Chapter 5
Similarity-based Learning

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Vectors

- Using a vector to represent a set of numbers

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

  - $\mathbf{x}$ is an n-dimension vector
  - In data analysis, we can use a vector to describe a data instance that consist of a set of features

Feature spaces

- The speed and agility ratings for 20 college athletes labelled with the decisions for whether they were drafted or not.
- Two features:
  - **Speed**
  - **Agility**

ID	Speed	Agility	Draft
1	2.50	6.00	No
2	3.75	8.00	No
3	2.25	5.50	No
4	3.25	8.25	No
5	2.75	7.50	No
6	4.50	5.00	No
7	3.50	5.25	No
8	3.00	3.25	No
9	4.00	4.00	No
10	4.25	3.75	No

ID	Speed	Agility	Draft
11	2.00	2.00	No
12	5.00	2.50	No
13	8.25	8.50	No
14	5.75	8.75	Yes
15	4.75	6.25	Yes
16	5.50	6.75	Yes
17	5.25	9.50	Yes
18	7.00	4.25	Yes
19	7.50	8.00	Yes
20	7.25	5.75	Yes

Feature spaces

- $\mathbf{x_2}$ and $\mathbf{x_{10}}$ are two college athletics of ID = 2 and ID = 10

$$\mathbf{x_2} = \begin{bmatrix} 3.75 \\ 8.00 \end{bmatrix}$$

$$\mathbf{x_{10}} = \begin{bmatrix} 4.25 \\ 3.75 \end{bmatrix}$$

Feature spaces

- Weather observation

Day	MinTemp	MaxTemp	Humidity	Rain
1	24	31	0.7	0.4
2	24	33	0.65	0.3
3	23	30	0.6	0.3
4	24	32	0.8	0.7
5	23	29	0.8	0.8
6	22	29	0.7	0.6
7	21	27	0.6	0.2

Feature spaces

- $\mathbf{x_3}$ and $\mathbf{x_6}$ are data instances of day 3 and day 6

$$\mathbf{x_3} = \begin{bmatrix} 23 \\ 30 \\ 0.6 \\ 0.3 \end{bmatrix}$$

$$\mathbf{x_6} = \begin{bmatrix} 22 \\ 29 \\ 0.7 \\ 0.6 \end{bmatrix}$$

Distance

- Difference between two vectors

  - $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$
  - $\mathbf{x} - \mathbf{y} = \begin{bmatrix} x_1 - y_1 \\ x_2 - y_2 \\ \vdots \\ x_n - yn \end{bmatrix}$

- How to quantize the difference? How do we estimate a number to describe the difference?
  - For measurement
  - For Comparison

Distance

- Given two vectors of n-dimension, **x** and **y**, a distance function *d* must conform to the following four criteria:
  - Non-negativity
    $d(\mathbf{x}, \mathbf{y}) \geq 0$
  - Identity
    $d(\mathbf{x}, \mathbf{y}) = 0 \leftrightarrow \mathbf{x} = \mathbf{y}$
  - Symmetry
    $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$
  - Triangular Inequality
    $d(\mathbf{x}, \mathbf{y}) \leq d(\mathbf{x}, \mathbf{z}) + d(\mathbf{y}, \mathbf{z})$

- We can use a distance function to describe **similarity** of two vectors

Distance

- L^p-norm

$$\|\mathbf{x}\|_{\boldsymbol{p}} = (|x_1|^p + |x_1|^p + \cdots + |x_n|^p)^{\frac{1}{p}}$$

  - p is a rational number and, in reduced form, has an even numerator.
    - L^0-norm
    - L^1-norm
    - L^2-norm
    - L^∞-norm
  - Minkoski distance

Distance

- L^2-norm
-

$$\|\mathbf{x}\|_2 = \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2} = \sqrt{\sum_{i=1}^{n} |x_i|^2}$$

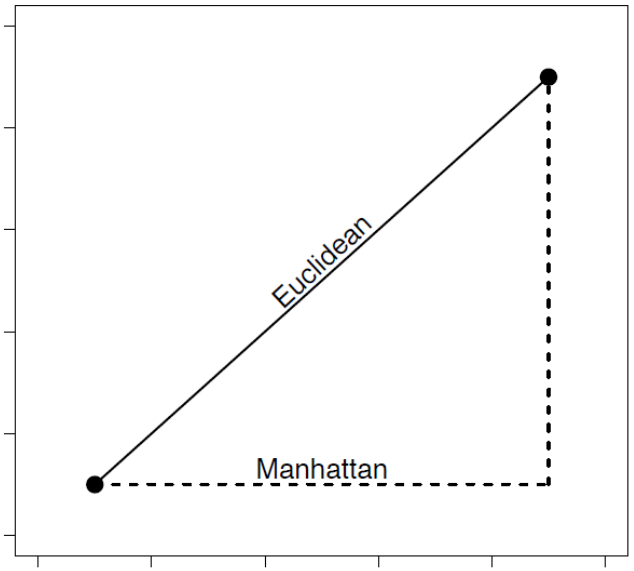
  - Euclidean distance
  - Euclidean norm
  - $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x} \cdot \mathbf{x}}$
  - $\frac{\partial \|\mathbf{x}\|_2}{\partial \mathbf{x}} = \frac{\mathbf{x}}{\|\mathbf{x}\|_2}$
  - $\frac{\partial \|\mathbf{x}\|_2}{\partial x_i} = \frac{x_i}{\|\mathbf{x}\|_2}, 1 \leq i \leq n$

Distance

- L^1-norm
-

$$\|\mathbf{x}\|_1 = |x_1| + |x_2| + \cdots + |x_n| = \sum_{i=1}^{n} |x_i|$$

  - Manhattan distance



Distance

- L^1-norm
  - $\mathbf{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$
    - $\|\mathbf{x}\|_2 = \sqrt{2} \approx 1.414$
    - $\|\mathbf{x}\|_1 = 2$
  - $\mathbf{y} = \mathbf{x} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$
    - $\|\mathbf{y}\|_2 = \sqrt{5} \approx 2.236$
    - $\|\mathbf{y}\|_1 = 3$
  - $\mathbf{z} = \mathbf{x} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$
    - $\|\mathbf{z}\|_2 = \sqrt{8} \approx 2.828$
    - $\|\mathbf{z}\|_1 = 4$

An element of x moves away from 0 by *d* the L_1 norm increases by *d*
➔ the difference between zero and nonzero elements is very important.

Distance

- L^{∞} -norm

$$\|\mathbf{x}\|_{\infty} = \max_i |x_i|$$

  - Bounded sequence

$$|x_i| \leq \|\mathbf{x}\|_{\infty}$$

  - Supremum

$$\|\mathbf{x}\|_{\infty} = \sup(|x_1|, |x_2|, \ldots, |x_n|)$$

    - The supremum of a subset **S** of a partially ordered set **T** is the least element in **T** that is greater than or equal to all elements of **S**

  - Infimum
    - The infimum of a subset **S** of a partially ordered set **T** is the greatest element in T that is less than or equal to all elements of S

Distance

- L^0-norm
  - Banach's definition:

$$\|\mathbf{x}\|_{\mathbf{0}} = \sum_{i=1}^{n} 2^{-i} \frac{|x_i|}{1 + |x_i|}$$

  - $\mathbf{x} = \begin{bmatrix} 1 \\ 0 \\ -4 \end{bmatrix}$
    - $\|\mathbf{x}\|_{\mathbf{0}} = \frac{\mathbf{1}}{\mathbf{2}} \frac{\mathbf{1}}{\mathbf{1+1}} + \frac{\mathbf{1}}{\mathbf{4}} \frac{\mathbf{0}}{\mathbf{1+0}} + \frac{\mathbf{1}}{\mathbf{8}} \frac{\mathbf{4}}{\mathbf{1+4}}$

$$= 0.25 + 0 + 0.1$$
$$= 0.35$$

Distance

- L^0-norm
  - Donoho's definition:

$$\|\mathbf{x}\|_{\mathbf{0}} = \sum_{i=1}^{n} |x_i|^0$$

- $\mathbf{x} = \begin{bmatrix} 1 \\ -4 \\ 0 \\ -2 \\ 0 \\ 0 \\ 0 \end{bmatrix}$
  - $\|\mathbf{x}\|_{\mathbf{0}} = \mathbf{3}$

This L^0-norm is used in information theory.
However, it is not a norm because it is not **homogeneous**.

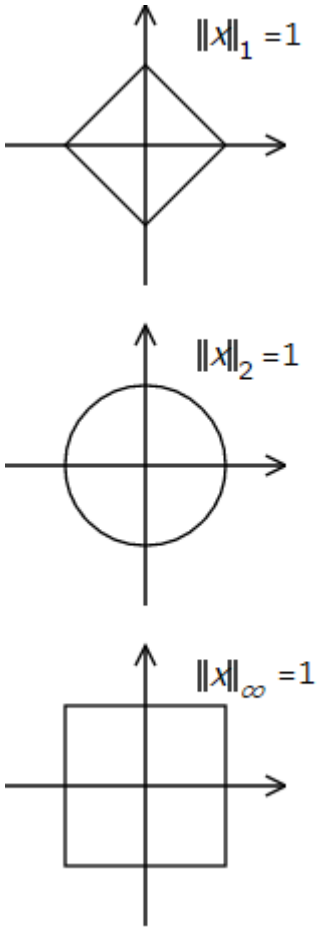
Homogeneous:

$$f(\alpha \mathrm{x}) = \alpha^k f(\mathrm{x})$$

α is a nonzero factor and *k* is an integer

Distance

- The spaces of one-distance of L^1, L^2, and L^∞

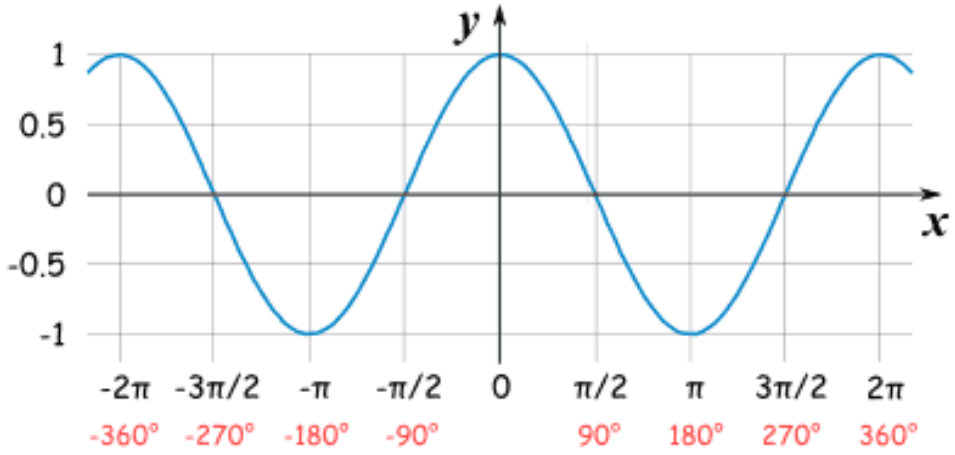


Distance

- cosθ

$$\mathbf{x}^{\mathbf{T}}\mathbf{y} = \|\mathbf{x}\|_2 \|\mathbf{y}\|_2 \cos\boldsymbol{\theta}$$

  - where θ is the angle between **x** and **y**.



Feature space normalization

- A dataset listing the salary and age information for customers and whether or not the purchased a pension plan

ID	Salary	Age	Purchased
1	53700	41	No
2	65300	37	No
3	48900	45	Yes
4	64800	49	Yes
5	44200	30	No
6	55900	57	Yes
7	48600	26	No
8	72800	60	Yes
9	45300	34	No
10	73200	52	Yes

Feature space normalization

- $\mathbf{x_1}$, $\mathbf{x_8}$, and $\mathbf{x_{10}}$ are three data instances of ID = 1, ID = 6, and ID 10.

$$\mathbf{x_1} = \begin{bmatrix} 53700 \\ 41 \end{bmatrix}, \mathbf{x_8} = \begin{bmatrix} 72800 \\ 60 \end{bmatrix}, \mathbf{x_{10}} = \begin{bmatrix} 73200 \\ 52 \end{bmatrix}$$

$$\mathbf{x_1} - \mathbf{x_8} = \begin{bmatrix} -19100 \\ -19 \end{bmatrix}$$

$$\|\mathbf{x_1} - \mathbf{x_8}\|_2 \approx 19100.01$$

$$\|\mathbf{x_1} - \mathbf{x_8}\|_1 = 19119$$

$$\cos\theta = 0.099$$

$\mathbf{x_1}$ is more similar to $\mathbf{x_8}$ than $\mathbf{x_{10}}$

$$\mathbf{x_1} - \mathbf{x_{10}} = \begin{bmatrix} -19500 \\ -11 \end{bmatrix}$$

$$\|\mathbf{x_1} - \mathbf{x_{10}}\|_2 \approx 19500.003$$

$$\|\mathbf{x_1} - \mathbf{x_{10}}\|_1 = 19511$$

$$\cos\theta = 0.093$$

Feature space normalization

- Range normalization
  - Given a value x in a range of $[x_{min}, x_{max}]$, the normalized value of x, x', can be estimated by the following equation

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}} (x'_{max} - x'_{min}) + x'_{min}$$

    - where $[x'_{min}, x'_{max}]$ is the range of normalization. In the most cases, $[x'_{min}, x'_{max}]$ = [0.0, 1.0], [-0.5, 0.5], or [-1.0, 1.0]

Feature space normalization

- Normalized data

Normalized Dataset			
ID	Salary	Age	Purch.
1	0.3276	0.4412	No
2	0.7276	0.3235	No
3	0.1621	0.5588	Yes
4	0.7103	0.6765	Yes
5	0.0000	0.1176	No
6	0.4034	0.9118	Yes
7	0.1517	0.0000	No
8	0.9862	1.0000	Yes
9	0.0379	0.2353	No
10	1.0000	0.7647	Yes

Feature space normalization

- $$\mathbf{x_1} = \begin{bmatrix} 0.3276 \\ 0.4412 \end{bmatrix}, \mathbf{x_8} = \begin{bmatrix} 0.9862 \\ 1.0 \end{bmatrix}, \mathbf{x_{10}} = \begin{bmatrix} 1.0 \\ 0.7647 \end{bmatrix}$$

$$\mathbf{x_1} - \mathbf{x_6} = \begin{bmatrix} -0.6586 \\ -0.5588 \end{bmatrix}$$

$$\|\mathbf{x_1} - \mathbf{x_6}\|_2 \approx 0.864$$

$$\|\mathbf{x_1} - \mathbf{x_6}\|_1 \approx 1.21$$

$\cos\theta = 0.99$

$$\mathbf{x_1} - \mathbf{x_{10}} = \begin{bmatrix} -0.6724 \\ -0.3235 \end{bmatrix}$$

$$\|\mathbf{x_1} - \mathbf{x_{10}}\|_2 \approx 0.746$$

$$\|\mathbf{x_1} - \mathbf{x_{10}}\|_1 \approx 0.9959$$

$\cos\theta = 0.96$

L1 and L2:

$\mathbf{x_1}$ is more similar to $\mathbf{x_{10}}$ than $\mathbf{x_8}$

$\cos\theta$:

$\mathbf{x_1}$ is more similar to $\mathbf{x_8}$ than $\mathbf{x_{10}}$

The Nearest Neighbor

- Input:
  - Training dataset
  - A **query** to be classified
- Algorithm
  1. Iterate across the instances in memory and find the instance that is shortest distance from the query position in the feature space.
  2. Make a prediction for the query equal to the value of the target feature of the nearest neighbor

The Nearest Neighbor

- Input:
  - Training dataset
  - A **query** to be classified
- Algorithm
  1. Iterate across the instances in memory and find the instance that is shortest distance from the query position in the feature space.
  2. Make a prediction for the query equal to the value of the target feature of the nearest neighbor

The Nearest Neighbor

- Training dataset:

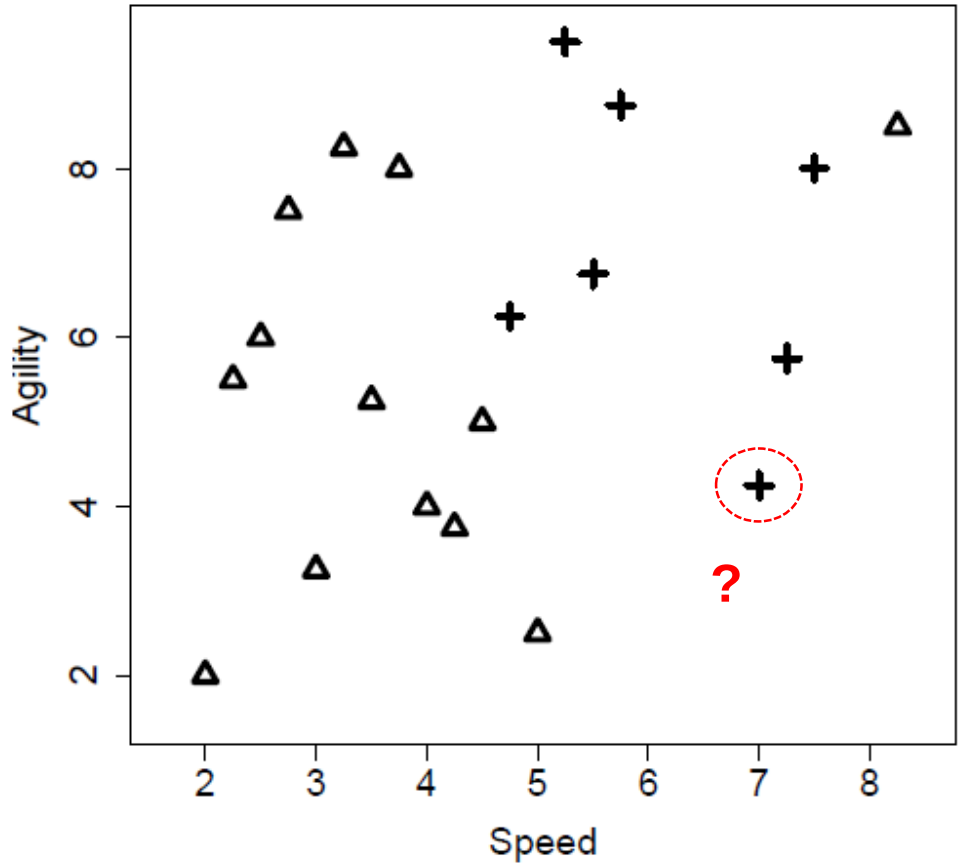
ID	Speed	Agility	Draft
1	2.50	6.00	No
2	3.75	8.00	No
3	2.25	5.50	No
4	3.25	8.25	No
5	2.75	7.50	No
6	4.50	5.00	No
7	3.50	5.25	No
8	3.00	3.25	No
9	4.00	4.00	No
10	4.25	3.75	No

ID	Speed	Agility	Draft
11	2.00	2.00	No
12	5.00	2.50	No
13	8.25	8.50	No
14	5.75	8.75	Yes
15	4.75	6.25	Yes
16	5.50	6.75	Yes
17	5.25	9.50	Yes
18	7.00	4.25	Yes
19	7.50	8.00	Yes
20	7.25	5.75	Yes

- Query:
  - Should we draft this guy?
    - **SPEED= 6.75, AGILITY= 3**

The Nearest Neighbor

- Figure of the training dataset
  - Δ: Draft = NO
  - +: Draft = YES
  - ?: the query



The Nearest Neighbor

- The L2 distances between the training data and the query

ID	SPEED	AGILITY	DRAFT	Dist.
18	7.00	4.25	yes	1.27
12	5.00	2.50	no	1.82
10	4.25	3.75	no	2.61
20	7.25	5.75	yes	2.80
9	4.00	4.00	no	2.93
6	4.50	5.00	no	3.01
8	3.00	3.25	no	3.76
15	4.75	6.25	yes	3.82
7	3.50	5.25	no	3.95
16	5.50	6.75	yes	3.95

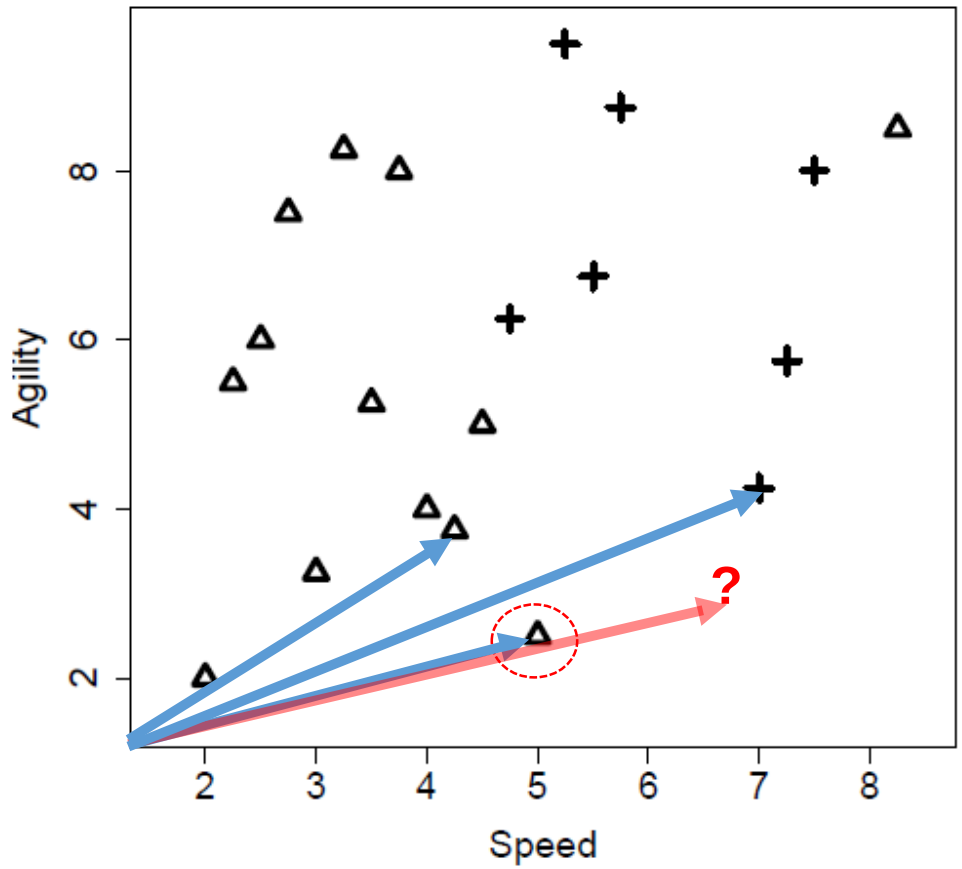
ID	SPEED	AGILITY	DRAFT	Dist.
11	2.00	2.00	no	4.85
19	7.50	8.00	yes	5.06
3	2.25	5.50	no	5.15
1	2.50	6.00	no	5.20
13	8.25	8.50	no	5.70
2	3.75	8.00	no	5.83
14	5.75	8.75	yes	5.84
5	2.75	7.50	no	6.02
4	3.25	8.25	no	6.31
17	5.25	9.50	yes	6.67

The Nearest Neighbor

- The L1 distances
  - **ID 18: 1.5**
  - ID 12: 2.25
  - ID 10: 3.25

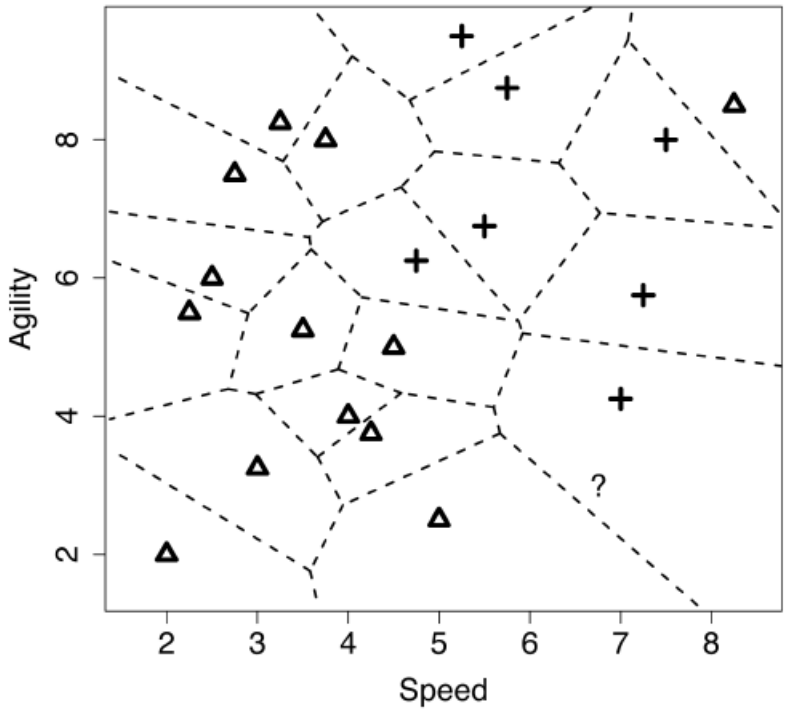
The Nearest Neighbor

- The cosine distances
  - **ID 12: 0.999**
  - ID 18: 0.992
  - ID 10: 0.954

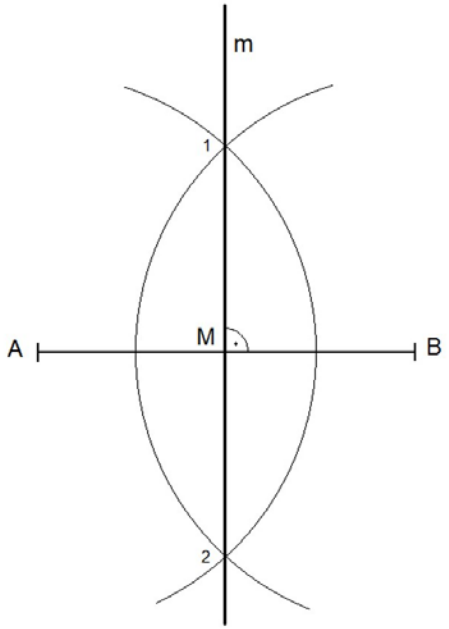


The Nearest Neighbor

- Voronoi tessellation



Perpendicular bisector



Order k with N samples:

Construction time: $O(k^2N\log N)$

Search time: $O(k + \log N_k)$, where N_k is the number of polygons.

Der-Tsai Lee, "On k-Nearest Neighbor Voronoi Diagrams in the Plane," *IEEE Transactions on Computers*, vol. C-31, no. 6, pp. 478-487, June 1982.

The Nearest Neighbor

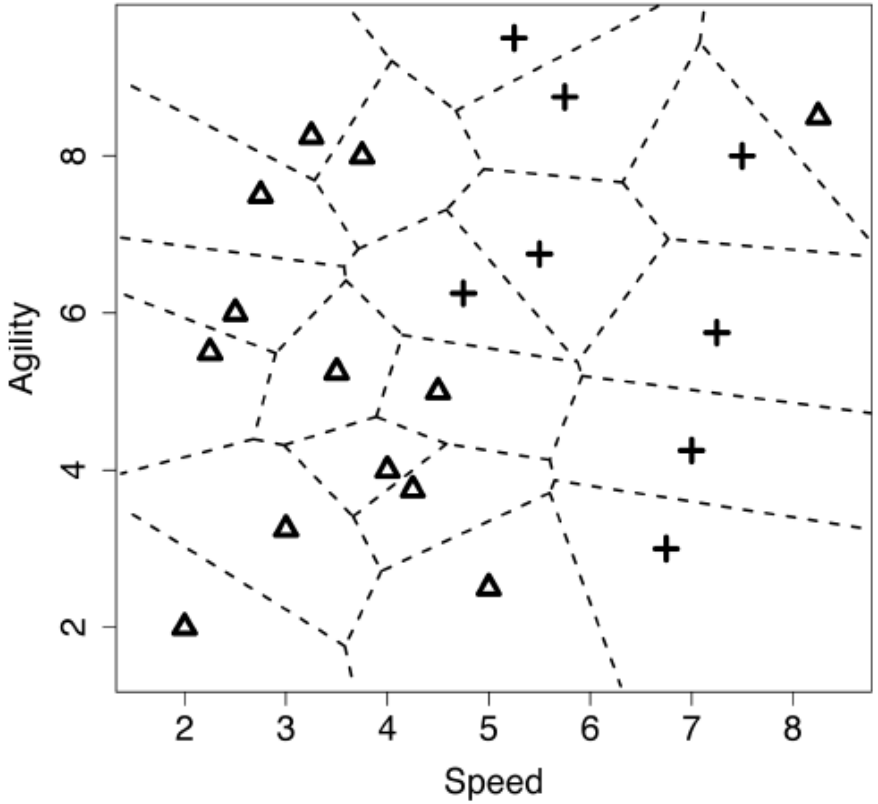
- Updating

ID	SPEED	AGILITY	DRAFT
1	2.50	6.00	no
2	3.75	8.00	no
3	2.25	5.50	no
4	3.25	8.25	no
5	2.75	7.50	no
6	4.50	5.00	no
7	3.50	5.25	no
8	3.00	3.25	no
9	4.00	4.00	no
10	4.25	3.75	no
11	2.00	2.00	no

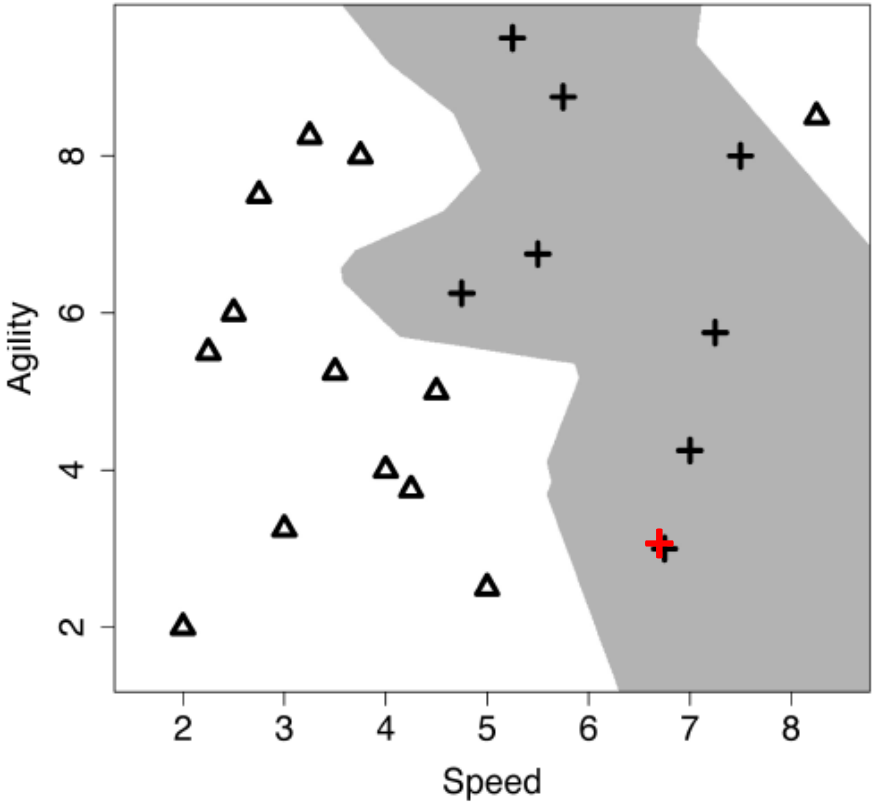
ID	SPEED	AGILITY	DRAFT
12	5.00	2.50	no
13	8.25	8.50	no
14	5.75	8.75	yes
15	4.75	6.25	yes
16	5.50	6.75	yes
17	5.25	9.50	yes
18	7.00	4.25	yes
19	7.50	8.00	yes
20	7.25	5.75	yes
21	6.75	3.00	yes

The Nearest Neighbor

- Updating



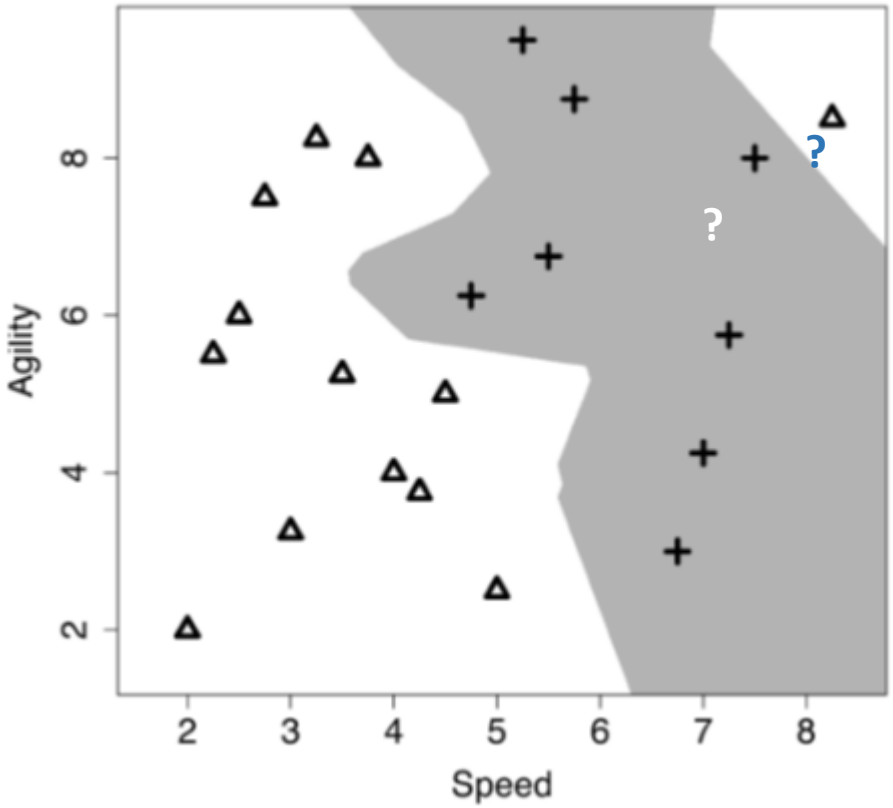
(a) Voronoi tessellation



(b) Decision boundary ($k = 1$)

The Nearest Neighbor

- Noisy
  - Query 1(blue ?):
    - Speed = 8.0
    - Agility = 8.0
    - ➔The NN is ID13 (8.25, 8.50)
    - ➔Draft = No
  - Query 2 (white ?):
    - Speed = 7.0
    - Agility = 7.0
    - ➔The NN is ID19 (7.5, 8.0)
    - ➔Draft = Yes



The K Nearest Neighbors, KNN

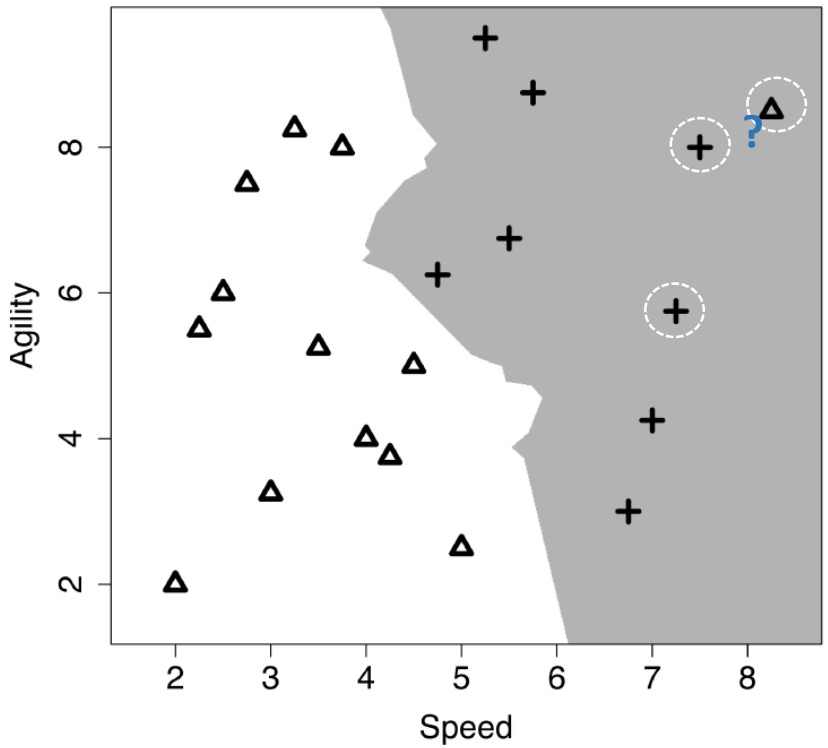
- KNN predicts the target level with the majority vote from the set of *k* nearest neightbors to the query **q**:

$$\mathbf{M}_{\boldsymbol{k}}(\mathbf{q}) = \mathbf{arg} \max_{\boldsymbol{l} \in \boldsymbol{levels}(\boldsymbol{t})} \sum_{\boldsymbol{i}=\mathbf{1}}^{\boldsymbol{k}} \boldsymbol{\delta}(\boldsymbol{t_i}, \boldsymbol{l})$$

  - where $\boldsymbol{\delta}(\boldsymbol{t_i}, \boldsymbol{l}) = \mathbf{1}$ if t_i equals to l and 0 otherwise

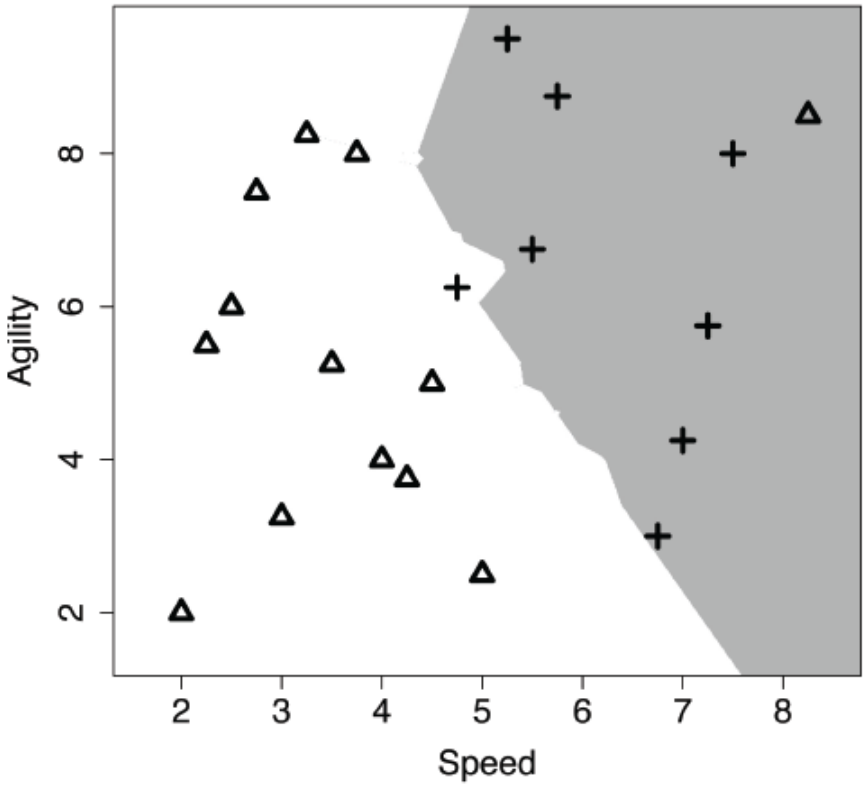
The K Nearest Neighbors, KNN

- *K* = 3
  - Query: Speed = 8.0, Agility = 8.0
    - Neighbors:
      - ID13 (8.25, 8.50, NO)
      - ID19 (7.5, 8.0, Yes)
      - ID13 (7.25, 5.75, Yes)
    - 2 Yes: 1 No
    - ➔Draft = Yes

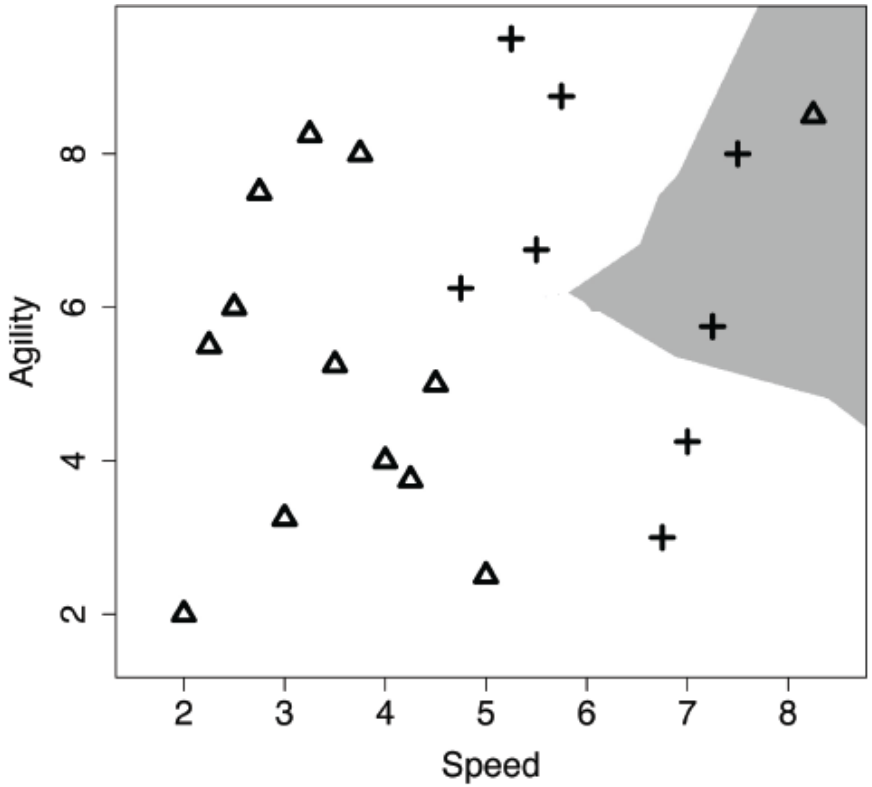


The K Nearest Neighbors, KNN

- K = 5



K = 15



The K Nearest Neighbors, KNN

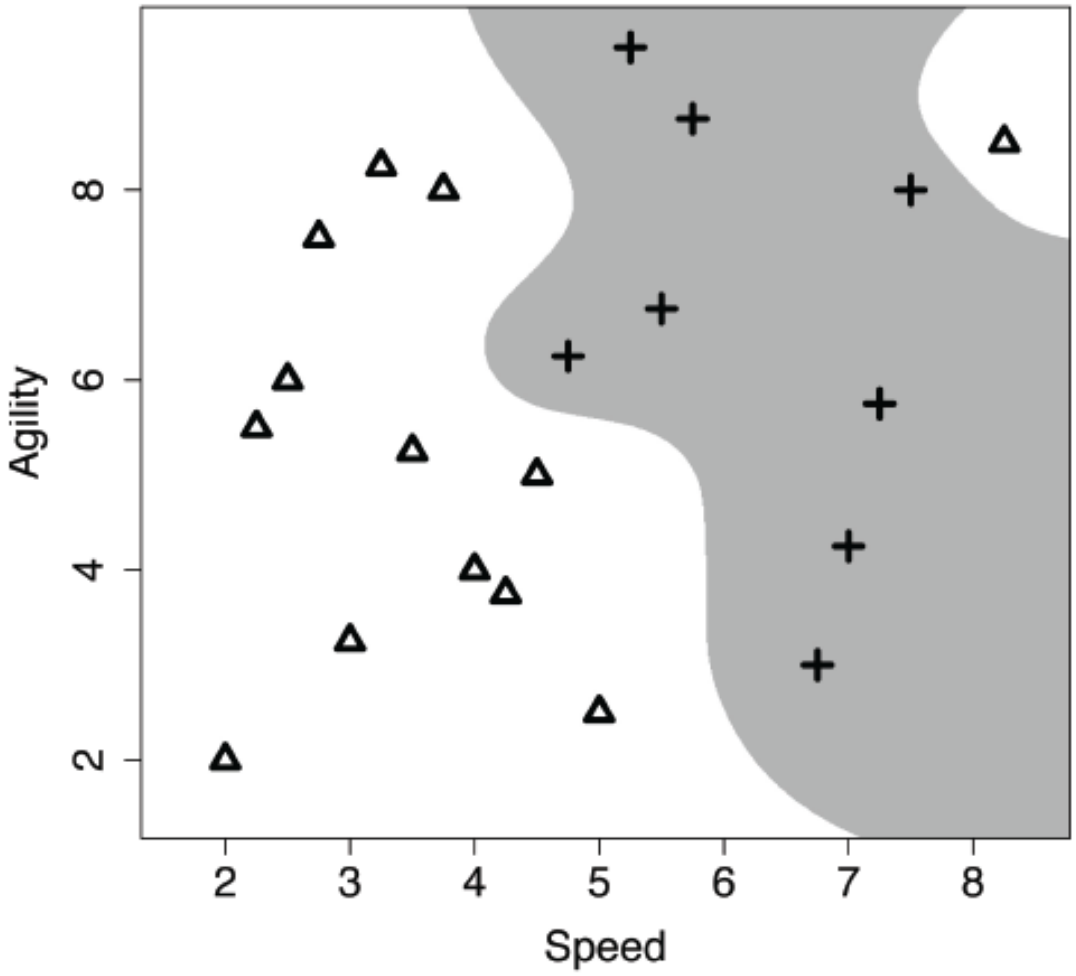
- Weighted KNN

$$\mathbf{M}_k(\mathbf{q}) = \arg \max_{l \in levels(t)} \sum_{i=1}^{k} \frac{1}{d(\mathbf{q}, \mathbf{x}_i)^2} \delta(t_i, l)$$

  - where $d(\mathbf{q}, \mathbf{x}_i)$ is a distance function

The K Nearest Neighbors, KNN

- Weighted KNN
  - K = 21



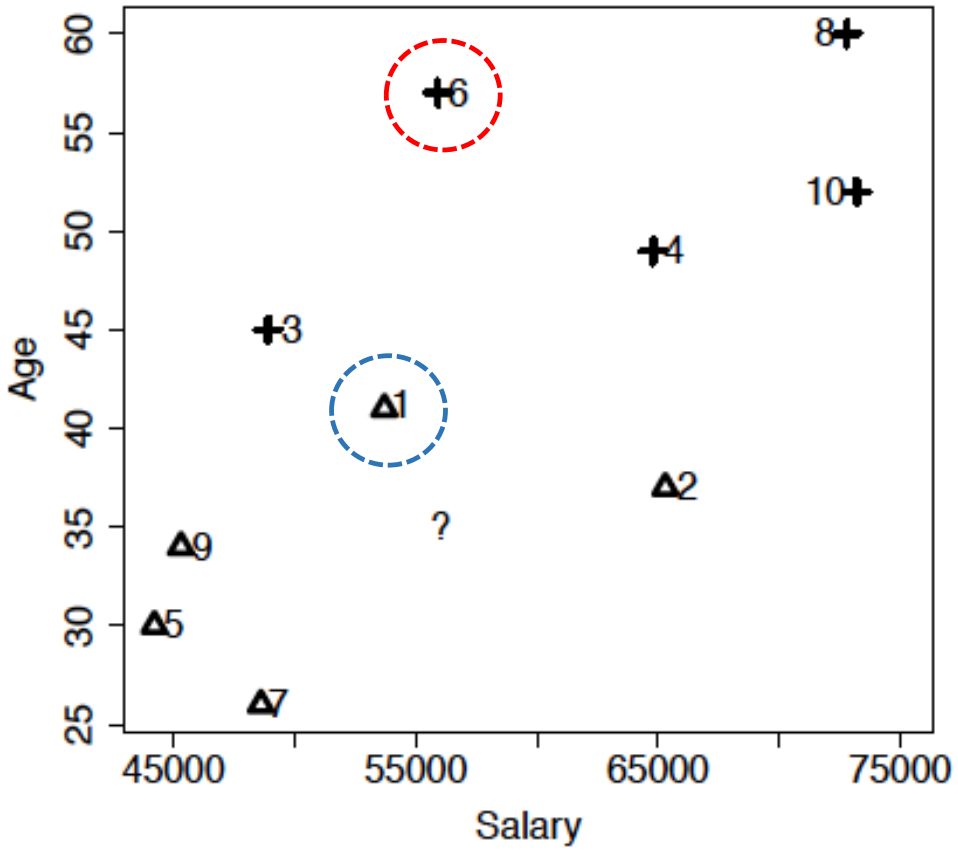
The K Nearest Neighbors, KNN

- KNN with data normalization
  - Customer dataset:

ID	Salary	Age	Purchased
1	53700	41	No
2	65300	37	No
3	48900	45	Yes
4	64800	49	Yes
5	44200	30	No
6	55900	57	Yes
7	48600	26	No
8	72800	60	Yes
9	45300	34	No
10	73200	52	Yes

The K Nearest Neighbors, KNN

- KNN without data normalization
  - Δ: Purchase = NO
  - +: Purchase = YES
  - ?: the query **q** = (56000, 35)
  - L^2-norm distance:
    - $d(\mathbf{q}, \mathbf{x}_1)$ = 2300.0078
    - $d(\mathbf{q}, \mathbf{x}_6)$ = 102.3914



The K Nearest Neighbors, KNN

- KNN without data normalization

ID	Salary	Age	Purch.	Salary and Age		Salary Only		Age Only	
				Dist.	Neigh.	Dist.	Neigh.	Dist.	Neigh.
1	53700	41	No	2300.0078	2	2300	2	6	4
2	65300	37	No	9300.0002	6	9300	6	2	2
3	48900	45	Yes	7100.0070	3	7100	3	10	6
4	64800	49	Yes	8800.0111	5	8800	5	14	7
5	44200	30	No	11800.0011	8	11800	8	5	5
6	55900	57	Yes	102.3914	1	100	1	22	9
7	48600	26	No	7400.0055	4	7400	4	9	3
8	72800	60	Yes	16800.0186	9	16800	9	25	10
9	45300	34	No	10700.0000	7	10700	7	1	1
10	73200	52	Yes	17200.0084	10	17200	10	17	8

The K Nearest Neighbors, KNN

- KNN with data normalization

	Normalized Dataset			Salary and Age		Salary Only		Age Only	
ID	Salary	Age	Purch.	Dist.	Neigh.	Dist.	Neigh.	Dist.	Neigh.
1	0.3276	0.4412	No	0.1935	1	0.0793	2	0.17647	4
2	0.7276	0.3235	No	0.3260	2	0.3207	6	0.05882	2
3	0.1621	0.5588	Yes	0.3827	5	0.2448	3	0.29412	6
4	0.7103	0.6765	Yes	0.5115	7	0.3034	5	0.41176	7
5	0.0000	0.1176	No	0.4327	6	0.4069	8	0.14706	3
6	0.4034	0.9118	Yes	0.6471	8	0.0034	1	0.64706	9
7	0.1517	0.0000	No	0.3677	3	0.2552	4	0.26471	5
8	0.9862	1.0000	Yes	0.9361	10	0.5793	9	0.73529	10
9	0.0379	0.2353	No	0.3701	4	0.3690	7	0.02941	1
10	1.0000	0.7647	Yes	0.7757	9	0.5931	10	0.50000	8

The K Nearest Neighbors, KNN

- In the most cases, the data should be normalized before the machine learning training
- Notice that the normalized data could lose the real data meaning

K-d tree

- k-d tree (k-dimensional tree)
  - A space-partitioning data structure for organizing points in a k-dimensional space.
  - Searching with multidimensional search key
  - A special case of binary space partitioning trees.
  - Performance:

Space	$O(n)$	$O(n)$
Search	$O(\log n)$	$O(n)$
Insert	$O(\log n)$	$O(n)$
Delete	$O(\log n)$	$O(n)$

Bentley, J. L. "Multidimensional binary search trees used for associative searching". Communications of the ACM. 18 (9): 509, 1975

K-d tree

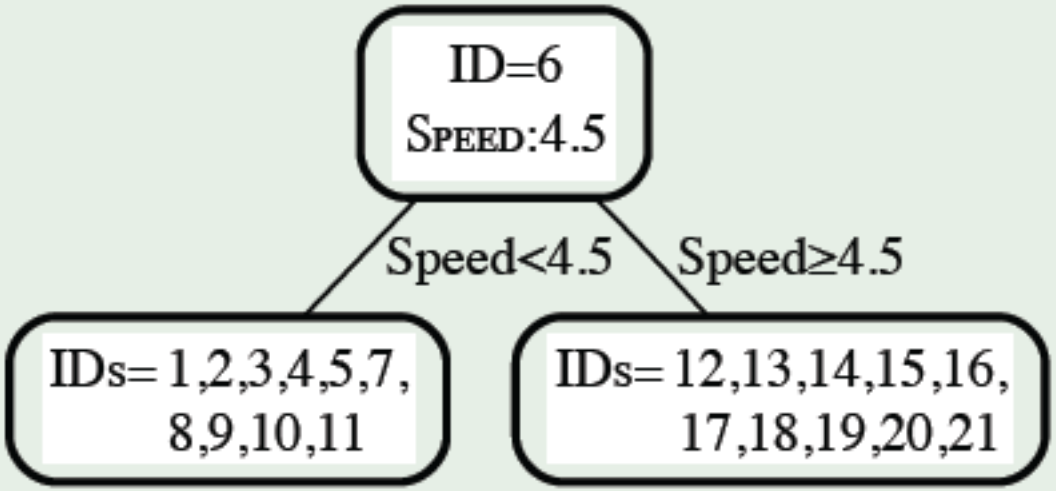
- Building a k-d tree
  - Dataset: college athletes
  - Dimension order:
    1. Speed
    2. Agility

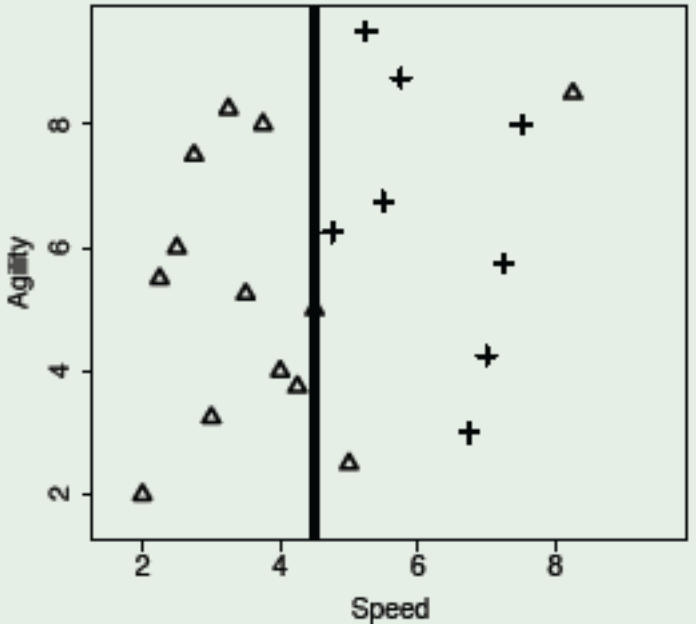
ID	Speed	Agility	Draft
1	2.50	6.00	No
2	3.75	8.00	No
3	2.25	5.50	No
4	3.25	8.25	No
5	2.75	7.50	No
6	4.50	5.00	No
7	3.50	5.25	No
8	3.00	3.25	No
9	4.00	4.00	No
10	4.25	3.75	No
11	2.00	2.00	No

ID	Speed	Agility	Draft
12	5.00	2.50	No
13	8.25	8.50	No
14	5.75	8.75	Yes
15	4.75	6.25	Yes
16	5.50	6.75	Yes
17	5.25	9.50	Yes
18	7.00	4.25	Yes
19	7.50	8.00	Yes
20	7.25	5.75	Yes
21	6.75	3.00	Yes

K-d tree

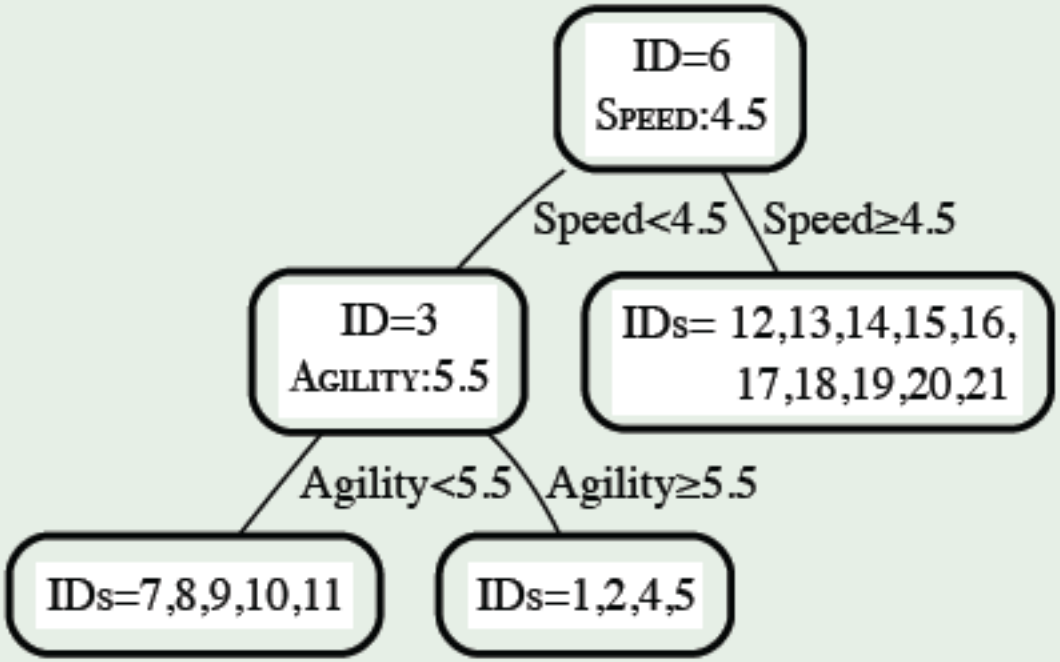
- Building a k-d tree
  - Splitting the first dimension: Speed
    - Using the median as the splitting pivot

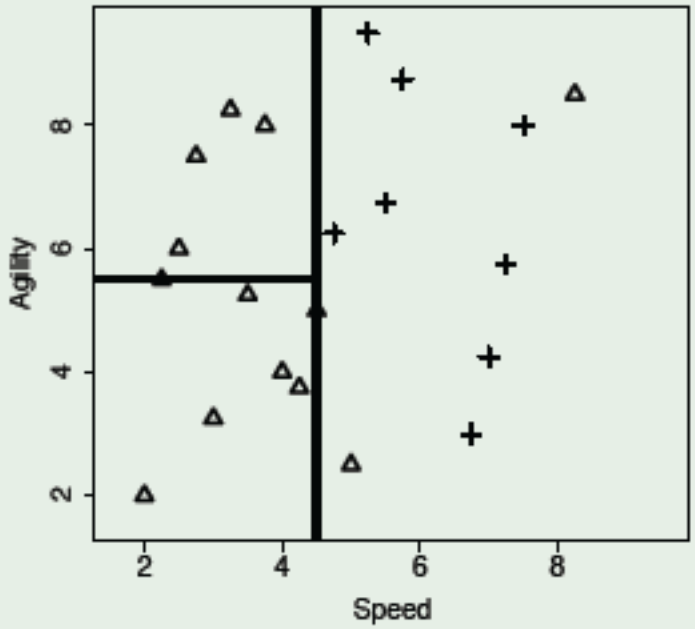




K-d tree

- Building a k-d tree
  - Splitting the second dimension: Agility



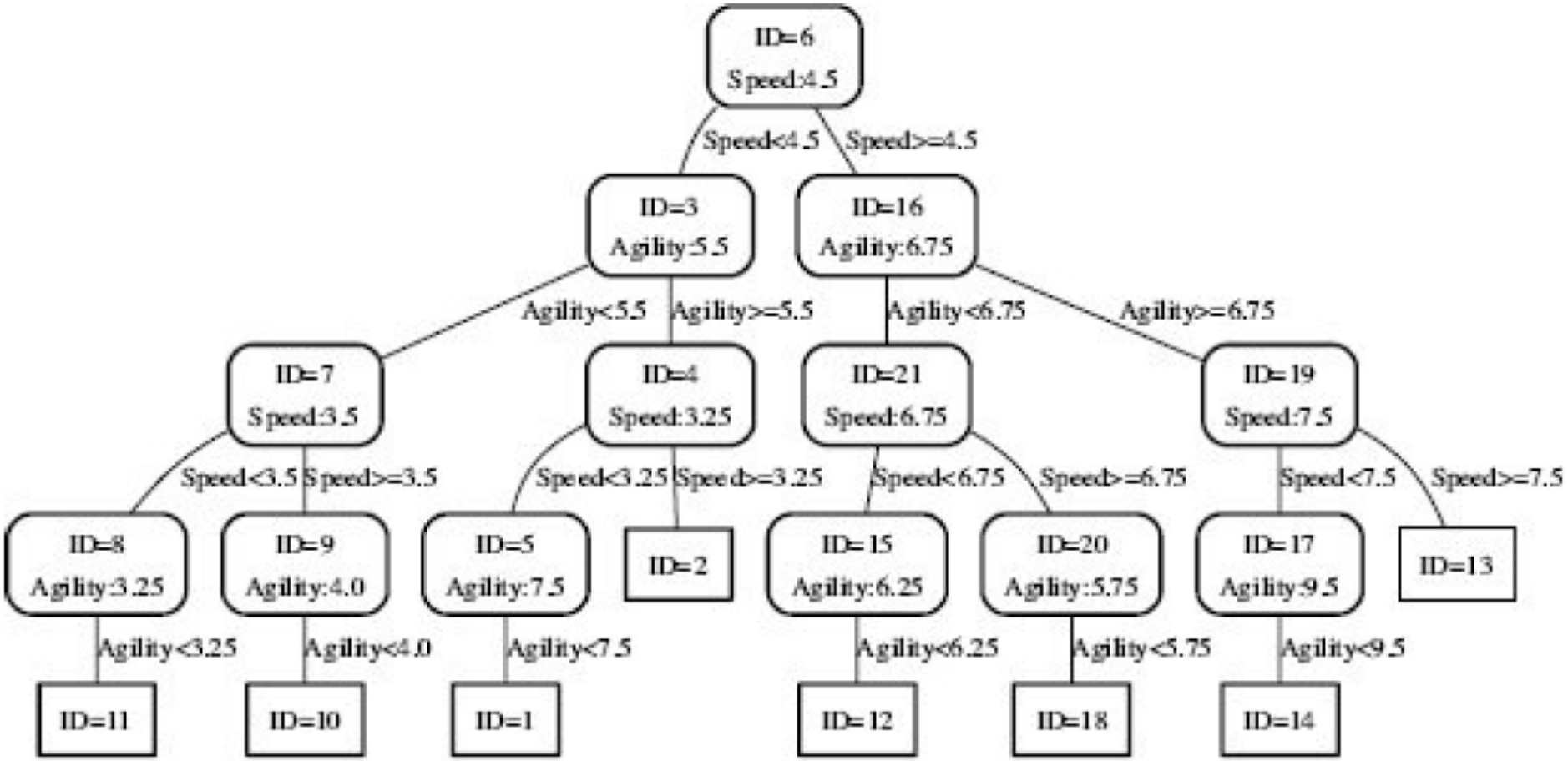


K-d tree

- Building a k-d tree
  1. Splitting d_1
  2. Splitting d_2
  3. …
  4. Splitting d_k
  5. If the number of items in a cell > 1, Repeat step 1; otherwise stop.

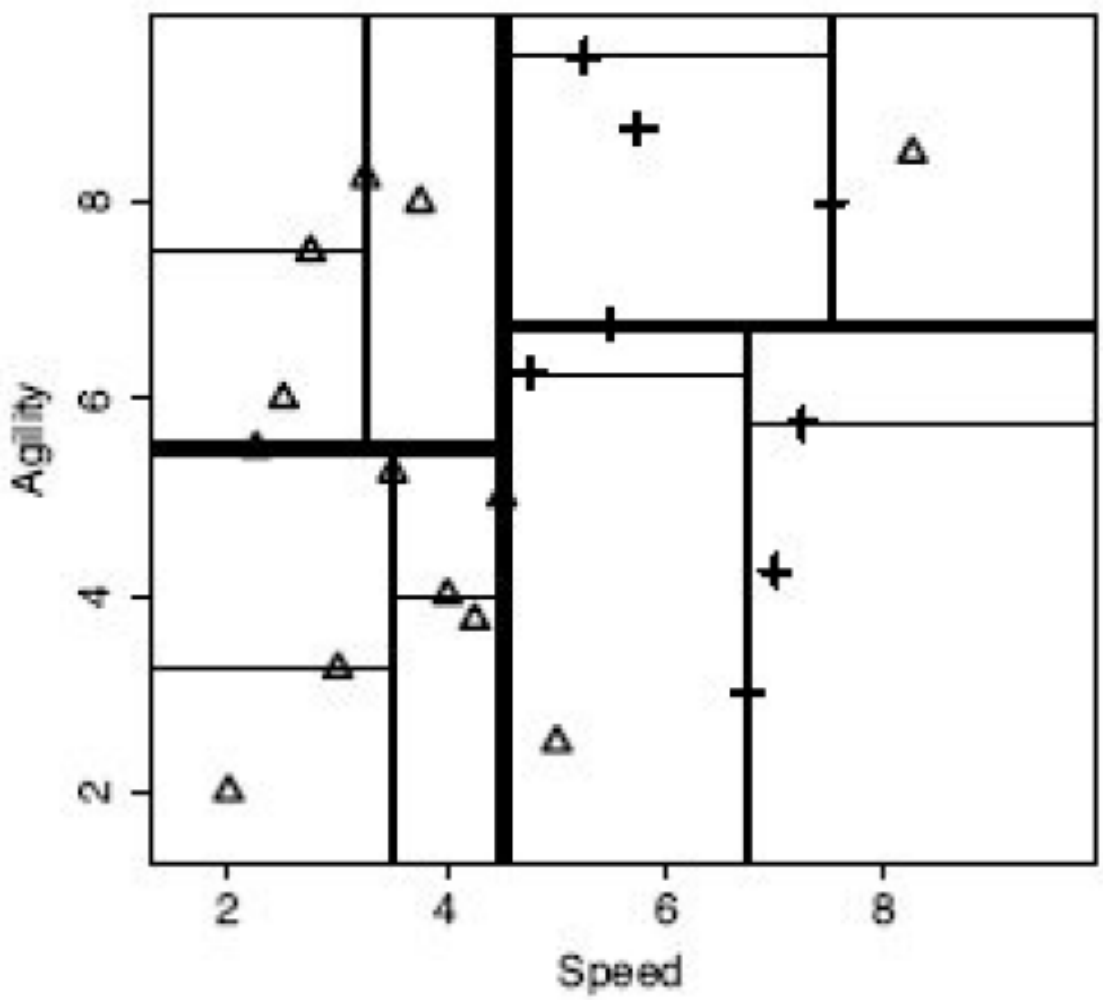
K-d tree

- Building a K-d tree
  - Final result



K-d tree

- Building a K-d tree
  - Final result



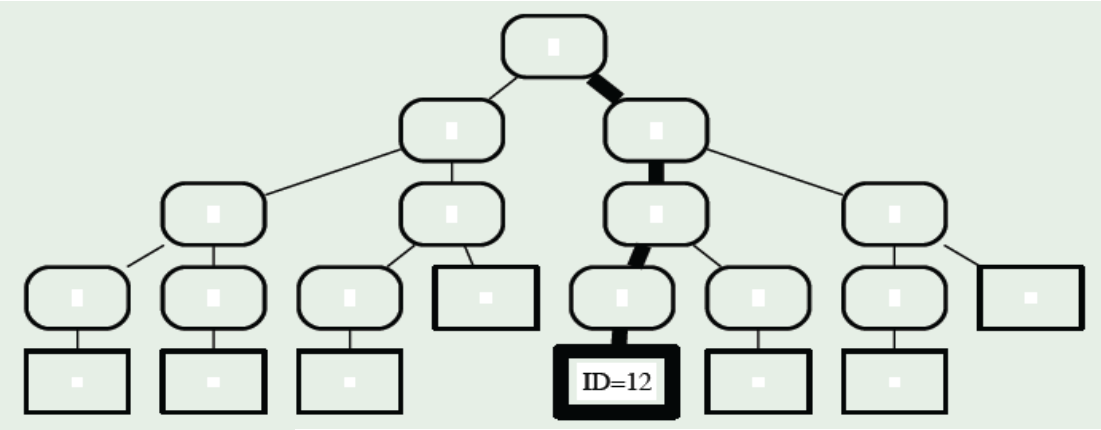
Finding the nearest neighbor by K-d tree

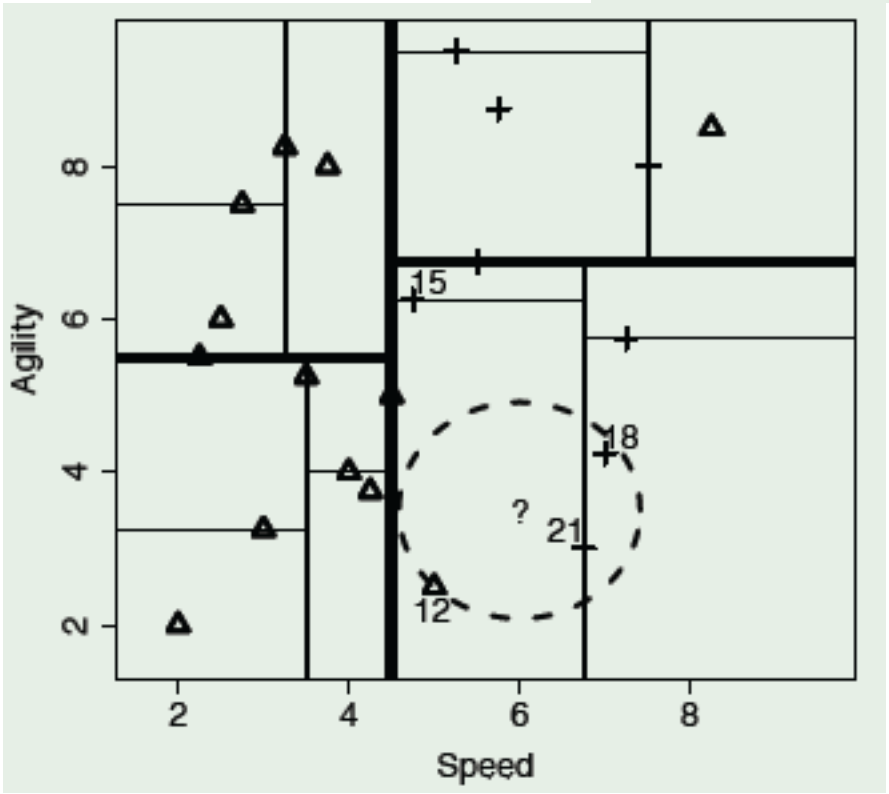
- Input:
  - Query: **q**
  - The root node of a K-d tree: **r**
- Algorithm
  1. The nearest neighbor, **t** = null
  2. The distance between **q** and **t,** $d_t = \infty$
  3. **x** = **descendTree**(**r**, **q**)
  4. while **x** != NULL do
  5. if d(**q**, **x**) < d_t ➔ **t** = **x**; d_t = d(**q**, **x**)
  6. if **boundaryDist**(**q**, **x**) < d_t ➔ **x** = **descendTree**(**x**, **q**)
  7. else ➔ **x** = **parent**(**x**)
  8. return **t**

descendTree(**x**, q): simple search from the node **x** to leaf
parent(**x**): returns the parent node of **x** and prune **x**
boundaryDist(**q**, **x**): comparing the distance between **q** and the hyperplane of **x** if **x** is a non-leaf node; otherwise, returns false.

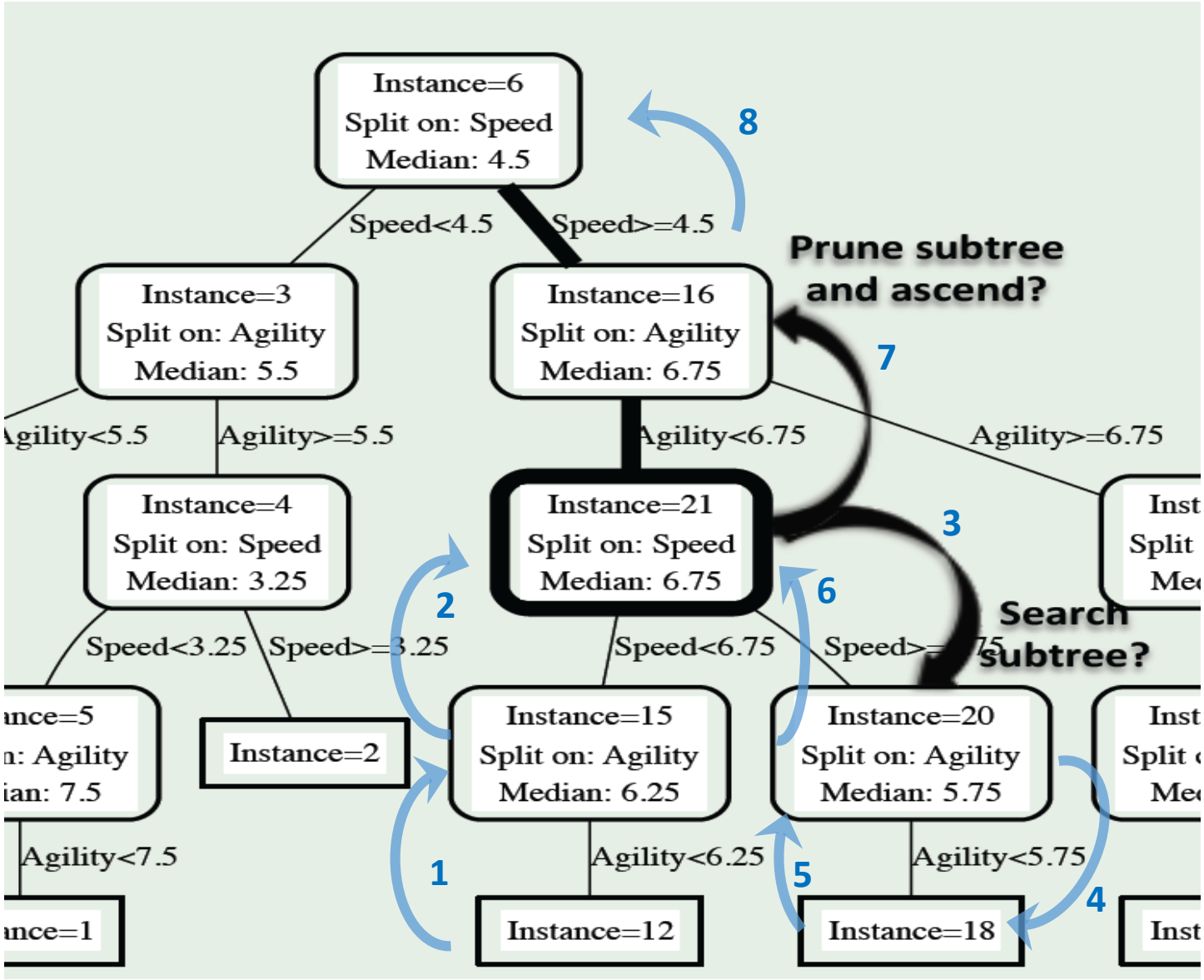
Finding the nearest neighbor by K-d tree

- **q** = (6.0, 3.5)



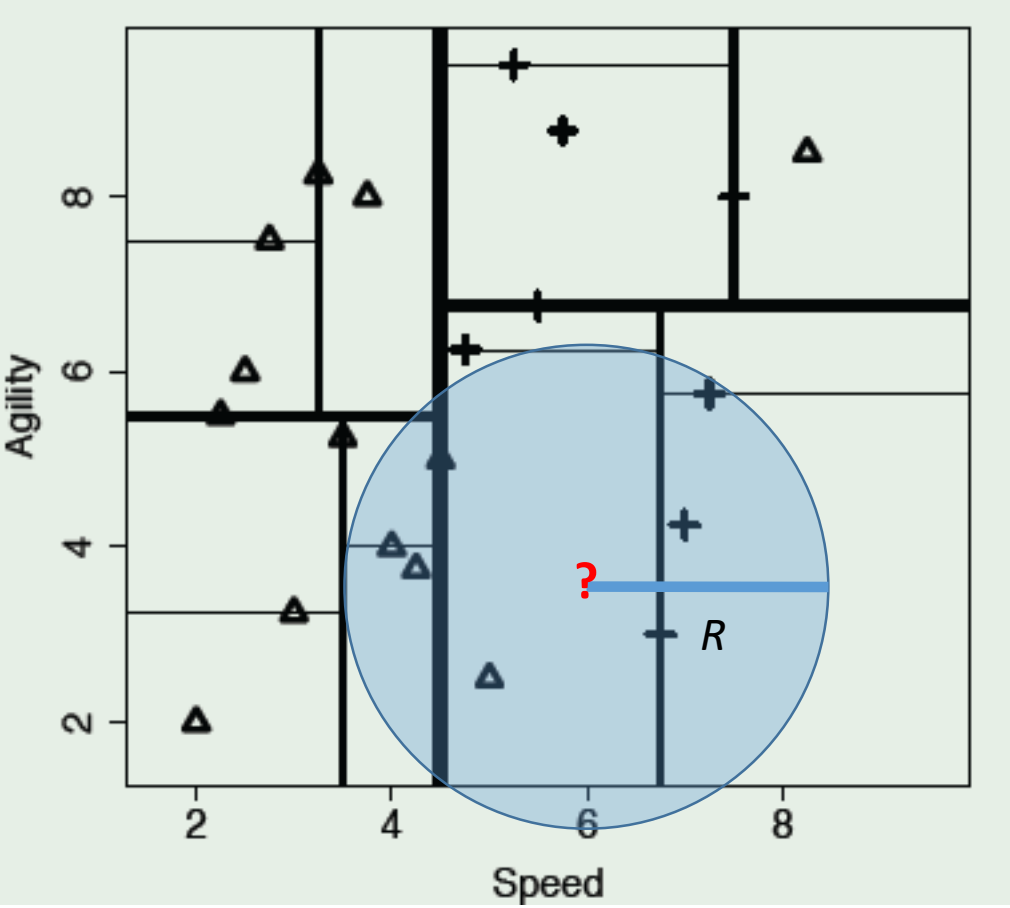


Finding the nearest neighbor by K-d tree



Finding the nearest neighbor by K-d tree

- K-NN by k-d tree
  - Let **t** be a ordered set with the capacity of *k*
- Given a radius *R*, finding the neighbors within a hypersphere $x_1^2 + x_2^2 + \cdots + x_k^2 = R$



Predicting Continuous Targets

- the average value in the neighborhood

$$\mathbf{M}_k(\mathbf{q}) = \frac{1}{k}\sum_{i=1}^{k} t_i$$

Predicting Continuous Targets

- Example:
  - A dataset of whiskeys listing the age (in years) and the rating (between 1 and 5, with 5 being the best) and the bottle price of each whiskey.

ID	Age	Rating	Price
1	0	2	30.00
2	12	3.5	40.00
3	10	4	55.00
4	21	4.5	550.00
5	12	3	35.00
6	15	3.5	45.00
7	16	4	70.00
8	18	3	85.00
9	18	3.5	78.00
10	16	3	75.00

ID	Age	Rating	Price
11	19	5	500.00
12	6	4.5	200.00
13	8	3.5	65.00
14	22	4	120.00
15	6	2	12.00
16	8	4.5	250.00
17	10	2	18.00
18	30	4.5	450.00
19	1	1	10.00
20	4	3	30.00

Predicting Continuous Targets

- Normalized data:

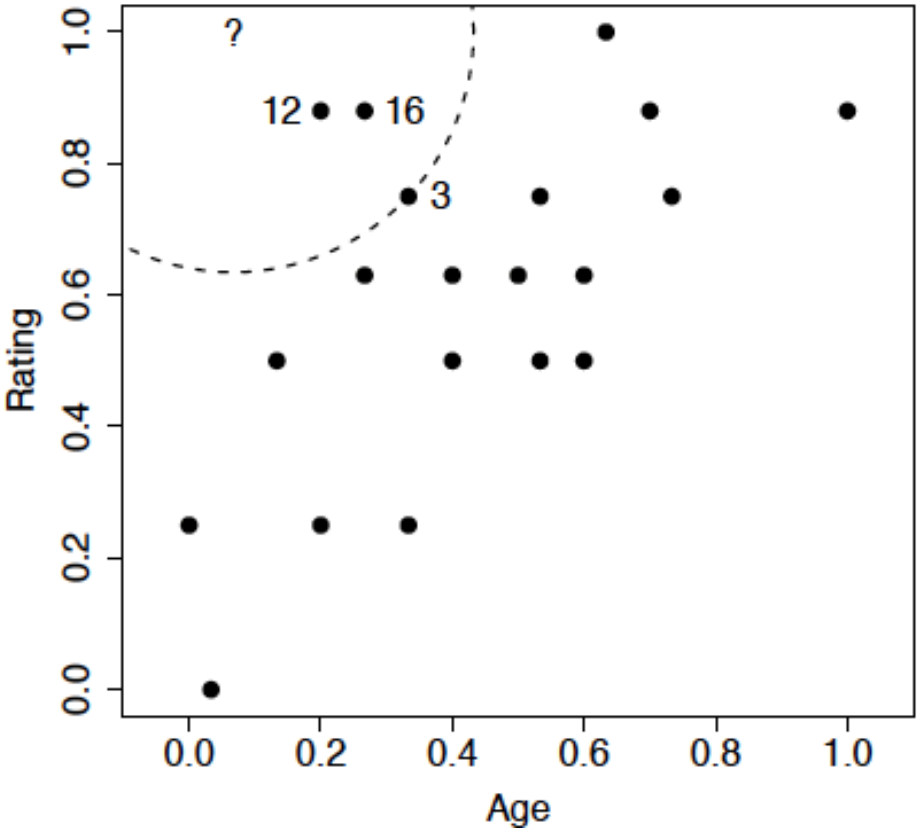
ID	Age	Rating	Price
1	0.0000	0.25	30.00
2	0.4000	0.63	40.00
3	0.3333	0.75	55.00
4	0.7000	0.88	550.00
5	0.4000	0.50	35.00
6	0.5000	0.63	45.00
7	0.5333	0.75	70.00
8	0.6000	0.50	85.00
9	0.6000	0.63	78.00
10	0.5333	0.50	75.00

ID	Age	Rating	Price
11	0.6333	1.00	500.00
12	0.2000	0.88	200.00
13	0.2667	0.63	65.00
14	0.7333	0.75	120.00
15	0.2000	0.25	12.00
16	0.2667	0.88	250.00
17	0.3333	0.25	18.00
18	1.0000	0.88	450.00
19	0.0333	0.00	10.00
20	0.1333	0.50	30.00

- Query: AGE = 0.0667 and RATING = 1.00
- K = 3

Predicting Continuous Targets

- Result



$$\frac{200.00 + 250.00 + 55.00}{3} = 168.33$$

Predicting Continuous Targets

- Weighted KNN for continuous targets

$$\mathbf{M}_k(\mathbf{q}) = \frac{\sum_{i=1}^{k} \frac{1}{d(\mathbf{q}, \mathbf{x}_i)^2} t_i}{\sum_{i=1}^{k} \frac{1}{d(\mathbf{q}, \mathbf{x}_i)^2}}$$

Similarity of binary features

- Example:
  - A binary dataset listing the behavior of two individuals on a website during a trial period and whether or not they subsequently signed-up for the website.

ID	Profile	FAQ	Help Forum	Newsletter	Liked	Signup
1	1	1	1	0	1	Yes
2	1	0	0	0	0	No

Similarity of binary features

- Example:
  - A binary dataset listing the behavior of two individuals on a website during a trial period and whether or not they subsequently signed-up for the website.

ID	Profile	FAQ	Help Forum	Newsletter	Liked	Signup
1	1	1	1	0	1	Yes
2	1	0	0	0	0	No

  - signup = ? if **q** = (1, 0, 1, 0, 0)

Similarity of binary features

- *CP*: co-presence <1, 1>
- *CA*: co-absence <0, 0>
- *PA*: presence-absence <1, 0>
- *AP*: absence-presence <0, 1>

		q	
		Pres.	Abs.
d$_1$	Pres.	CP=2	PA=0
	Abs.	AP=2	CA=1

		q	
		Pres.	Abs.
d$_2$	Pres.	CP=1	PA=1
	Abs.	AP=0	CA=3

Similarity of binary features

- Russel-Rao similarity
  - The ratio between the number of CP and the total number of binary features considered.

$$S_{RR}(\mathbf{q}, \mathbf{x}) = \frac{CP(\mathbf{q}, \mathbf{x})}{|\mathbf{q}|}$$

  - where $|\mathbf{q}|$ is the total number of binary features

  - Example:

$$S_{RR}(\mathbf{q}, \mathbf{d_1}) = \frac{2}{5} = 0.4$$

$$S_{RR}(\mathbf{q}, \mathbf{d_2}) = \frac{1}{5} = 0.2$$

    - $\mathbf{q}$ is more similar to $\mathbf{d}_1$ then $\mathbf{d}_2$.

		q	
		Pres.	Abs.
$\mathbf{d}_1$	Pres.	CP=2	PA=0
	Abs.	AP=2	CA=1

		q	
		Pres.	Abs.
$\mathbf{d}_2$	Pres.	CP=1	PA=1
	Abs.	AP=0	CA=3

Similarity of binary features

- Sokal-Michener similarity
  - the ratio between the total number of CP and CA, and the total number of binary features considered.

$$S_{SM}(\mathbf{q}, \mathbf{x}) = \frac{CP(\mathbf{q}, \mathbf{x}) + CA(\mathbf{q}, \mathbf{x})}{|\mathbf{q}|}$$

  - Example:

$$S_{SM}(\mathbf{q}, \mathbf{d_1}) = \frac{2+1}{5} = 0.6$$

$$S_{SM}(\mathbf{q}, \mathbf{d_2}) = \frac{1+3}{5} = 0.8$$

    - **q** is more similar to $\mathbf{d}_2$ then $\mathbf{d}_1$.

		q	
		Pres.	Abs.
$\mathbf{d}_1$	Pres.	CP=2	PA=0
	Abs.	AP=2	CA=1

		q	
		Pres.	Abs.
$\mathbf{d}_2$	Pres.	CP=1	PA=1
	Abs.	AP=0	CA=3

Similarity of binary features

- Jaccard similarity
  - ignoring CA

$$S_J(\mathbf{q}, \mathbf{x}) = \frac{CP(\mathbf{q}, \mathbf{x})}{CP(\mathbf{q}, \mathbf{x}) + PA(\mathbf{q}, \mathbf{x}) + AP(\mathbf{q}, \mathbf{x})}$$

  - Example:

$$S_J(\mathbf{q}, \mathbf{d_1}) = \frac{2}{2 + 0 + 2} = 0.5$$

$$S_J(\mathbf{q}, \mathbf{d_2}) = \frac{1}{1 + 1 + 0} = 0.5$$

    - **q** is equally similar to $\mathbf{d}_1$ and $\mathbf{d}_2$.

		q	
		Pres.	Abs.
$\mathbf{d}_1$	Pres.	CP=2	PA=0
	Abs.	AP=2	CA=1

		q	
		Pres.	Abs.
$\mathbf{d}_2$	Pres.	CP=1	PA=1
	Abs.	AP=0	CA=3

Other Similarity

- Cosine similarity

$$S_{cos}(\mathbf{q}, \mathbf{x}) = \frac{\mathbf{q} \cdot \mathbf{x}}{|\mathbf{q}||\mathbf{x}|}$$

Other Similarity

- Mahalanobis distance

$$d_M(\mathbf{q}, \mathbf{x}) = \sqrt{(\mathbf{q} - \mathbf{x})^T \boldsymbol{\Sigma}^{-1} (\mathbf{q} - \mathbf{x})}$$

  - where $\boldsymbol{\Sigma}$ is a covariance matrix

$$\boldsymbol{\Sigma} = \begin{bmatrix} var(x_1) & cov(x_1, x_2) & \cdots & cov(x_1, x_k) \\ cov(x_2, x_1) & var(x_2) & & cov(x_2, x_k) \\ \vdots & & \ddots & \vdots \\ cov(x_n, x_1) & cov(x_n, x_2) & \cdots & var(x_k) \end{bmatrix},$$

  if the number of features is *k*,

$$cov(a, b) = \frac{1}{n-1} \sum_{i=1}^{n} ((a_i - \bar{a}) \times (b_i - \bar{b})),$$

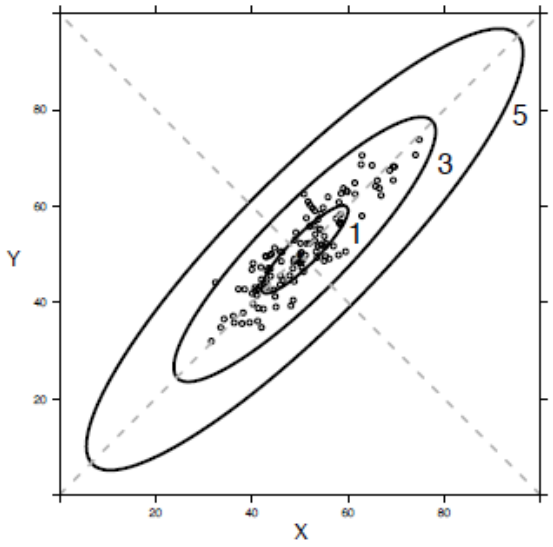
$$var(a) = cov(a, a)$$

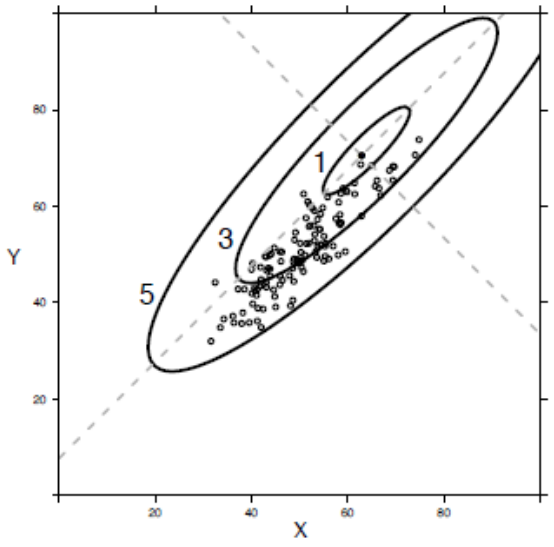
  - *n* is the number of data;
  - $\bar{a}$ and $\bar{b}$ are the averages of feature *a* and *b* respectively.

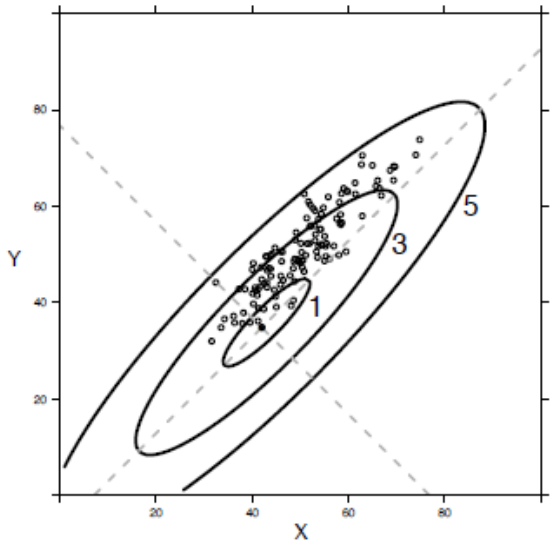
Covariance matrix generalizes the notion of variance to multiple dimension

Other Similarity

- Mahalanobis distance
  - Similar to Euclidean distance, the mahalanobis distance squares the differences of the features.
  - But it also rescales the differences (using the inverse covariance matrix) so that all the features have unit variance and the effects of covariance is removed.







K-Means Clustering

- Clustering *n* data points **X** into *k* disjoint subsets S_i containing n_i data points so as to minimize the sum-of-squares criterion.

$$\mathbf{X} = \{\boldsymbol{x_1}, \boldsymbol{x_2}, \ldots, \boldsymbol{x_n}\}, \mathbf{S} = \{\boldsymbol{S_1}, \boldsymbol{S_2}, \ldots, \boldsymbol{S_k}\}$$

$$\underset{\boldsymbol{S}}{\operatorname{argmin}} \sum_{\boldsymbol{i=1}}^{\boldsymbol{k}} \sum_{\boldsymbol{x \in S_i}} \|\boldsymbol{x} - \boldsymbol{\mu_i}\|^{\mathbf{2}}$$

- where $\boldsymbol{\mu_i}$ is the center of $\boldsymbol{S_i}$
- *K*-means clustering is a type of **unsupervised learning**, which is used when data without defined categories.
- References:
  - https://en.wikipedia.org/wiki/K-means_clustering
  - http://mathworld.wolfram.com/K-MeansClusteringAlgorithm.html
  - https://www.datascience.com/blog/k-means-clustering
  - http://www.saedsayad.com/clustering_kmeans.htm

K-Means Clustering

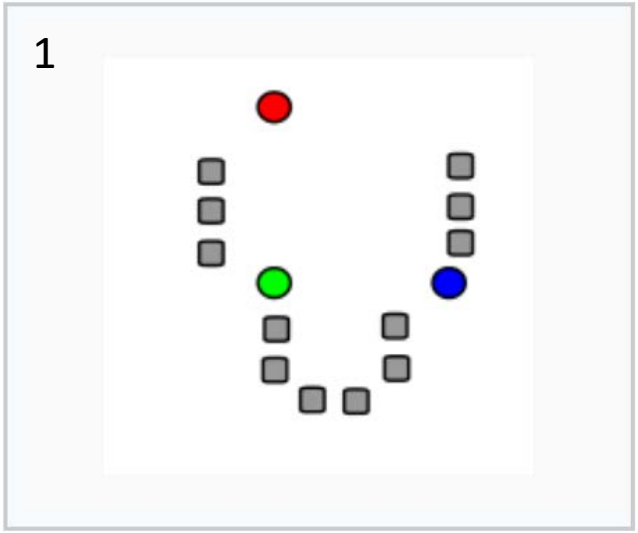
- Standard algorithm

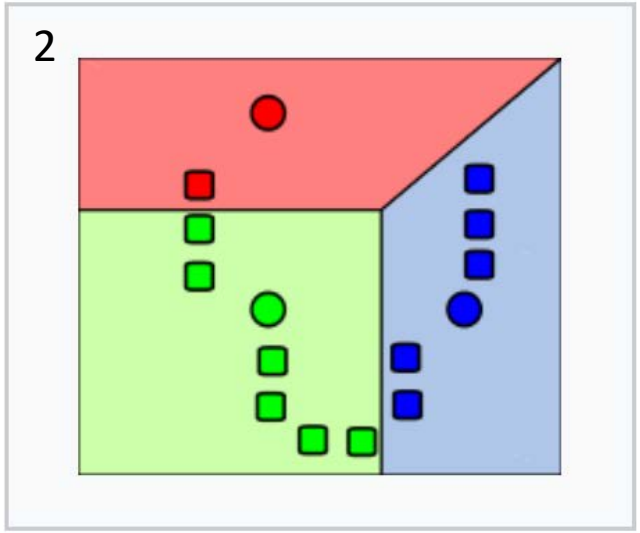
  Input: **X** and *k.*

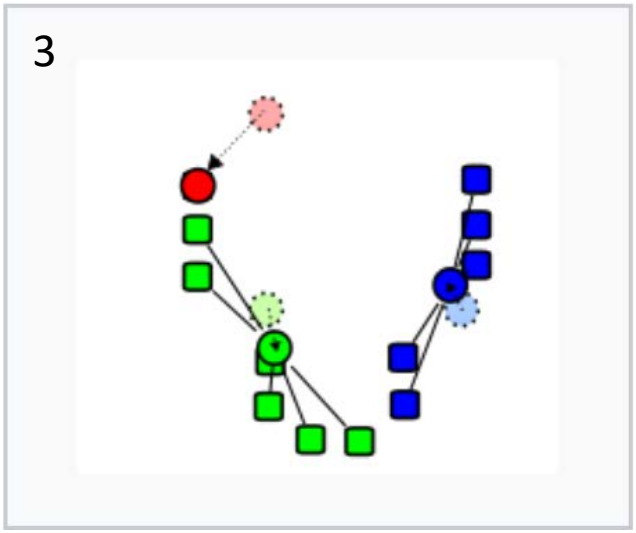
  1. Select *k* points at random as cluster centers.
     - These *k* points may not ∈ **X**
  2. Assign data instances to their closest cluster center according to the Euclidean distance function.
     - Generating **S**
     - Voronoi diagram
  3. Updating the cluster center by the mean of data instances in each cluster.
  4. Repeat steps 2 and 3 until a stopping criteria is met:
     - No data points change clusters.
     - The sum of the distances is minimized.
     - Some maximum number of iterations is reached.

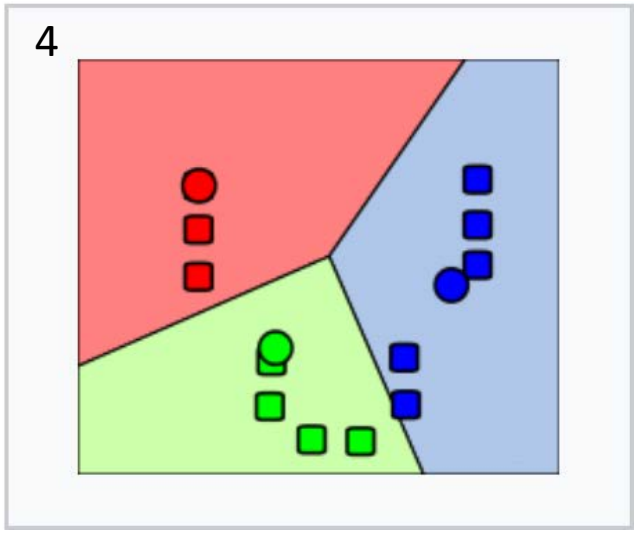
K-Means Clustering

- Standard algorithm







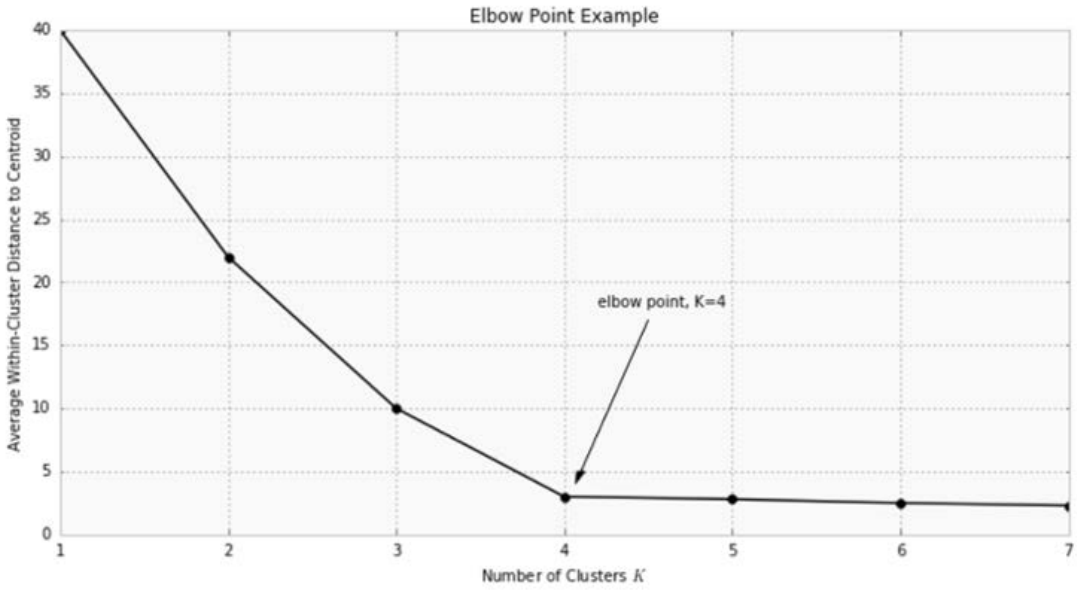


K-Means Clustering

- How to decide *k*?
  - There is no perfect method for determining exact value of *K.*
  - An approximate algorithm
    - Increasing the *k* will always reduce the distance to data points
    - Calculating

$$\alpha_k = \frac{1}{k}\sum_{i=1}^{k}\sum_{x \in S_i} \|x - \mu_i\|^2$$

    - Select *k* while $\frac{d\alpha_k}{dk}$ less than a small number



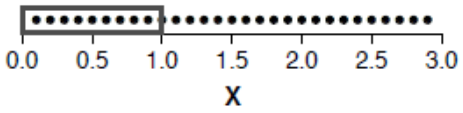
K-Means Clustering

- Applications
  - Segment by purchase history
  - Segment by activities on a web-based application
  - Define personas based on interests
  - Detect activity types in motion sensors
  - Group images
  - Separate audio

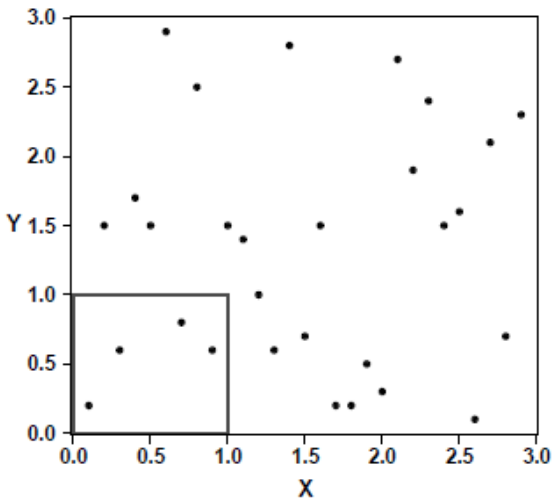
Feature Selection

- The curse of dimensionality
  - $density = k^{\frac{1}{m}}$
    - *k* = the number of data instances
    - *m* = the number of dimensions

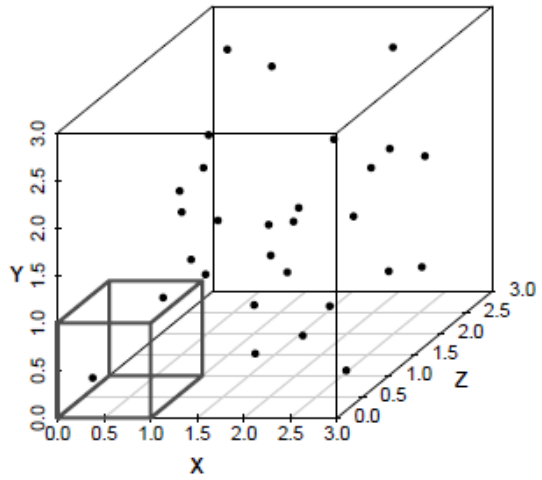
$density = 10^{\frac{1}{1}} = 10$



$density = 4^{\frac{1}{2}} = 2$



$density = 2^{\frac{1}{3}} = 1.2599$



- if we fix *k* = 10➔ 2D:

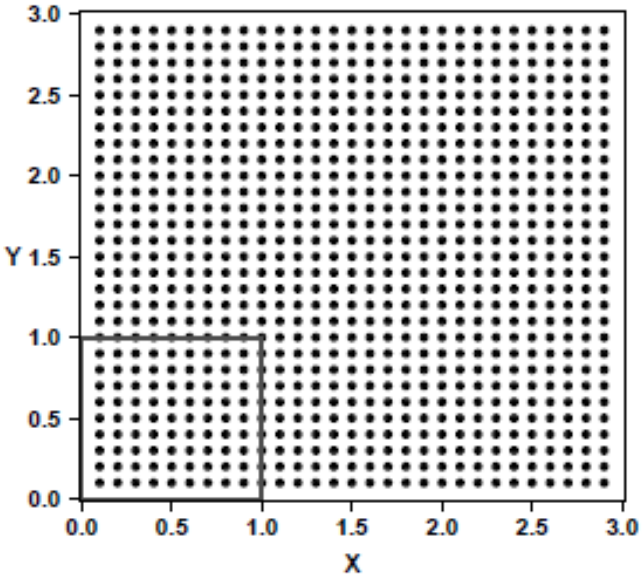
$density = 10^{\frac{1}{2}} = 3.1623$

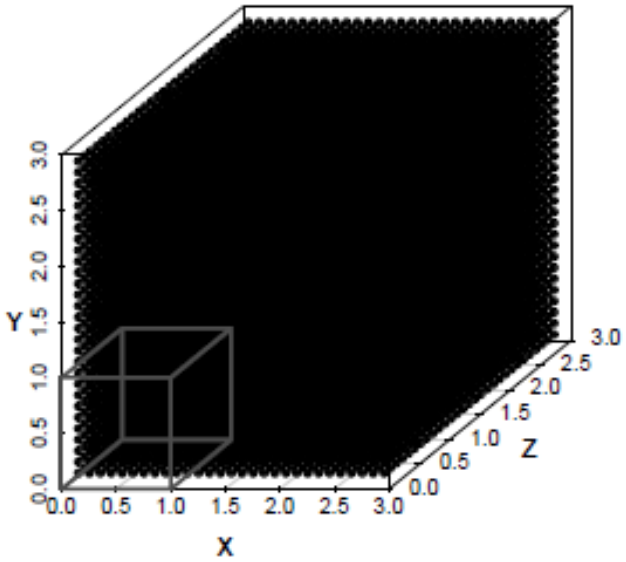
3D:

$density = 10^{\frac{1}{3}} = 2.1544$

Feature Selection

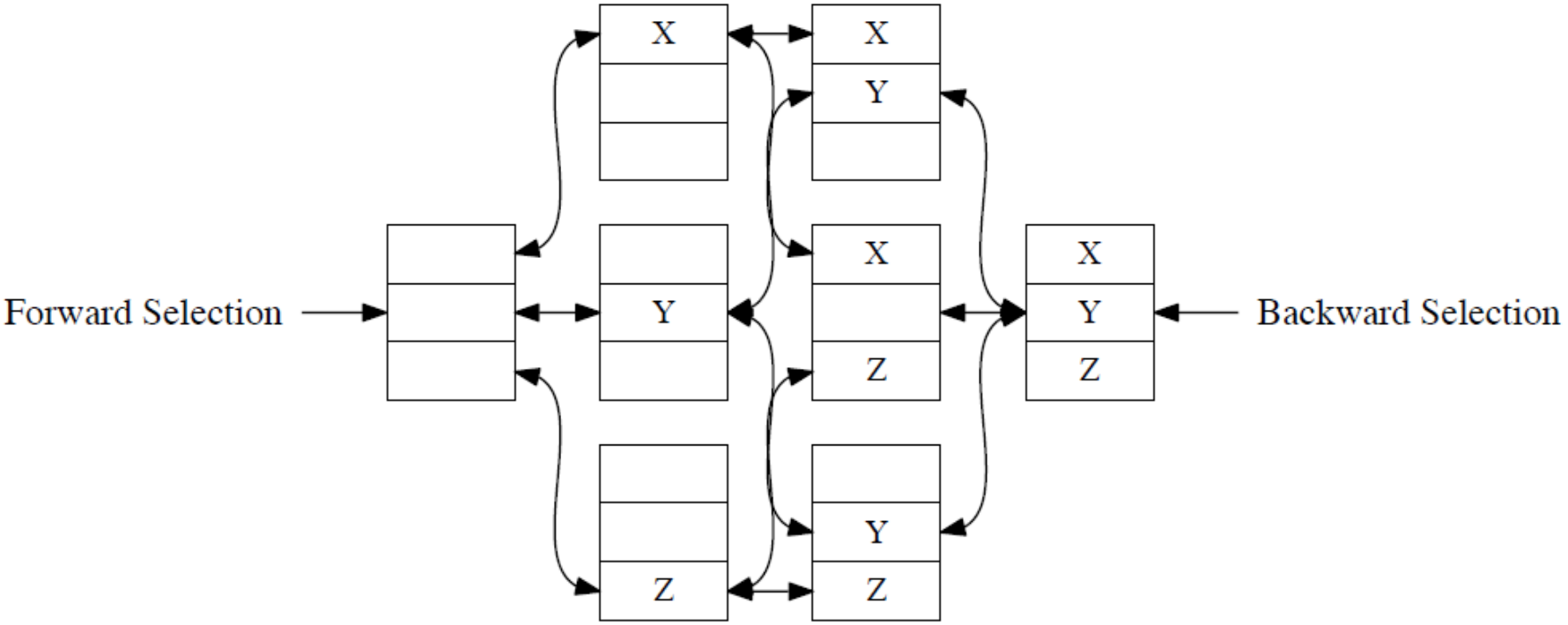
- The curse of dimensionality
  - if we fix *density* = 10
    - 1D: $k = 10$
    - 2D: $k^{\frac{1}{2}} = 10 \rightarrow k = 100$
    - 3D: $k^{\frac{1}{3}} = 10 \rightarrow k = 1000$





Feature Selection

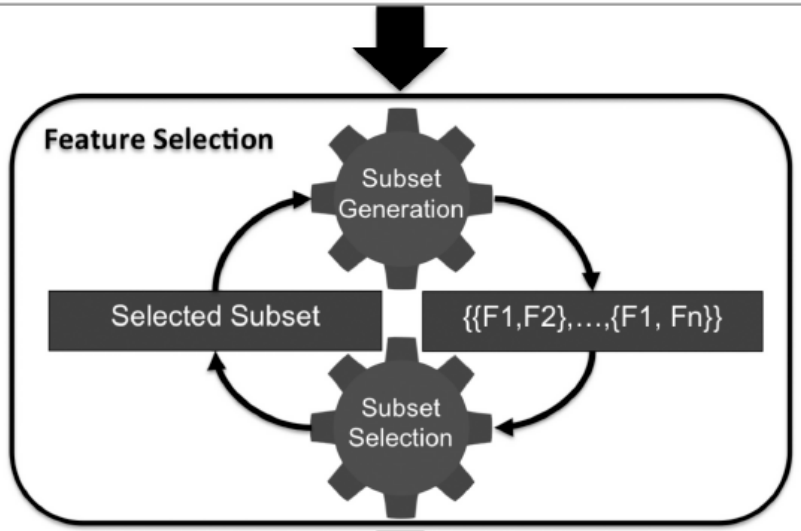
- Feature subset



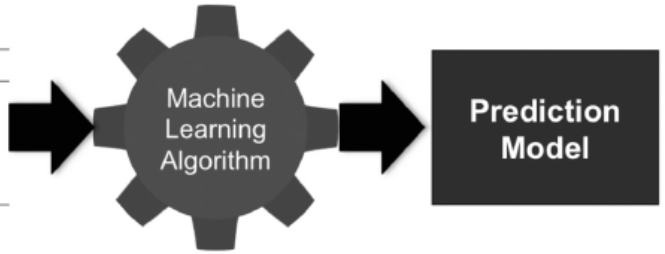
Feature Selection

- Iterative feature selection

ID	F1	F2	F3	...	F150	F151	...	F227	F228	...	F387	...	Fn	Target
1	-	-	-	...	-	-	...	-	-	...	-	...	-	-
2	-	-	-	...	-	-	...	-	-	...	-	...	-	-
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
K	-	-	-	...	-	-	...	-	-	...	-	...	-	-

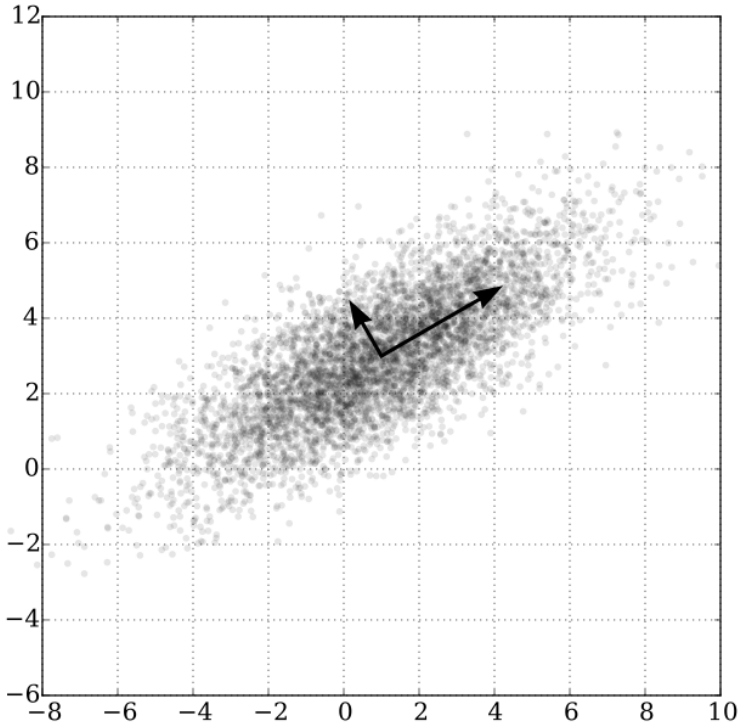


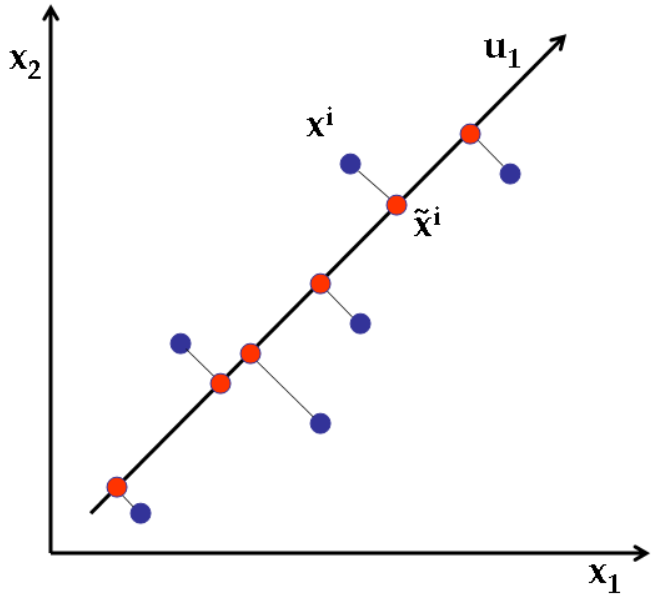
ID	F2	F150	F227	F387	Target
1	-	-	-	-	-
2	-	-	-	-	-
...	...	...	...	...	...
K	-	-	-	-	-



PCA

- Principal component analysis
  - The main linear technique for **dimensionality reduction**.
  - It performs a linear mapping of the data to a **lower-dimensional space** in such a way that the variance of the data in the low-dimensional representation is maximized.





PCA

- Each data instance has *n* features
  - $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$,
  - $\mathbf{x}^{\mathrm{T}} = [x_1 \quad x_2 \quad \cdots \quad x_n]$
- *m* data instances➔ $m \times n$ matrix
  - $\boldsymbol{A} = \begin{bmatrix} \mathbf{x_1}^{\mathrm{T}} \\ \mathbf{x_2}^{\mathrm{T}} \\ \vdots \\ \mathbf{x_m}^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & & \ddots & \\ x_{m1} & x_{m2} & & x_{mn} \end{bmatrix}$

PCA

- M is a symmetric matrix if $M^{\mathrm{T}} = M$
  - $A^{\mathrm{T}}A$ is a symmetric matrix
    - Because $(A^{\mathrm{T}}A)^{\mathrm{T}} = A^{\mathrm{T}}A$

- U is an unitary matrix if $U^*U = UU^* = I$
  - where I is the identity matrix
  - *: conjugate transpose
    - if $\boldsymbol{A} = \begin{bmatrix} 1 & -2-3i \\ 1+4i & 5i \end{bmatrix}, \boldsymbol{A}^* = \begin{bmatrix} 1 & 1-4i \\ -2+3i & -5i \end{bmatrix}$

- Q is an orthogonal matrix if $Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I$ and Q is a square matrix with real entries

PCA

- $\boldsymbol{A}$ is an $m \times n$ matrix
  - Column space: $\boldsymbol{A}\mathbf{x}$, where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$
    - a space of $m \times 1$ matrices
  - Row space: $\mathbf{x}\boldsymbol{A}$, where $\mathbf{x} = [x_1, x_2, \ldots, x_m]$
    - a space of $1 \times n$ matrices

PCA

- $\boldsymbol{A}$ is an $m \times n$ matrix
  - An eigenvector of A is a non-zero vector $\mathbf{v}$ such that

$$\boldsymbol{A}\mathbf{v} = \lambda\mathbf{v}$$

or

$$\mathbf{v}^{\mathrm{T}}\boldsymbol{A} = \lambda\mathbf{v}^{\mathrm{T}}$$

  - The scalar λ is the eigenvalue corresponding to $\mathbf{v}$
  - Given a non-zero real number s, $s\mathbf{v}$ and $\mathbf{v}$ have the same eigenvalue
    - $\boldsymbol{A}\mathbf{v} = \lambda\mathbf{v}$
    - $\boldsymbol{A}(s\mathbf{v}) = \lambda(s\mathbf{v})$
  - We often let every eigenvector is normalized (the length is one)

PCA

- Linearly independent
  - A set of n vectors, $V = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$
  - V is linearly independent if
    $a_1\mathbf{v}_1 + a_2\mathbf{v}_2 + \ldots + a_n\mathbf{v}_n$ = zero vector, can only be satisfied by all a_i are zeros

- Suppose that A has n linearly independent eigenvectors,
  - $\boldsymbol{A}$ is an $m \times n$ matrix
  - Q is an $n \times n$ matrix = $[\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n]$
  - $\boldsymbol{\Lambda}$ is an $n \times n$ diagonal matrix with n eigenvalue
  - $AQ = Q\boldsymbol{\Lambda}$

PCA

- Every **real symmetric matrix** can be decomposed as follows
  - $\boldsymbol{A}$ is an $n \times n$ real symmetric matrix
  - $A = Q \Lambda Q^{\mathrm{T}}$
    - Q contains n orthogonal eigenvectors
      - $Q Q^{\mathrm{T}} = I$
    - Λ is an $n \times n$ diagonal matrix contains n eigenvalues

PCA

- Singular value decomposition, SVD
  - Every real matrix has a singular value decomposition
    - A is an $m \times n$ matrix
    - $A = UDV^{\mathrm{T}}$
      - U is an $m \times m$ matrix, $UU^{\mathrm{T}} = U^{\mathrm{T}}U = I$
      - D is an $m \times n$ diagonal matrix
      - V is an $n \times n$ matrix, $VV^{\mathrm{T}} = V^{\mathrm{T}}V = I$
  - But the same is not true of the eigenvalue decomposition.
    - For example, if a matrix is not square, the eigendecomposition is not defined, and we must use a singular value decomposition instead.

PCA

- $\boldsymbol{A}$ is an $m \times n$ real matrix
  - $A = UDV^{\mathrm{T}}$
- $A^{\mathrm{T}}A$ is an $n \times n$ real symmetric matrix
  - $A^{\mathrm{T}}A = (UDV^{\mathrm{T}})^{\mathrm{T}}UDV^{\mathrm{T}} = VDU^{\mathrm{T}}UDV^{\mathrm{T}} = VD^2V^{\mathrm{T}}$
  - $Q = V$
  - $\Lambda = D^2$
- AA^{T} has the same property

PCA

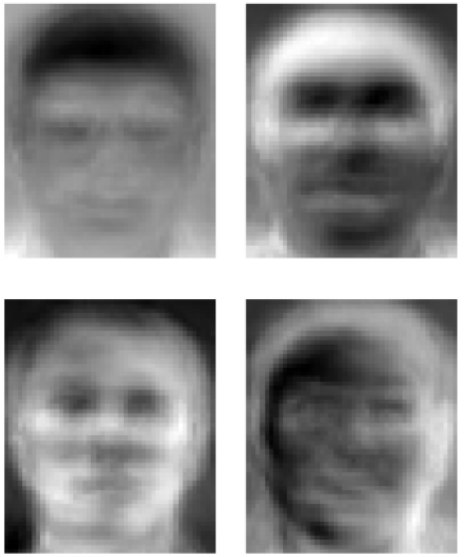
- The center of *m* data instances
  - $\bar{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m} \mathbf{x}_i$
- *m* data instances➔ $m \times n$ matrix
  - m data instances
  - n dimensions (features)
  - $\boldsymbol{A} = \begin{bmatrix} (\mathbf{x_1} - \bar{\mathbf{x}})^{\mathrm{T}} \\ (\mathbf{x_2} - \bar{\mathbf{x}})^{\mathrm{T}} \\ \vdots \\ (\mathbf{x_m} - \bar{\mathbf{x}})^{\mathrm{T}} \end{bmatrix}$
  - $A^{\mathrm{T}}A$ ($n \times n$) is the covariance matrix to describe the data variance of all dimensions (features)

PCA

- PCA
  - $A^{\mathrm{T}}A = Q\Lambda Q^{\mathrm{T}}$
    - where $\Lambda = \begin{bmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{bmatrix}, \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$
    - $Q = [\mathbf{v_1} \quad \mathbf{v_2} \quad \cdots \quad \mathbf{v_n}]$
  - The data can be represented by in a space with the basis of Q
    - $\mathbf{y}^{\mathrm{T}} = (\mathbf{x} - \bar{\mathbf{x}})^{\mathrm{T}}Q$
    - The axis $\mathbf{v_1}$ is more importance than $\mathbf{v_2}$
    - Choose $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_k}$, where λ_k larger than a threshold, we call these axes are principal components

PCA Example: Face Recognition

- L. Sirovich; M. Kirby (1987). "Low-dimensional procedure for the characterization of human faces". *Journal of the Optical Society of America A*. 4 (3): 519–524.
- Eigenfaces
  - Eigenvectors of a training set of *m* face images
  - Each image: $r \times c$ pixels ➔ let $n = r \times c$ ➔a vector of *n* intensities
  - The average of *m* face images➔$\bar{\mathbf{x}}$
  - *m* face images - $\bar{\mathbf{x}}$ ➔ $A = m \times n$ matrix
  - Finding the eigenvectors of $A^{\mathrm{T}}A$
  - Each eigenvector consists of *n* intensities
  - eigenvectors ➔ eigenfaces



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PCA Example: Face Recognition

- Choose the principal components

$$\bar{\lambda} = (\lambda_1 + \lambda_n + \cdots + \lambda_n)$$

  - Given a threshold *t*, we choose *k* principal components such that

$$\frac{(\lambda_1+\lambda_n+\cdots+\lambda_k)}{\bar{\lambda}} > t$$

  - Therefore, each training face image can be represented by
    - $\mathbf{y}^{\mathrm{T}} = (\mathbf{x} - \bar{\mathbf{x}})^{\mathrm{T}} Q$
    - ➔$\mathbf{y}^{\mathbf{T}} Q^{\mathbf{T}} = (\mathbf{x} - \bar{\mathbf{x}})^{\mathrm{T}}$
    - ➔$\mathbf{x} = Q\boldsymbol{y} + \bar{\mathbf{x}}$
    - $y_1\times$ 1st eigenface + $y_2\times$ 2nd eigenface + … + $y_k\times$ k^{th} eigenface

PCA Example: Face Recognition

- Face recognition
  - input face: $\mathbf{z}$
  - $\mathbf{w^T} = (\mathbf{z} - \bar{\mathbf{x}})^{\mathrm{T}} Q$
  - Find the nearest neighbour of $\mathbf{w^T}$ from the transformed training set (all $\mathbf{y}$)

PCA Example: Feature Analysis

- Reference:
  - Jeff Jauregui "Principal component analysis with linear algebra", 2012.
- Sibley's Bird Database of North American birds
- 100 bird species. ➔ $m = 100$
- In studying **the size of a bird**, each specie should be observed by three features: **length**, **wingspan**, and **weight**. ➔ $n = 3$



PCA Example: Feature Analysis

- $A^{\mathrm{T}}A = \begin{bmatrix} 91.43 & 171.92 & 297.99 \\ 545.21 & 373.92 & 545.21 \\ 297.99 & 171.92 & 1297.26 \end{bmatrix}$

- ➔$\lambda_1 = 1626.52, \lambda_2 = 128.99, \lambda_3 = 7.10$

- ➔$\mathbf{v}_1 = \begin{bmatrix} 0.22 \\ 0.41 \\ 0.88 \end{bmatrix}, \mathbf{v_2} = \begin{bmatrix} 0.25 \\ 0.85 \\ -0.46 \end{bmatrix}, \mathbf{v_3} = \begin{bmatrix} 0.97 \\ -0.32 \\ -0.08 \end{bmatrix}$
- Which of the feature is most significant in determining a bird's "size"?

PCA Example: Feature Analysis

- The third entry, weight, of $\mathbf{v}_1$ is the largest
  - Weight is the most significant.
  - Wingspan is the next most important factor in determining a bird's size.
- $\mathbf{v}_2$ is also telling us something
  - Some birds are large size with small wingspan and large weight ➔ stoutness birds