Machine Learning

(Học máy – IT3190E)

Khoat Than

School of Information and Communication Technology

Hanoi University of Science and Technology

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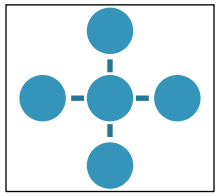
Contents

Classification problem

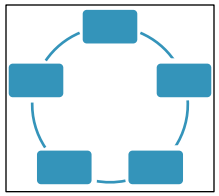
- **Supervised learning:** learn a function y = f(x) from a given training set $\{\{x_1, x_2, \ldots, x_N\}; \{y_1, y_2, \ldots, y_N\}\}$ so that $y_i \cong f(x_i)$ for every i.
  - Each training instance has a label/response.
- **Multiclass classification/categorization:** output y is only one from a pre-defined set of labels
  - y in {normal, spam}
  - y in {fake, real}

Which class does the object belong to?

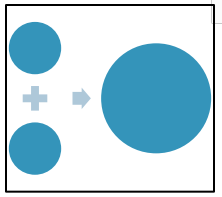
Class a



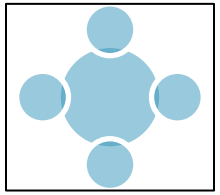
Class a



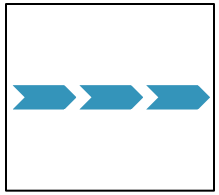
Class b



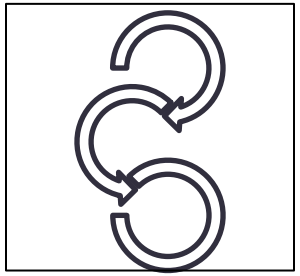
Class a



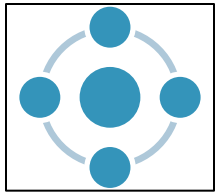
?



Class b



Class a



Neighbor-based learning (1)

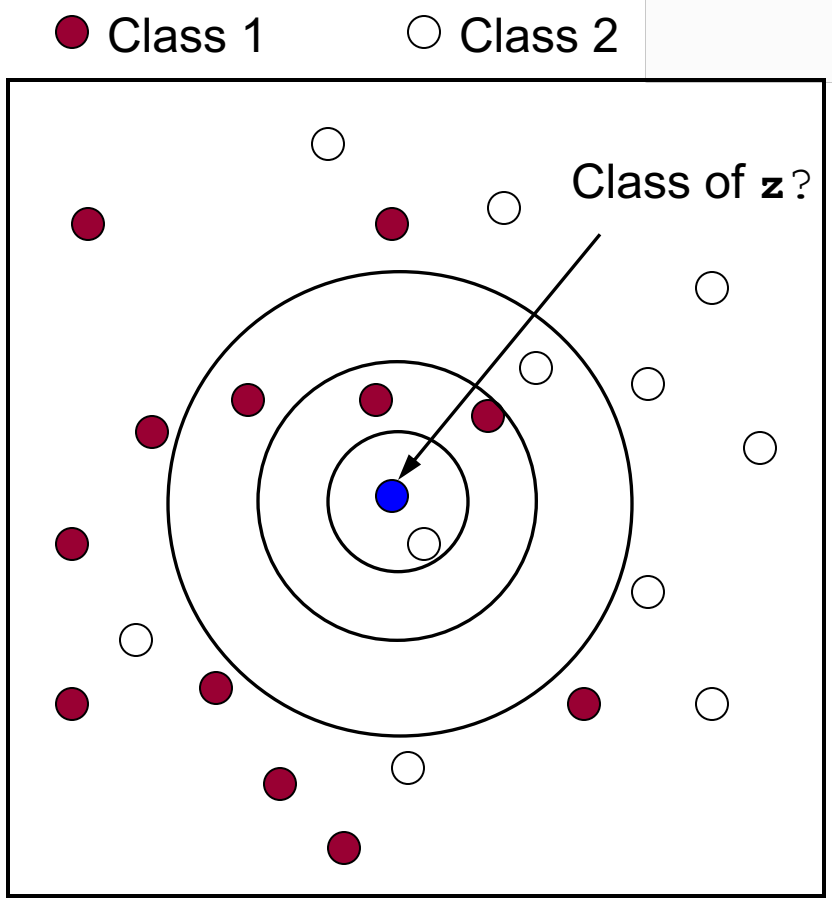
- *K-nearest neighbors* (KNN) is one of the most simple methods in ML. Some other names:
  - Instance-based learning
  - Lazy learning
  - Memory-based learning
- Main ideas:
  - There is no specific assumption on the function to be learned.
  - Learning phase just stores all the training data.
  - Prediction for a new instance is based on its nearest neighbors in the training data.
- Thus KNN is called a *non-parametric method*.
  (no specific assumption on the classifier/regressor)

Neighbor-based learning (2)

- Two main ingredients:
  - The **similarity measure** (distance) between instances/objects.
  - The **neighbors** to be taken in prediction.
- *Under some conditions, KNN can achieve the Bayes-optimal error which is the performance limit of any methods.* [Gyuader and Hengartner, JMLR 2013]
  - Even 1-NN (with some simple modifications) can reach this performance. [Kontorovich & Weiss, AISTATS 2015]
- KNN is close to ***Manifold learning***.

KNN: example

- Take 1 nearest neighbor?
  - Assign **z** to class 2.
- Take 3 nearest neighbors?
  - Assign **z** to class 1.
- Take 5 nearest neighbors?
  - Assign **z** to class 1.



KNN for classification

- Data representation:
  - Each observation is represented by a vector in an n-dimensional space, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$. Each dimension represents an attribute/feature/variate.
  - There is a set C of predefined labels.
- Learning phase:
  - Simply save all the training data **D**, with their labels.
- Prediction: for a new instance **z**.
  - *For each instance **x** in **D**, compute the distance/similarity between **x** and **z**.*
  - *Determine a set NB(**z**) of the nearest neighbors of **z**.*
  - *Using majority of the labels in NB(**z**) to predict the label for **z**.*

KNN for regression

- Data representation:
  - Each observation is represented by a vector in an n-dimensional space, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$. Each dimension represents an attribute/feature/variate.
  - The output y is a real number.
- Learning phase:
  - Simply save all the training data **D**, with their labels.
- Prediction: for a new instance **z**.
  - *For each instance* **x** *in* ***D****, compute the distance/similarity between* **x** *and* **z**.
  - *Determine a set NB(***z***) of the nearest neighbors of* **z***, with* $|NB(z)| = k$.
  - *Predict the label for* **z** *by* $y_z = \frac{1}{k} \sum_{x \in NB(z)} y_x$

KNN: two key ingredients (1)

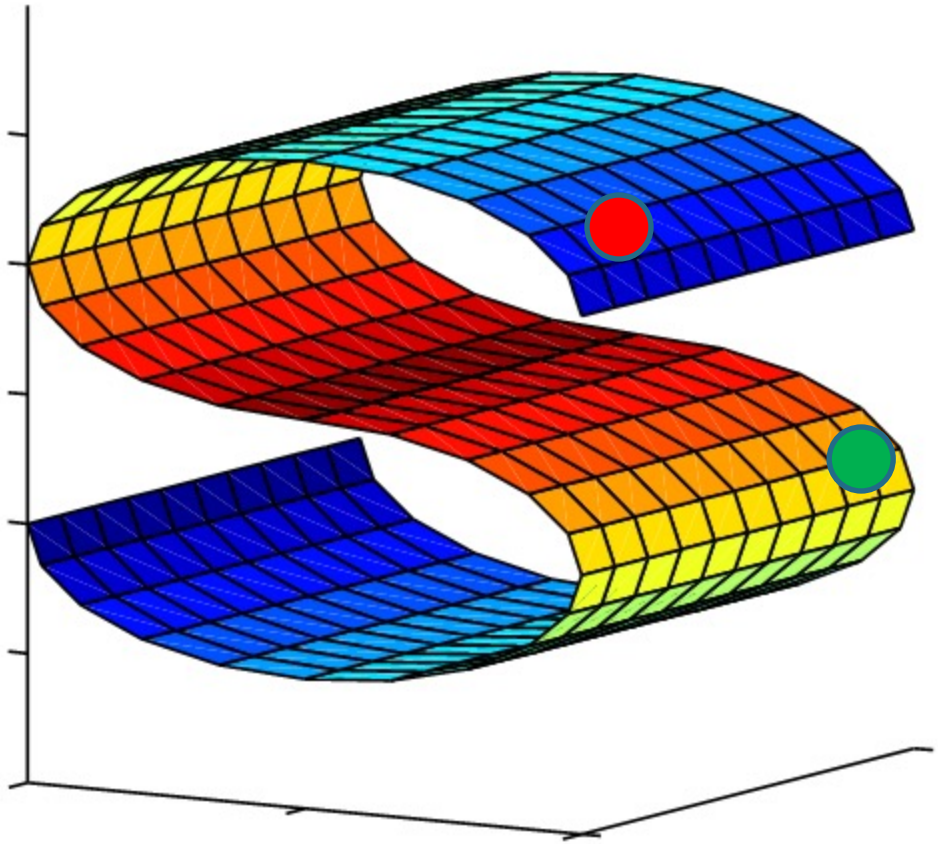
Different thoughts,

Different views

Different measures

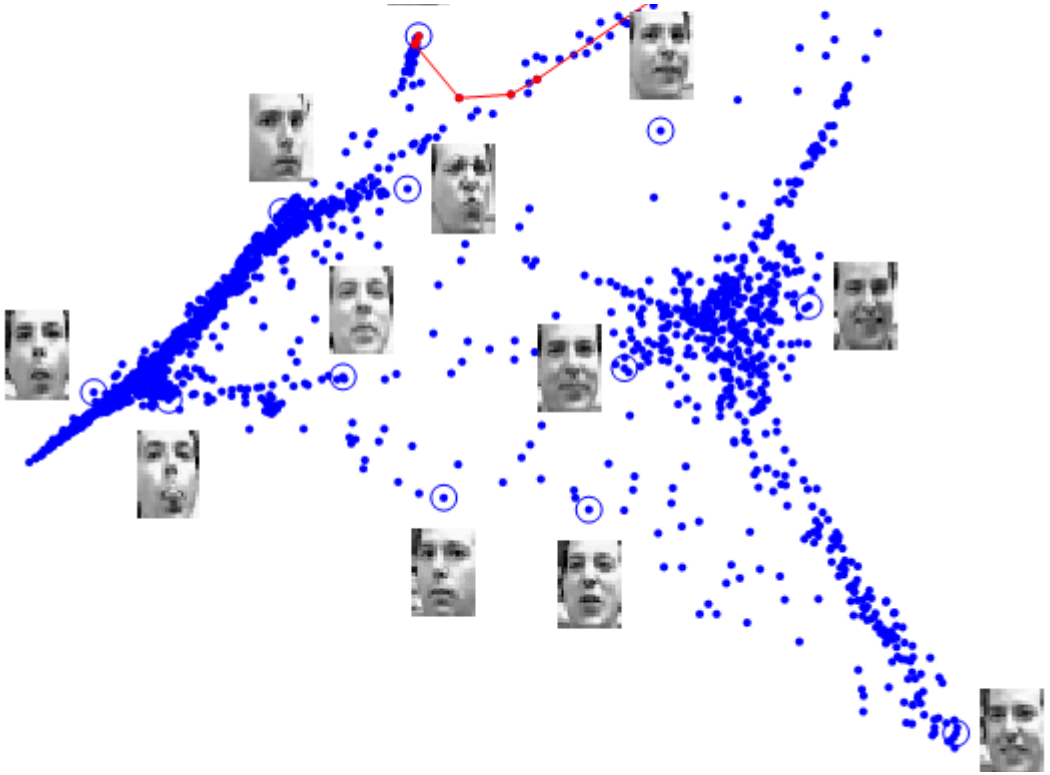
KNN: two key ingredients (2)

- The **distance/similarity** measure
  - Each measure implies a view on data
  - Infinite many measures !!!
  - What measure should be?



KNN: two key ingredients (3)

- The set NB(**z**) of **nearest neighbors.**
  - How many neighbors are enough?
  - How can we select NB(**z**)?
    (by choosing k or restricting the area?)



KNN: 1 or more neighbors?

- In theory, *1-NN can be among the best methods under some conditions*. [Kontorovich & Weiss, AISTATS 2015]
  - KNN is Bayes optimal under some conditions: Y bounded, large training size M, and the true regression function being continuous, and

$$k \to \infty, (k/M) \to 0, (k/\log M) \to +\infty$$

- In practice, we should use more neighbors for prediction (k>1), but not too many:
  - To avoid noises/errors in only one nearest neighbor.
  - Too many neighbors migh break the inherent structure of the data manifold, and thus prediction might be bad.

Distance/similarity measure (1)

- The distance measure:
  - Plays a very important role in KNN.
  - Indicates how we assume/suppose the distribution of our data.
  - Be determined once, and does not change in all prediction later.
- Some common distance measures:
  - *Geometric distance:* usable for problems with real inputs
  - *Hamming distance:* usable for problems with binary inputs, such as x in {0; 1}

Distance/similarity measure (2)

- Some geometric distances:
  - Minkowski (L_p-norm):
  $$d(x,z) = \left(\sum_{i=1}^{n} |x_i - z_i|^p \right)^{1/p}$$
  - Manhattan (L_1-norm):
  $$d(x,z) = \sum_{i=1}^{n} |x_i - z_i|$$
  - Euclid (L_2-norm):
  $$d(x,z) = \sqrt{\sum_{i=1}^{n} (x_i - z_i)^2}$$
  - Chebyshev (max norm):
  $$d(x,z) = \lim_{p \to \infty} \left(\sum_{i=1}^{n} |x_i - z_i|^p \right)^{1/p}$$
  $$= \max_i |x_i - z_i|$$

Distance/similarity measure (3)

- Hamming distance:
  - for problems with binary inputs
  - such as **x** = (1,0,0,1,1)

$$d(x,z) = \sum_{i=1}^{n} Difference(x_i, z_i)$$

$$Difference(a,b) = \begin{cases} 1, if\ (a \neq b) \\ 0, if\ (a = b) \end{cases}$$

- Cosine measure:
  - Suitable for some problems with textual inputs.

$$d(x,z) = \frac{x^T z}{\|x\| . \|z\|}$$

KNN: attribute normalization

- Normalizing the attributes is sometimes important to get good predictiveness in KNN.
  - No normalization implies that the magnitude of an attribute might play a heavy role, and artificially overwhelms the other attributes. Ex.:

$$d(x,z) = \sqrt{\sum_{i=1}^{n} (x_i - z_i)^2}$$

    - x = (`Age`=20, `Income`=12000, `Height`=1.68)
    - z = (`Age`=40, `Income`=1300, `Height`=1.75)
    - $d(\boldsymbol{x}, \boldsymbol{z})$ = $[(20-40)^2 + (12000-1300)^2 + (1.68-1.75)^2]^{0.5}$
  - This is unrealistic and unexpected in some applications.
- Some common normalizations:
  - Make all values of x_j in [-1; 1];
  - Make all values of x_j to have empirical mean 0 and variance 1.

KNN: attribute weighting

- Weighting the attributes is sometimes important for KNN.
  - No weight implies that the attributes play an equal role, e.g., due to the use of the Euclidean distance:

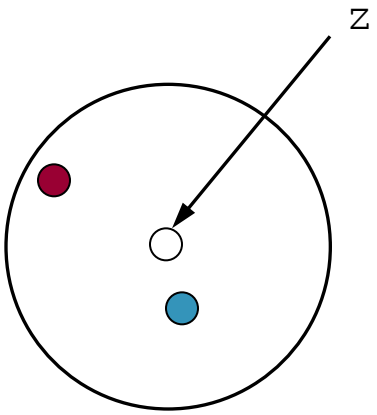
$$d(x,z)=\sqrt{\sum_{i=1}^{n}(x_i-z_i)^2} \longrightarrow d(x,z)=\sqrt{\sum_{i=1}^{n}w_i(x_i-z_i)^2}$$

  - This is unrealistic in some applications, where an attribute might be more important than the others in prediction.
  - Some weights (w_i) on the attributes might be more suitable.
- How to decide the weights?
  - Base on the knowledge domain about your problem.
  - Learn the weights automatically from the training data.

KNN: weighting neighbors (1)

$$y_z = \frac{1}{k} \sum_{x \in NB(z)} y_x$$

- Prediction of labels miss some information about neighbors.
  - The neighbors in NB(**z**) play the same role with respect to the different distances to the new instance.
  - This is unrealistic in some applications, *where closer neighbors should play more important role than the others.*
- Using the distance as weights in prediction might help.
  - Closer neighbors should have more effects.
  - Farther points should have less effects.



KNN: weighting neighbors (2)

- Let v be the weights to be used.
  - *v(**x**,**z**) can be chosen as the inverse of the distance from **x** to **z**, d(**x**,**z**).*
  - Some examples:

$$v(x,z) = \frac{1}{\alpha + d(x,z)} \qquad v(x,z) = \frac{1}{\alpha + [d(x,z)]^2} \qquad v(x,z) = e^{-\frac{d(x,z)^2}{\sigma^2}}$$

- For classification:

$$c_z = \arg\max_{c_j \in C} \sum_{x \in NB(z)} v(x,z).Identical(c_j, c_x) \qquad Identical(a,b) = \begin{cases} 1, if\,(a=b) \\ 0, if\,(a \neq b) \end{cases}$$

- For regression:

$$y_z = \frac{\sum_{x \in NB(z)} v(x,z).y_x}{\sum_{x \in NB(z)} v(x,z)}$$

KNN: limitations/advantages

- Advantages:
  - *Low cost for the training phase.*
  - *Very flexible in choosing the distance/similarity measure:* we can use many other measures, such as Kullback-Leibler divergence, Bregman divergence,…
  - *KNN is able to reduce some bad effects from noises when k > 1.*
  - *In theory, KNN can reach the best performance among all regression methods, under some conditions.*
    (this might not be true for other methods)
- Limitations:
  - Have to find a suitable distance/similarity measure for your problem.
  - Prediction requires intensive computation.

References

- A. Kontorovich and Weiss. A Bayes consistent 1-NN classifier. *Proceedings of the 18th International Conference on Artificial Intelligence and Statistics (AISTATS). JMLR: W&CP volume 38*, 2015.
- A. Guyader, N. Hengartner. On the Mutual Nearest Neighbors Estimate in Regression. *Journal of Machine Learning Research* 14 (2013) 2361-2376.
- L. Gottlieb, A. Kontorovich, and P. Nisnevitch. Near-optimal sample compression for nearest neighbors. *Advances in Neural Information Processing Systems*, 2014.

Exercises

- What is the different between KNN and OLS?
- Is KNN prone to overfitting?
- How to make KNN work with sequence data?
  (each instance is a sequence)