

Applied Machine Learning

Course number: W207

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Applied Machine Learning

Lecture 3 ...

- *K-Nearest Neighbors*
- *Probability review*
 - *Conditional probability*
 - *Independence*
- *Naïve Bayes*
 - *Application to text data and spam detection*

Instance-based representation

- Simplest form of learning: *rote learning*
 - Training instances are *searched for* instance that *most closely resembles new instance*
 - The *instances* themselves *represent the knowledge*
 - Also called *instance-based* learning
- Similarity function defines what's "learned"
- Instance-based learning is *lazy learning*
- Methods: *nearest-neighbor, k-nearest-neighbor, ...*

Instance-based representation

- In **instance-based classification**, each new instance is compared with existing ones using a distance metric
- The **closest** existing instance is used to **assign the class to the new one**
- This is called the *nearest-neighbor* classification method
- Sometimes more than one nearest neighbor is used, and the **majority class** of the **closest k neighbors** (or the distance weighted average if the class is numeric) is assigned to the new instance
- This is the *k-nearest-neighbor* method.

The distance function

- Simplest case: **one numeric attribute**
 - Distance is the **difference** between the two attribute values involved (or a function thereof)
- Several **numeric attributes**: normally, **Euclidean distance** is used and attributes are normalized
- **Nominal attributes**: distance is set to 1 if values are different, 0 if they are equal
- Are all attributes equally important?
 - **Weighting** the attributes might be necessary

Instance-based learning

- In instance-based learning the **distance function defines what is learned**

- Most instance-based schemes use ***Euclidean distance***:

$$\sqrt{(a_1^{(1)} - a_1^{(2)})^2 + (a_2^{(1)} - a_2^{(2)})^2 + \dots + (a_k^{(1)} - a_k^{(2)})^2}$$

$\mathbf{a}^{(1)}$ and $\mathbf{a}^{(2)}$: two instances with k attributes

- **Note:** taking the square root is not required when comparing distances
- Other popular metric: ***city-block metric (aka Manhattan)***
 - Adds differences without squaring them

Manhattan Distance

Taxicab geometry

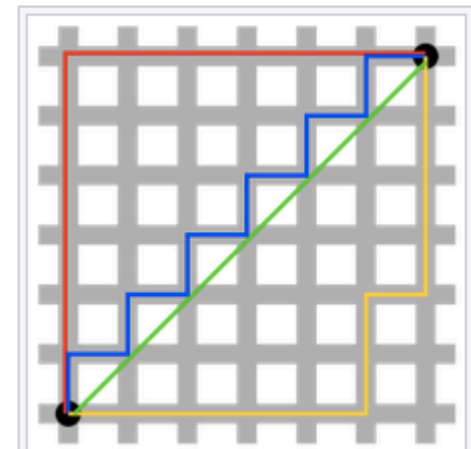
From Wikipedia, the free encyclopedia
(Redirected from [Manhattan distance](#))

A **taxicab geometry**, considered by [Hermann Minkowski](#) in 19th-century Germany, is a form of [geometry](#) in which the usual distance function or [metric](#) of [Euclidean geometry](#) is replaced by a new metric in which the [distance](#) between two points is the sum of the [absolute differences](#) of their [Cartesian coordinates](#).

The **taxicab metric** is also known as **rectilinear distance**, **L_1 distance** or **ℓ_1 norm** (see [\$L^p\$ space](#)), **snake distance**, **city block distance**, **Manhattan distance** or **Manhattan length**, with corresponding variations in the name of the geometry.^[1] The latter names allude to the [grid layout of most streets](#) on the island of [Manhattan](#), which causes the shortest path a car could take between two intersections in the [borough](#) to have length equal to the intersections' distance in taxicab geometry.

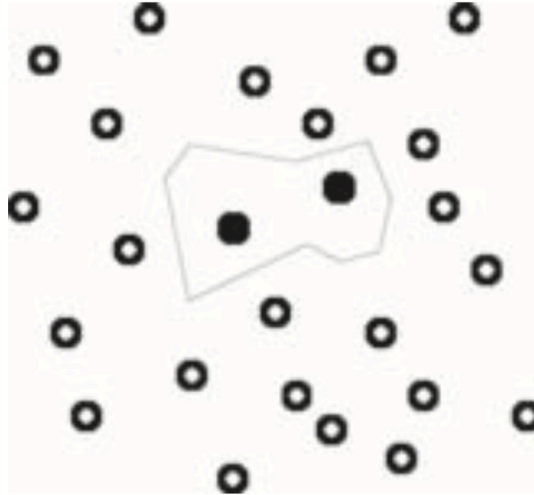
Contents [\[hide\]](#)

- [1 Formal definition](#)
- [2 Properties](#)

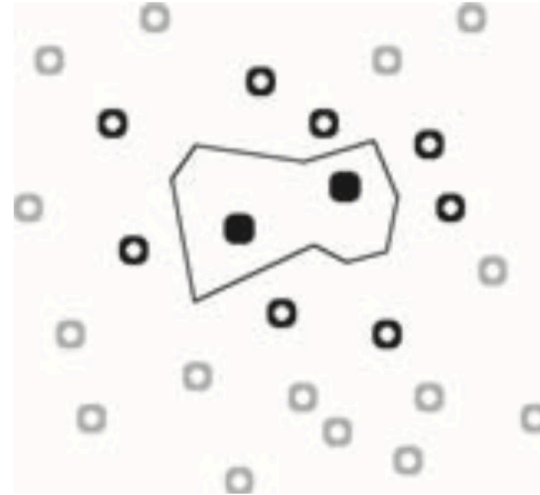


Taxicab geometry versus Euclidean distance: In taxicab geometry, the red, yellow, and blue paths all have the shortest length of 12. In Euclidean geometry, the green line has length $6\sqrt{2} \approx 8.49$, and is the unique shortest path.

Learning prototypes



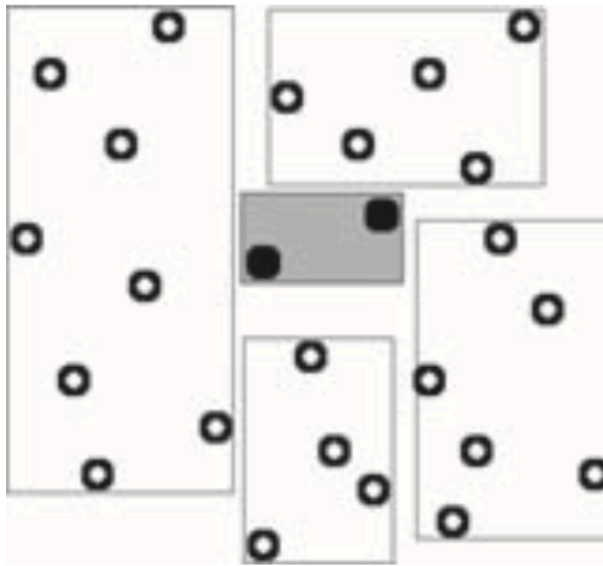
(a)



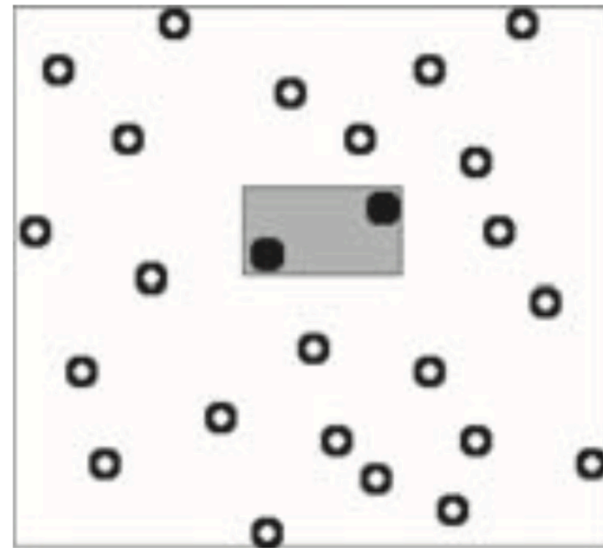
(b)

- Only those **instances involved in a decision** need to be **stored**
- **Noisy** instances should be **filtered out**
- Idea: only use *prototypical* examples

Rectangular generalizations



(c)



(d)

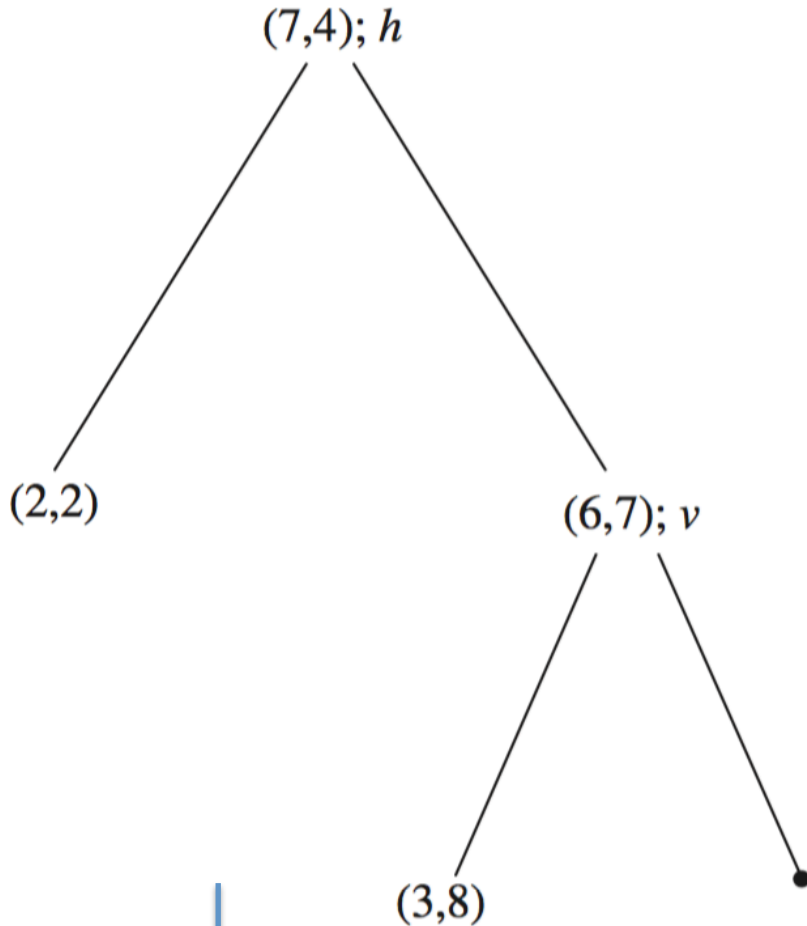
- Nearest-neighbor rule is **used outside** rectangles
- **Rectangles are rules!** (But they can be more conservative than “normal” rules.)
- **Nested rectangles** are **rules with exceptions**

Finding nearest neighbors efficiently

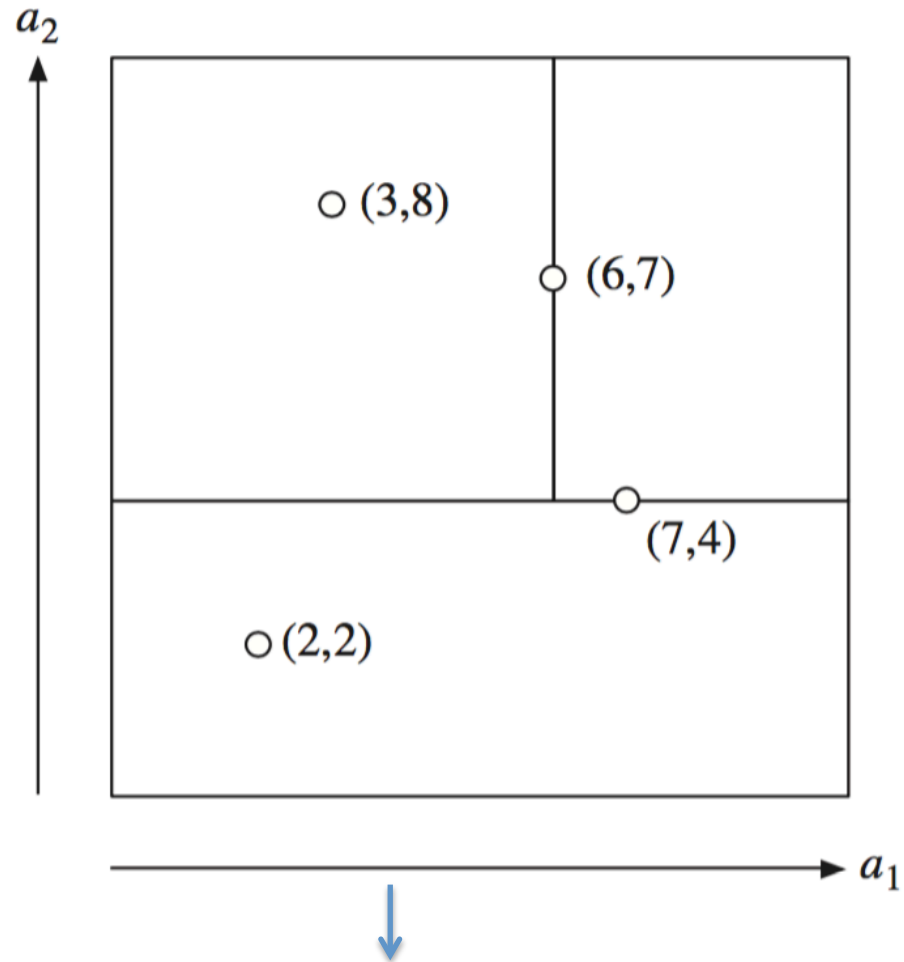
- Simplest way of finding nearest neighbor:
linear scan of the data
 - Classification takes time proportional to the product of the number of instances in training and test sets
- Nearest-neighbor search can be done more efficiently using appropriate data structures
- Two methods that represent training data in a tree structure are:

kD-trees and *ball trees*

kD-tree example



Shows an example with $k = 2$



Shows the **four training instances** it represents, along with the **hyperplanes that constitute the tree**

Discussion of nearest-neighbor learning

- Often **very accurate**
- **Assumes all attributes are equally important**
 - Remedy: attribute **selection**, attribute **weights**, or attribute **scaling**
- **Possible remedies** against noisy instances:
 - Take a **majority vote** over the k nearest neighbors
 - **Remove noisy instances** from dataset (difficult!)
- Statisticians have used k -NN since the early 1950s
 - If $n \rightarrow \infty$ and $k/n \rightarrow 0$, classification error approaches minimum
- k D-trees can become **inefficient when the number of attributes is too large**
- Ball trees are instances *may* help; they are instances of ***metric trees***

Model selection criteria

- Model selection criteria attempt to find a good compromise between:
 - The complexity of a model
 - Its prediction accuracy on the training data
- Reasoning: a good model is a simple model that achieves high accuracy on the given data
- Also known as *Occam's Razor*:

“the best theory is the smallest one that describes all the facts”

William of Ockham, born in the village of Ockham in Surrey (England) about 1285, was the most influential philosopher of the 14th century and a controversial theologian.

Elegance vs. errors

- **Theory 1: very simple**, elegant theory that explains the data almost perfectly
- **Theory 2: significantly more complex** theory that reproduces the data without mistakes ... *(is it more elegant?)*
- **Theory 1 is probably preferable**
- Classical example: Kepler's three laws on planetary motion
 - Less accurate than Copernicus's latest refinement of the Ptolemaic theory of epicycles on the data available at the time

Simplicity first

- Simple algorithms often work very well!
- There are many kinds of simple structure, e.g.:
 - One attribute does all the work
 - All attributes contribute equally & independently
 - Logical structure with a few attributes suitable for tree
 - An independent set of simple logical rules
 - Relationships between groups of attributes
 - A weighted linear combination of the attributes
 - Strong neighborhood relationships based on distance
 - Clusters of data in unlabeled data
 - Bags of instances that can be aggregated
- Success of method depends on the domain

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