We can then proceed as follows : for each $\mathbf{x} \in \mathbb{R}^d$ and each $i = 1, \dots, n$, let $d_i(\mathbf{x})$ be the distance between $\mathbf{x}$ and $\mathbf{x}_i$: $d_i(\mathbf{x}) = d(\mathbf{x}_i, \mathbf{x})$. We define the first statistic of rank $r_1(\mathbf{x})$ as the index of the nearest neighbor of $\mathbf{x}$ amongst $\mathbf{x}_1, \dots, \mathbf{x}_n$, that is,

$$r_1(\mathbf{x}) = i^* \qquad \text{if and only if} \qquad d_{i*}(\mathbf{x}) = \min_{1 \leqslant i \leqslant n} d_i(\mathbf{x}).$$

By recursion, we can define $r_k(\mathbf{x})$ for any $1 \leqslant k \leqslant n$:

$$r_k(\mathbf{x}) = i^* \quad \text{if and only if} \quad d_{i*}(\mathbf{x}) = \min_{\substack{1 \leqslant i \leqslant n \\ i \notin \{r_1, \dots, r_{k-1}\}}} d_i(\mathbf{x}). \tag{1}$$

The set of k-nearest neighbors of $\mathbf{x}$ is then : $V_k(\mathbf{x}) = \{\mathbf{x}_{r_1}, \dots, \mathbf{x}_{r_k}\}$. Finally, the decision function to classify $\mathbf{x}$ is a vote by majority, solving :

$$\hat{f}_k(\mathbf{x}) \in \arg\max_{y \in \mathcal{Y}} \left(\sum_{j=1}^{k} \mathbb{1}_{\{y_{r_j} = y\}} \right). \tag{2}$$

The module `sklearn.neighbors` (http://scikit-learn.org/stable/modules/neighbors.html) implements the algorithms based on nearest neighbors.

3) Fill the `KNNClassifier` to reimplement the decision function described above. Check your predictions by comparing them to the results of `KNeighborsClassifier` of `scikit-learn`, on one, then all of the toy datasets introduced above.

For quicker computation, you will now use the functions from `scikit-learn` instead of your implementation. For now, you will use the classical Euclidean distance $d(\mathbf{x}, \mathbf{v}) = \|\mathbf{x} - \mathbf{v}\|_2$.

4) Vary k. What happens when $k = 1$? $k = n$? Plot these cases on one dataset. When is the decision frontier simple ? complicated ?
5) What is the fraction of errors on your training data when $k = 1$? and on test data ?
6) Plot the error curves as a function of k on one of the datasets for n taking values 100, 500 and 1000. What is the best k ? Is it the same for all datasets ? Be careful to evaluate the error on the testing data. You can use the class `ErrorCurve`.
7) What are the pros and cons of this method ?
8) Apply this method the the DIGITS dataset with different choices of $k \geqslant 1$. Refer to http://scikit-learn.org/stable/_downloads/plot_digits_classification.py to load the data.
9) Compute the confusion matrix $(\mathbb{P}\{Y = i, C_k(X) = j\})_{i,\,j}$ associated to your classifier C_k. Refer to http://scikit-learn.org/stable/auto_examples/plot_confusion_matrix.html.
10) Propose a method to choose k and implement it. You can use `LOOCurve`.
11) A popular variant is to use weights for the j-th neighbor : $e^{-d_j^2(\mathbf{x})/h}$ (for a scalar parameter $h > 0$ controlling the level of weighting) : we replace Equation (2) by :

$$\hat{f}_k(\mathbf{x}) \in \arg\max_{y \in \mathcal{Y}} \left(\sum_{j=1}^{k} \exp\left(-\frac{d_j^2(\mathbf{x})}{h} \right) \mathbb{1}_{\{y_{r_j} = y\}} \right). \tag{3}$$

Implement this version in your `KNNClassifier` and compare to `scikit-learn` (passing the `weights` function as a parameter to the constructor of `KNeighborsClassifier`). You could get inspiration from `_weight_func` of `scikit-learn` : https://github.com/scikit-learn/scikit-learn/blob/master/sklearn/neighbors/tests/test_neighbors.py. Test the impact of h on the classification frontiers.

- To go further -

Global details available at [HTF09, Chapitre 13]. For a theoretical understanding of the method, refer to [DGL96, Chapitre 11], and for the limits of the method when $k = 1$, http://certis.enpc.fr/%7Edalalyan/Download/DM1.pdf. Finally, for algorithmic considerations, one can read http://scikit-learn.org/stable/modules/neighbors.html#brute-force and following paragraphs.

Références

[DGL96] L. Devroye, L. Györfi, and G. Lugosi. *A probabilistic theory of pattern recognition*, volume 31 of *Applications of Mathematics (New York)*. Springer-Verlag, New York, 1996. 3

[HTF09] T. Hastie, R. Tibshirani, and J. Friedman. *The elements of statistical learning*. Springer Series in Statistics. Springer, New York, second edition, 2009. http://www-stat.stanford.edu/~tibs/ElemStatLearn/. 3