Unsupervised Learning

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We have seen so far...

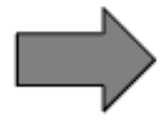
- Until now we have seen supervised methods, in which a human **training** (supervision) was needed
- Training was given as a **large set of examples**
- Each example was an association from a set of **input variables** (X) to an **output variable** (y)

Price	Rooms	SQM
700000	5	230

City
Rome

- Now we will see **unsupervised methods**, in which no training is involved. They are used to:
  - Mine frequent patterns to make **associations** between examples
  - Group together similar objects creating **clusters**
  - Find latent variables to meaningfully **represent** the examples

Price	Rooms	SQM
700000	5	230



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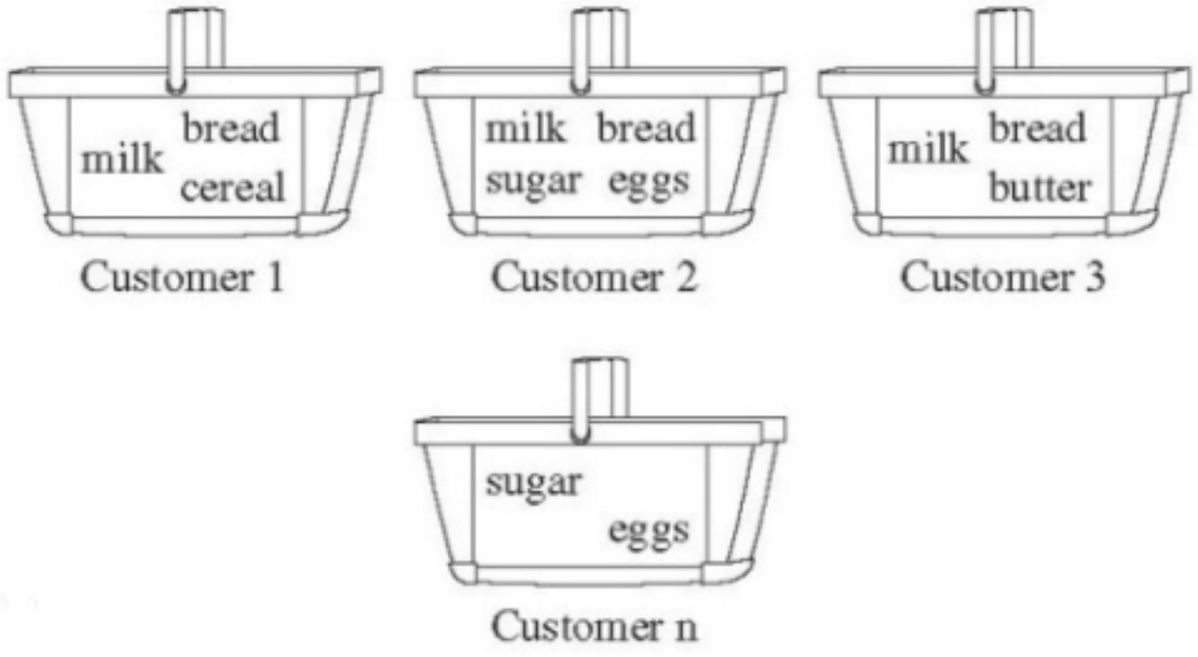
Mining frequent patterns

- Mine frequent patterns to make **associations** between examples allows to discover new relations from data.
- Frequent patterns are patterns that appear frequently in a data set.
- This kind of technique can be applied in different scenarios, such as:
  - Marketing basket analysis (frequent patterns in products buying)
  - Bioinformatics (associating genes and diseases)
  - Intrusion detection systems (finding malicious activities)

Market basket analysis

- A typical example of frequent pattern mining is market basket analysis.
- This process analyzes customer **buying habits** by finding associations between the different items that customers place in their “shopping baskets”
- For instance, if customers are buying milk, how likely are they **to buy also** bread (and what kind of bread) on the same trip to the supermarket?



Example: AllElectronics

- As a manager of an *AllElectronics* branch you wonder: “Which groups or sets of items are customers likely to purchase on a given trip to the store?”
- To answer your question, market basket analysis may be performed on the data of customer transactions at your store.
- You can then use the results to design a smart store layout
  - Items that are frequently purchased together can be placed in proximity to encourage the combined sale of such items.
  - Example: if customers who purchase computers also tend to buy antivirus software at the same time, then placing the hardware display close to the software display may help increase the sales of one or both items.

Association Rules

- Transactions data can be analyzed for buying patterns that reflect items that are frequently associated (purchased together).
- These patterns can be represented in the form of **association rules**.
- For example, the information that *customers who purchase computers also tend to buy antivirus software at the same time* is represented in the following **association rule**:

```
computer => antivirus_software [support = 2%, confidence = 60%].
```

- *[support = 2%]* means that in the 2% of all the transactions, computer and antivirus software are bought together.
- *[confidence = 60%]* means that 60% of the people who bought a computer also bought an antivirus software at the same time.

Support & Confidence

- We can now have a more formal look at the two measures.
- Let *A* be a set of items (can be a singlet {*computer*})
- Let *B* be a set of items (can be a singlet {*antivirus_software*})
- The rule $A \Rightarrow B$ holds in the transactions set with **support** *s*, where *s* is the percentage of all transactions, that **contains** $A \cup B$

$$support(A \Rightarrow B) = P(A \cup B)$$

- The rule $A \Rightarrow B$ holds in the transactions set with **confidence** *c*, where *c* is the percentage of transactions containing *A*, that also contain B

$$confidence(A \Rightarrow B) = P(B|A)$$

Mining strong association rules

- Association rules are considered **strong** if they satisfy **both**:
  1. A **minimum support threshold**.
  2. A **minimum confidence threshold**.
- These thresholds can be set by users or domain experts.
- In general, **association rule mining** can be viewed as a two-step process:

1. **Find all frequent itemsets** *A*: by definition, each of these itemsets will occur at least as frequently as a predetermined minimum support (if *A* doesn't satisfy the threshold, neither will *A*U*B* : if milk is not among the transactions, neither is milk and coffee).

2. **Generate strong association rules** from the frequent itemsets *A* to *B*: By definition, these rules must satisfy minimum support and minimum confidence.

Example: AllElectronics data

- Consider the following transactions data for *AllElectronics*:

Transaction ID	Item set
T100	{Item1, Item2, Item5}
T200	{Item2, Item4}
T300	{Item2, Item3}
T400	{Item1, Item2, Item4}
T500	{Item1, Item3}
T600	{Item2, Item3}
T700	{Item1, Item3}
T800	{Item1, Item3}
T900	{Item1, Item2, Item3, Item5}
T1000	{Item1,Item2,Item3}

- We set minimum support 30% and confidence 80%.

Example: iteration 1

- We first consider the *support* of itemsets with cardinality 1:

1-Itemsets	Support
{Item1}	70%
{Item2}	70%
{Item3}	70%
{Item4}	20%
{Item5}	20%

- The itemsets that **does not** satisfy minimum support are pruned.
- The itemsets that **does** satisfy minimum support are taken in the next iteration.

Example: iteration 2

- We now consider the *support* of itemsets with cardinality 2:

2-Itemsets	Support
{Item1, Item2}	40%
{Item1, Item3}	50%
{Item2, Item3}	40%

- All itemsets satisfy minimum support threshold and are taken in the next iteration.

Example: iteration 3

- We now consider the *support* of itemsets with cardinality 3:

3-Itemsets	Support
{Item1, Item2,Item3}	20%

- The itemset **does not** satisfy minimum support are pruned
- We stop the iterations as there can be no larger itemsets.
- We have therefore found the largest frequent itemsets as:

2-Itemsets	Support
{Item1, Item2}	40%
{Item1, Item3}	50%
{Item2, Item3}	40%

Example: association rules

- We found the frequent itemsets {Item1,Item2}, {Item1,Item3}, {Item2,Item3}
- What are the **association rules** that can be generated from the above frequent itemsets?
  - {Item1} ⇒ {Item2} [support=40%]
  - {Item2} ⇒ {Item1} [support=40%]
  - {Item1} ⇒ {Item3} [support=50%]
  - {Item3} ⇒ {Item1} [support=50%]
  - {Item2} ⇒ {Item3} [support=40%]
  - {Item3} ⇒ {Item2} [support=40%]
- We already computed their support in the search for frequent itemsets, therefore we know that minimum support is satisfied.
- We now go back to the data to compute their confidence and check if they are **strong association rules** (confidence ≥ 70%)

Example: confidence

Trans. ID	Item set
T100	{Item1, Item2, Item5}
T200	{Item2, Item4}
T300	{Item2, Item3}
T400	{Item1, Item2, Item4}
T500	{Item1, Item3}
T600	{Item2, Item3}
T700	{Item1, Item3}
T800	{Item1, Item3}
T900	{Item1, Item2, Item3, Item5}
T1000	{Item1,Item2,Item3}

- We can compute confidence with the support values we already computed.

$$confidence(A \Rightarrow B) = P(B|A) = \frac{support(A \cup B)}{support(A)}$$

- {Item1} ⇒ {Item2} [support=40%, confidence=4/7= 57%]
- {Item2} ⇒ {Item1} [support=40%, confidence=4/7= 57%]
- {Item1} ⇒ {Item3} [support=50%, confidence=5/7= 71%]
- {Item3} ⇒ {Item1} [support=50%, confidence=5/7= 71%]
- {Item2} ⇒ {Item3} [support=40%, confidence=4/7= 57%]
- {Item3} ⇒ {Item2} [support=40%, confidence=4/7= 57%]

Mining association rules: recap

- We have seen how to iteratively find frequent itemsets and filter them by minimum support and minimum confidence rules.
- The algorithm we used to find strong association rules is called ***a priori* algorithm**.
- The *a priori* property says that ***if a set cannot pass a test, all of its supersets will fail the same test as well.*** This allowed us to prune and reduce the search space.

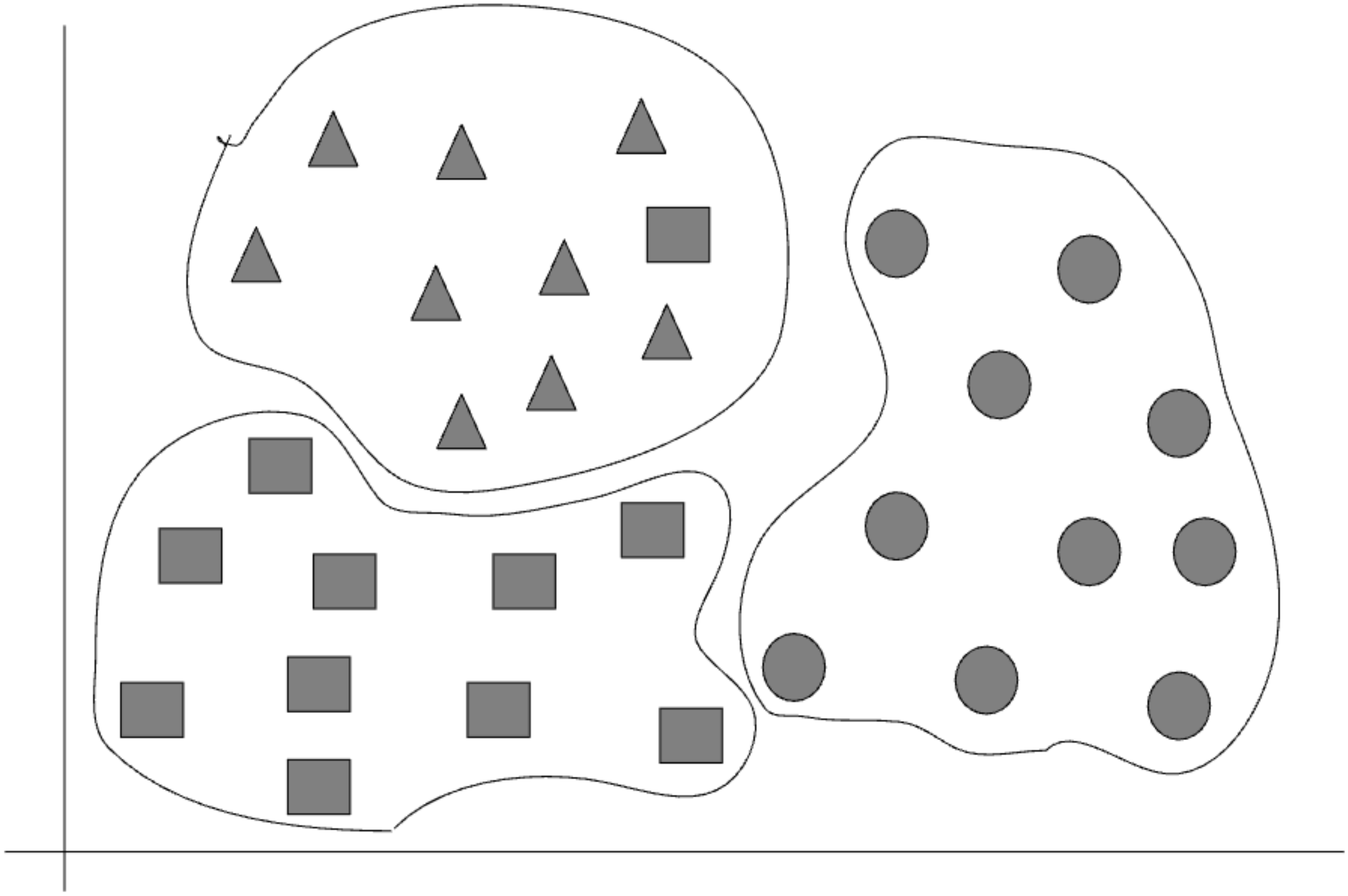
- **Association rules mining** of itemsets is an example of ***unsupervised learning* task.**
- We will now see how items (or, more generally, objects) can be *clustered* together based on their common features.
- This method is called **clustering.**

Clustering

- Goal of clustering is to group together similar objects (documents, patients, houses) into “clusters”, depending on their features:
  - usually, they are **grouped together if they belong to the same “category”** but...
  - **categories** are **not known**!

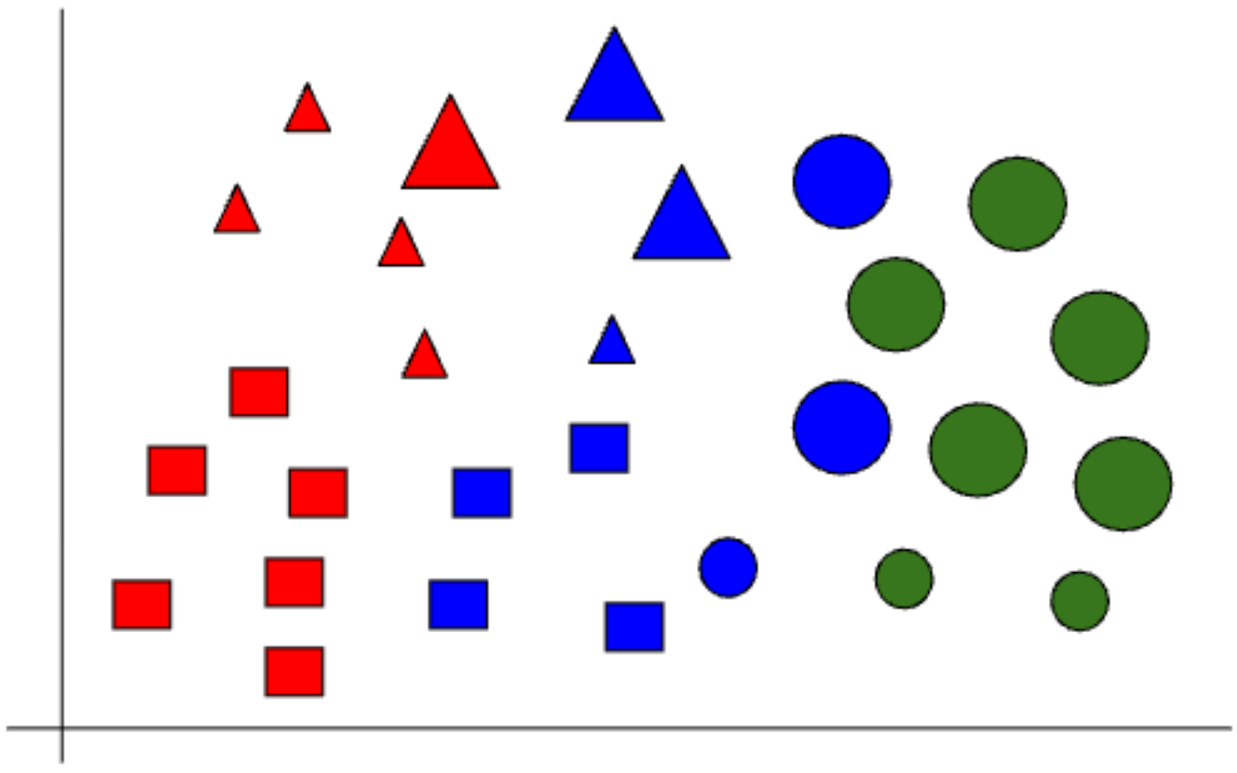
- Clustering has no “ground truth” since:
  - it’s an unsupervised technique: there is no labeled data.
  - evaluation depends on perspective, may be different for different people.
  - being without supervision restrictions, it may find new, unknown common features shared by objects: ***pattern discovery.***

Clustering example



Clustering Bias (1)

- It's common to say that clusters are "in the eye of the beholder":
  - are the terms "horse" and "car" similar?
  - in the previous example the clustering bias was the shape of each object, it was obvious.
  - with more features it may be less obvious.



Clustering Bias (2)

- It's common to say that clusters are "in the eye of the beholder":
  - are the terms "horse" and "car" similar?
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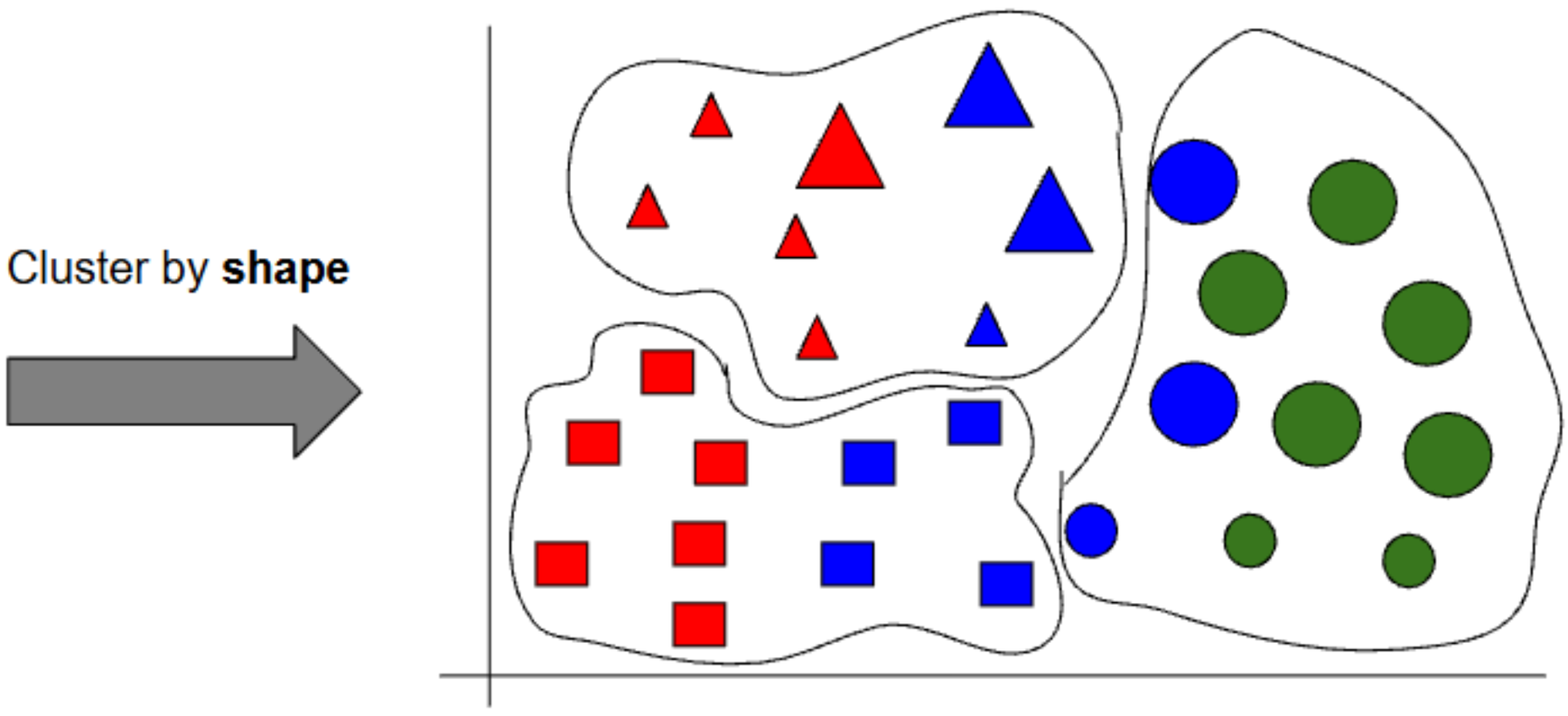
  - with more features it may be less obvious.

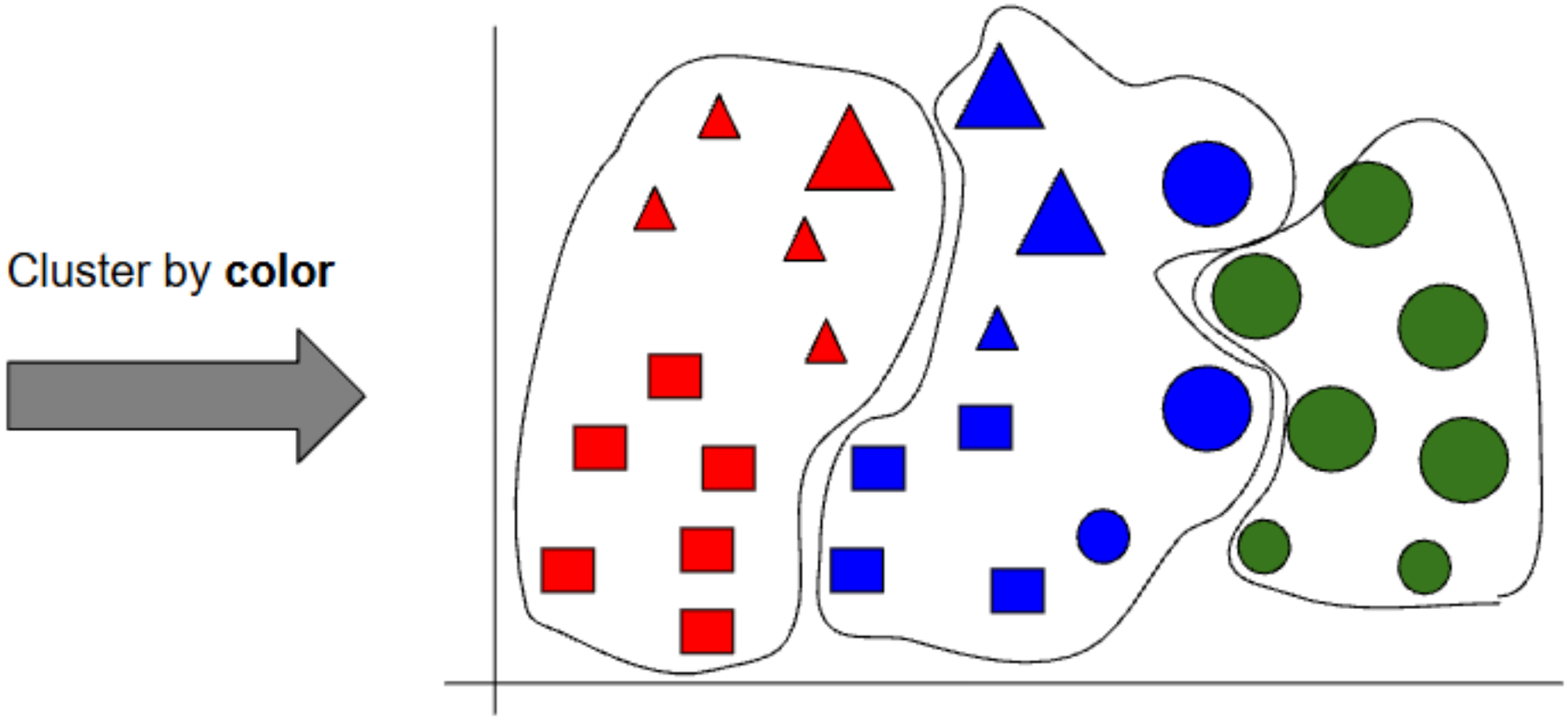
Cluster by **shape**



Clustering Bias (3)

- It's common to say that clusters are "in the eye of the beholder":
  - are the terms "horse" and "car" similar?
  - in the previous example the clustering bias was the shape of each object, it was obvious.
  - with more features it may be less obvious.

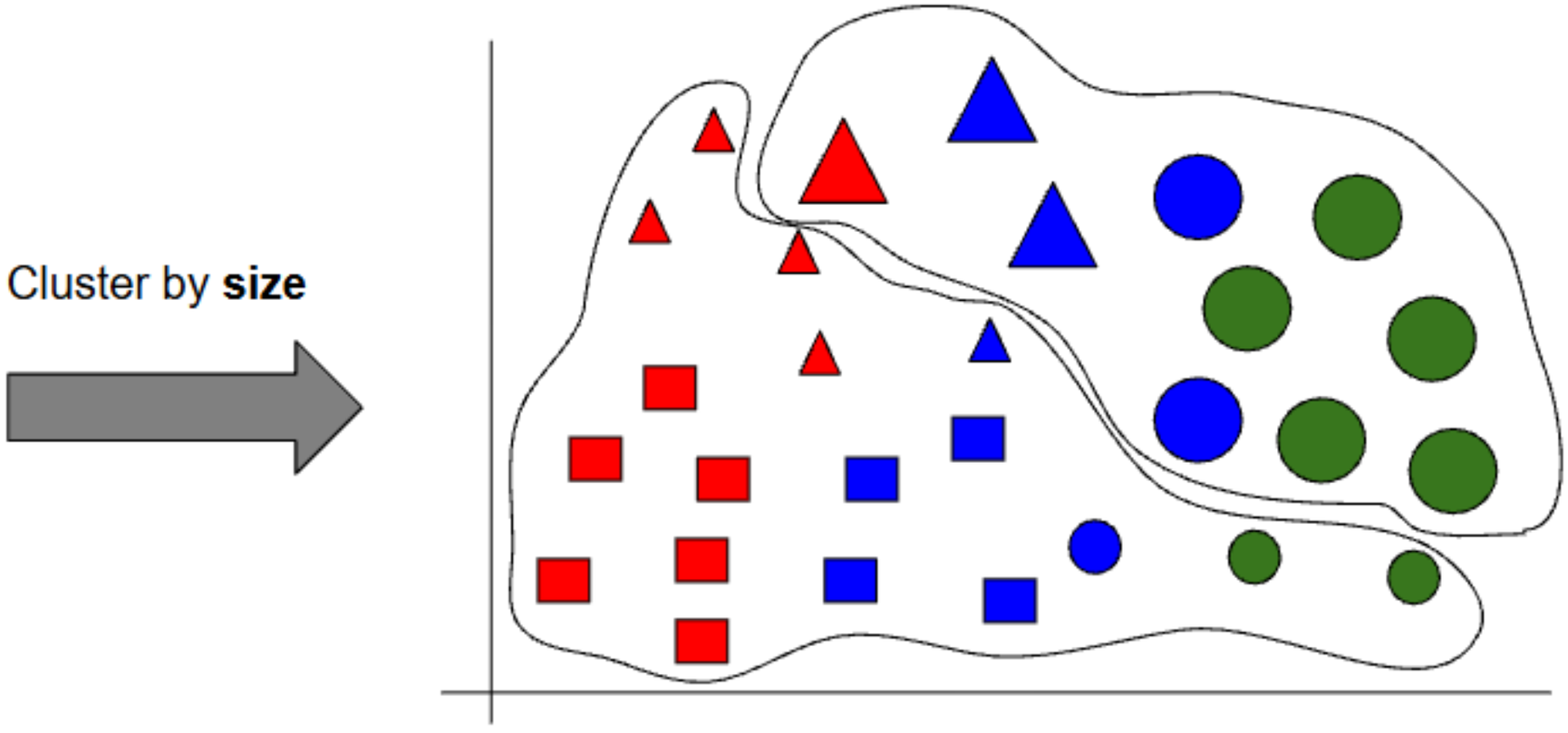
Cluster by **color**



Clustering Bias (4)

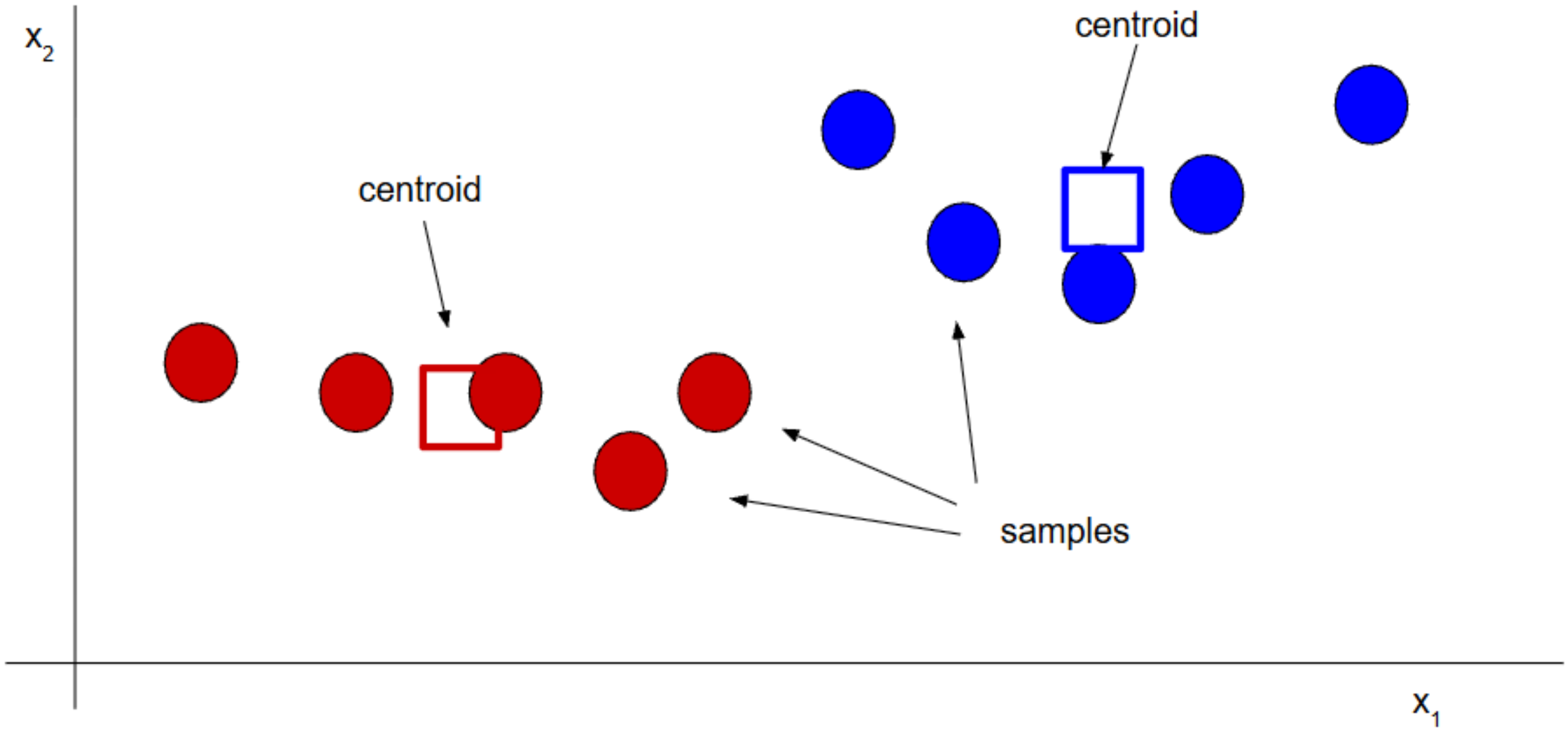
- It's common to say that clusters are "in the eye of the beholder":
  - are the terms "horse" and "car" similar?
  - in the previous example the clustering bias was the shape of each object, it was obvious.
  - with more features it may be less obvious.

Cluster by **size**



k-means

- k-means clustering aims to partition n samples into k clusters in which each sample **belongs to the cluster with the nearest mean**, serving as a prototype of the cluster.



k-means

- Algorithm for k-means starts with a “weak” clustering that is **refined** in many rounds **until nothing changes**.
- The parameter k is user-defined (number of clusters)

ALGORITHM

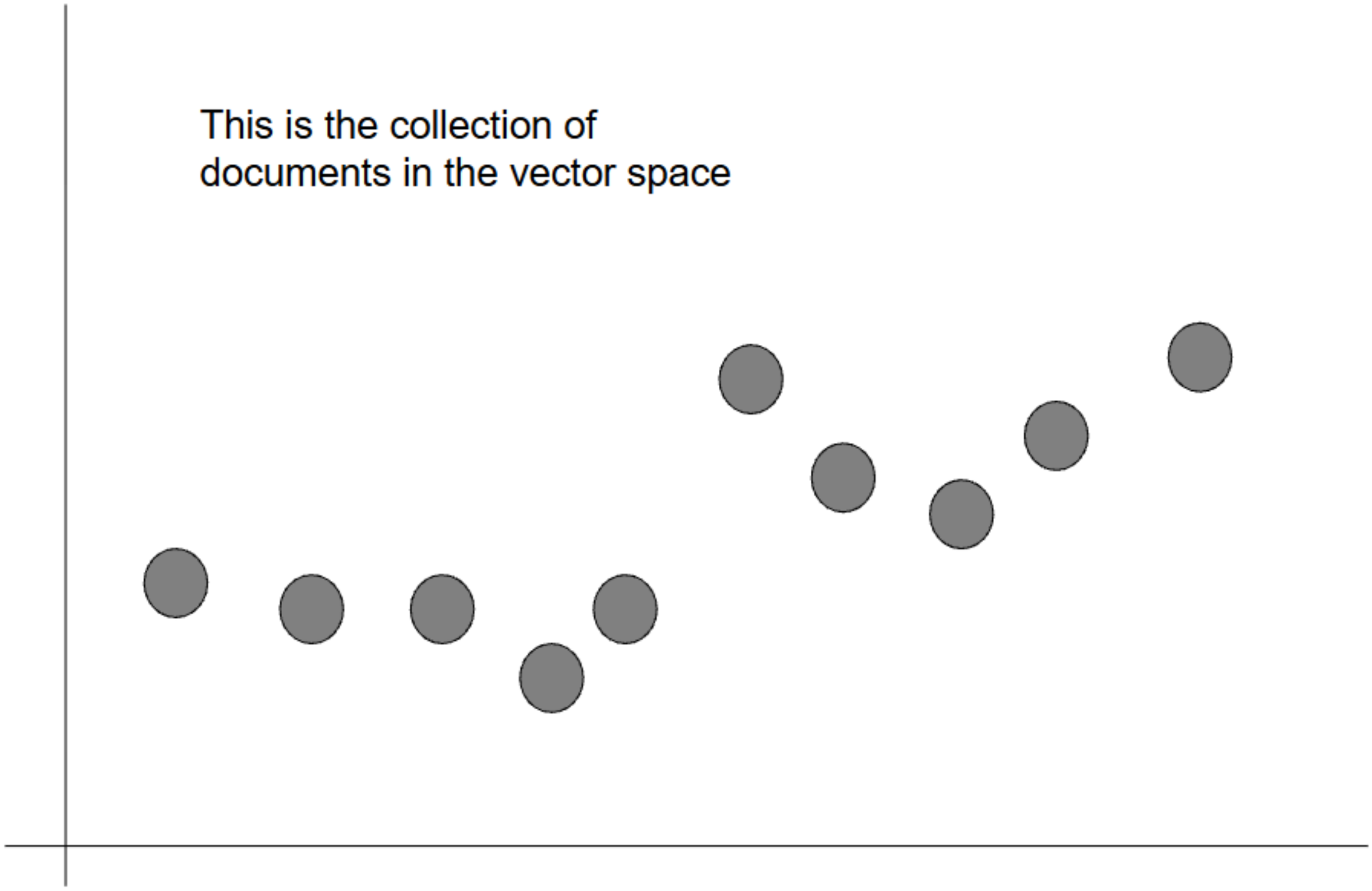
```
samples = [(x11,x12),...,(xm1,xm2)] #our dataset of m samples in 2-dimension space
centroids = pick_random(samples,k) #pick k random samples as centroids
for each sample in samples: #first weak clustering
     cluster[sample] = nearest(sample,centroids) #assign to nearest centroids
anychange = True

while (anychange):
     anychange = False
     centroids = [mean(cluster1),...,mean(clusterk)] #recompute centroids
     for each sample in samples:
          if cluster[sample] != nearest(sample,centroids): #we should move
               cluster[sample] = nearest(sample,centroids)
               anychange = True
```

k-means convergence

- There are at most k^m ways to partition m data points into k clusters
- k^m is a large but finite number
- For each iteration of the algorithm, we produce a new clustering based only on the old clustering.
- At each round there can be one of two cases:
  1. The old clustering is the same as the new → the iteration stops
  2. The new clustering is different → the distance between the samples and the centroids is lower
- If the old clustering is the same as the new, then the next clustering will again be the same.
- If the new clustering is different from the old then the newer one has a lower cost

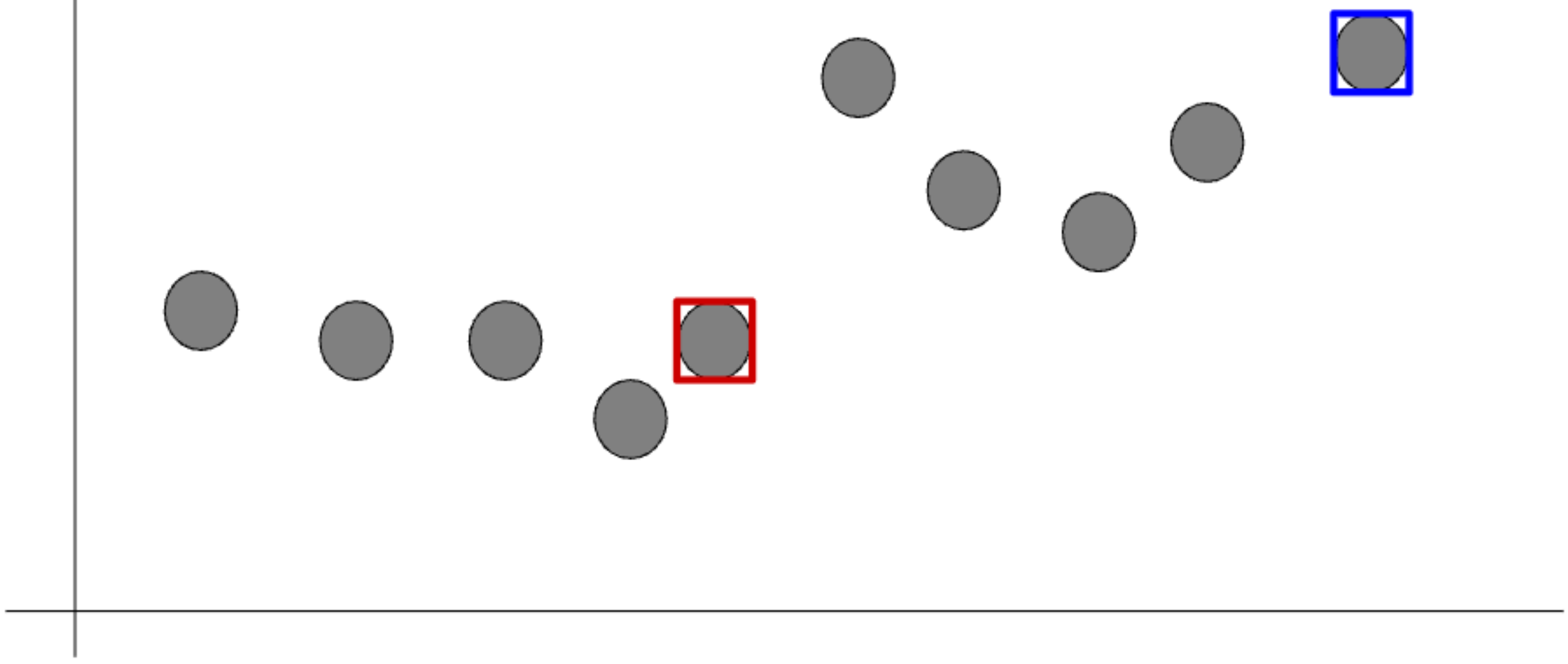
k-means: example

This is the collection of
documents in the vector space



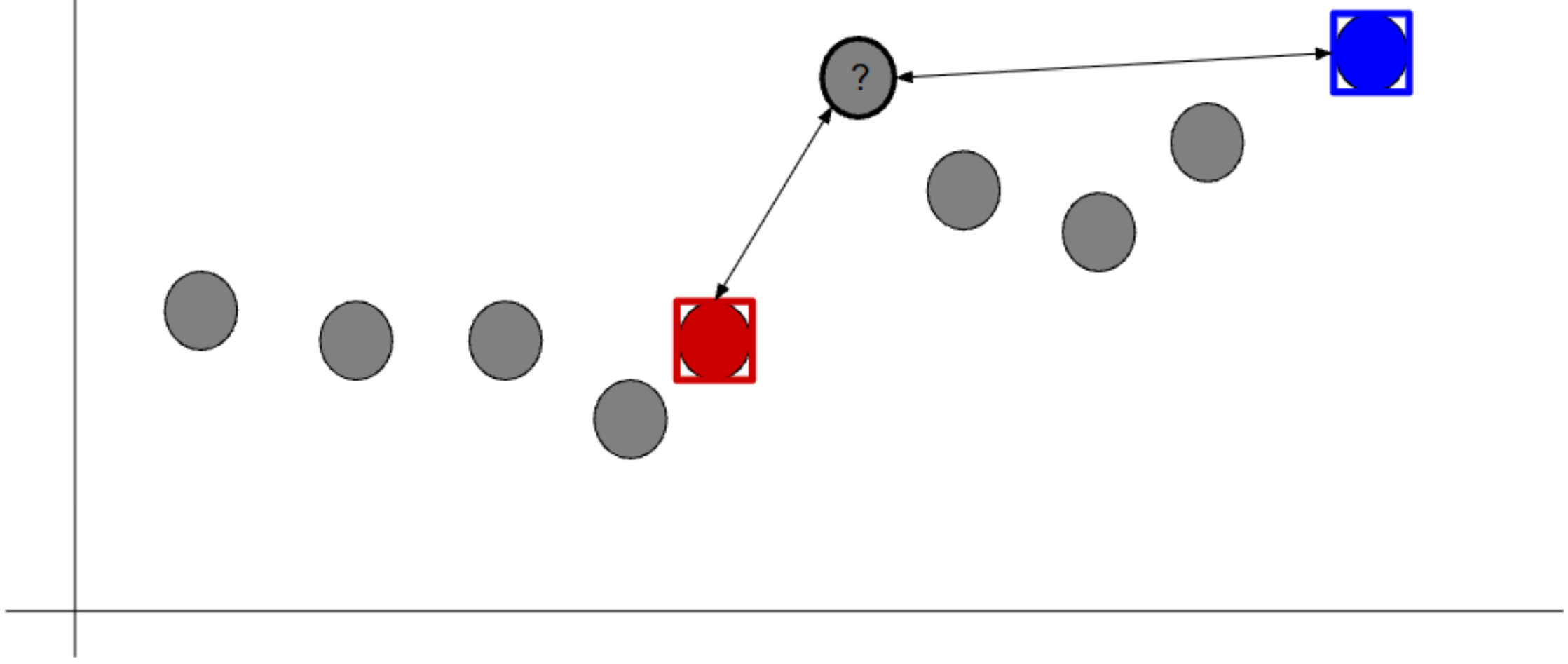
k-means: first round

The hyperparameter k is set to 2
in this example.
We pick 2 random documents
as centroids.



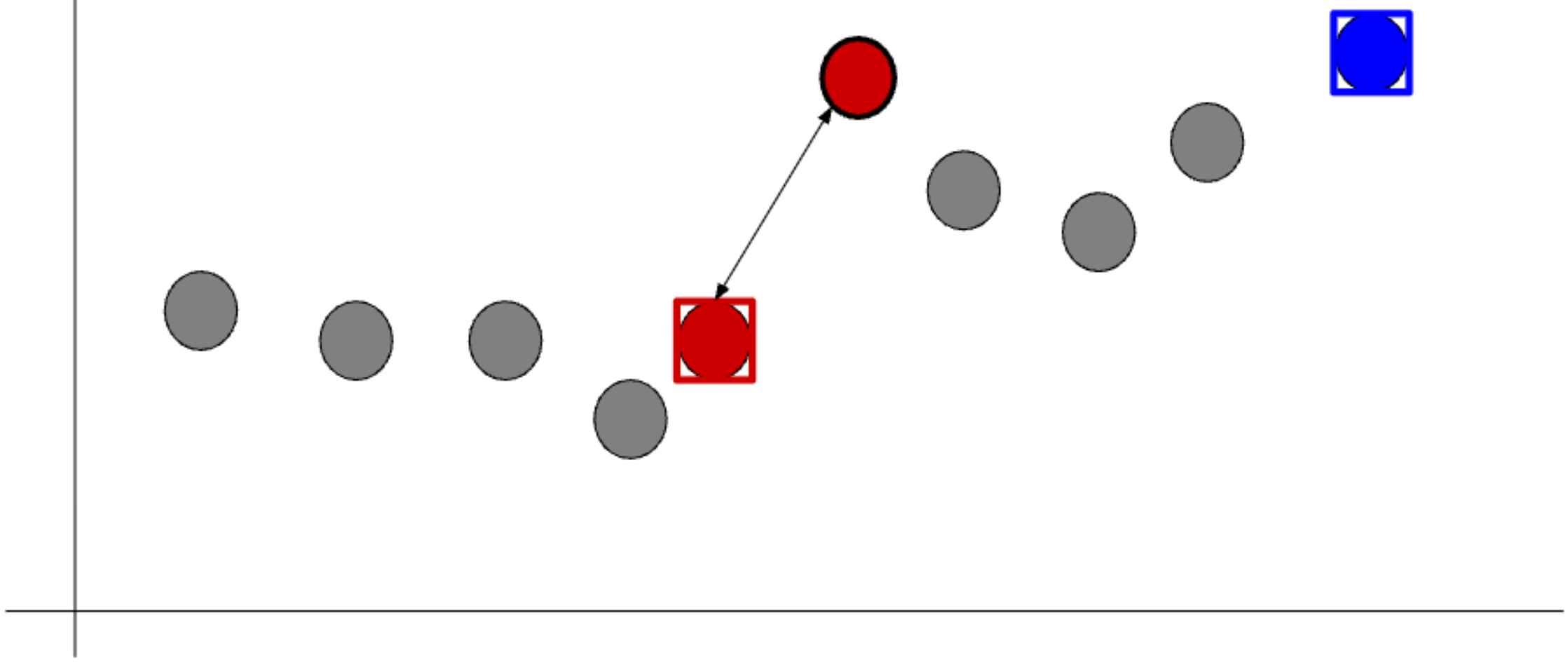
k-means: first round

Each document is assigned to the cluster of the nearest centroid.



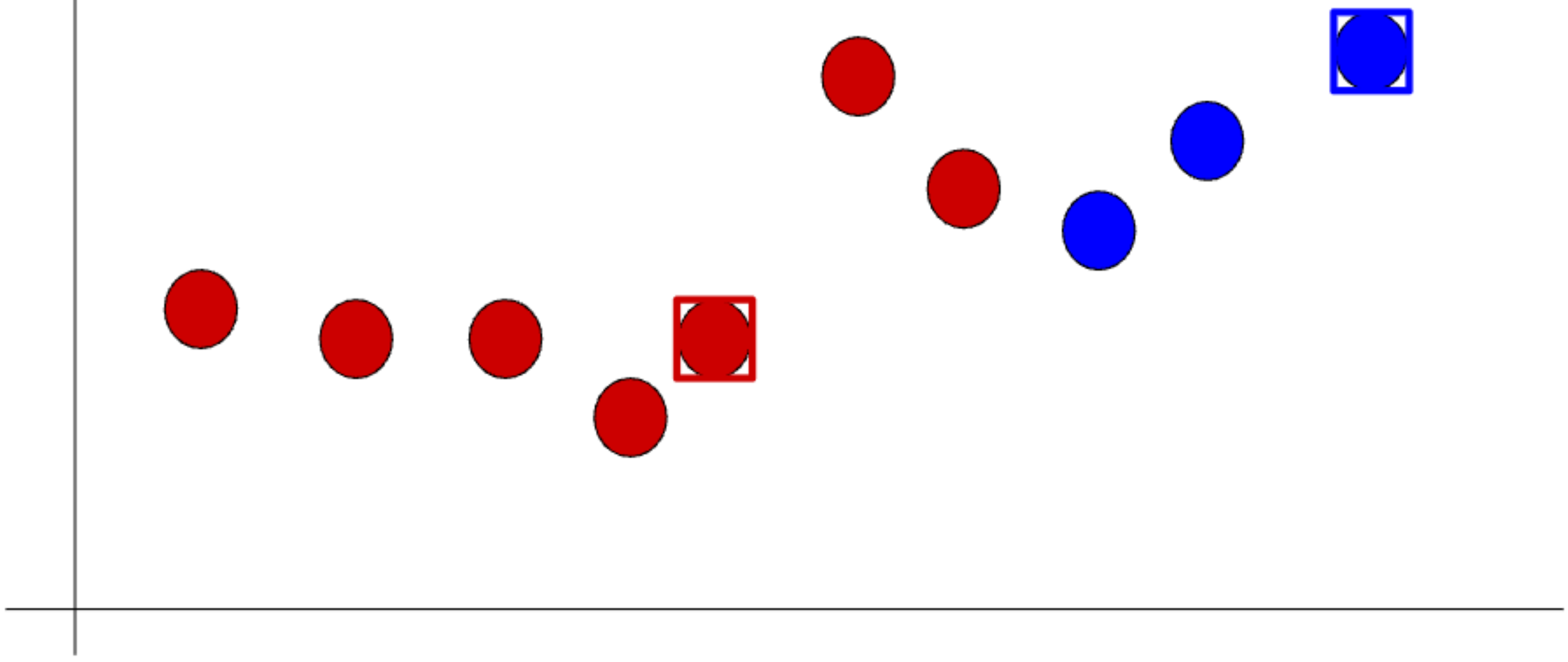
k-means: first round

Each document is assigned to the cluster of the nearest centroid.



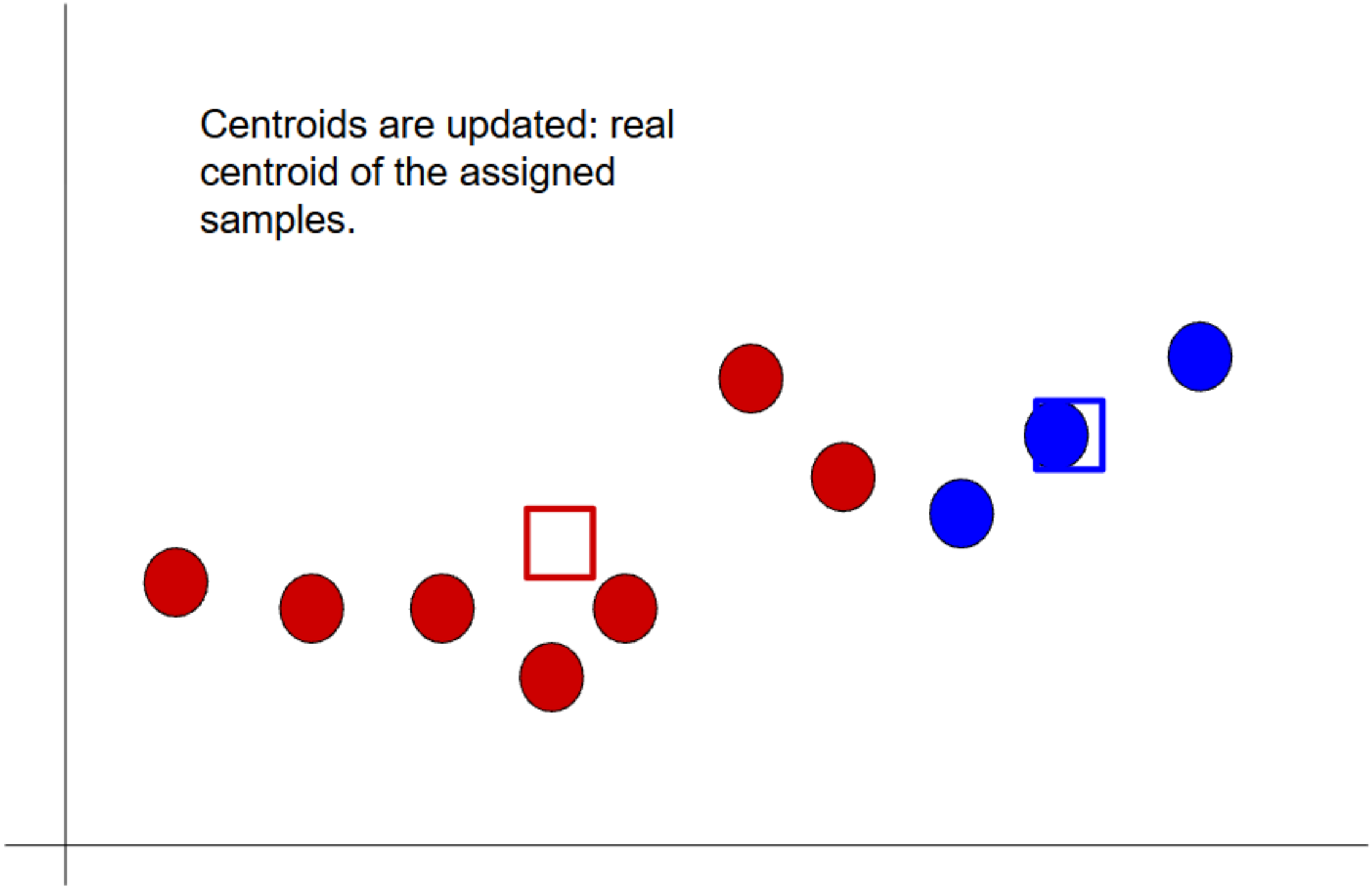
k-means: first round

Each document is assigned to the cluster of the nearest centroid.



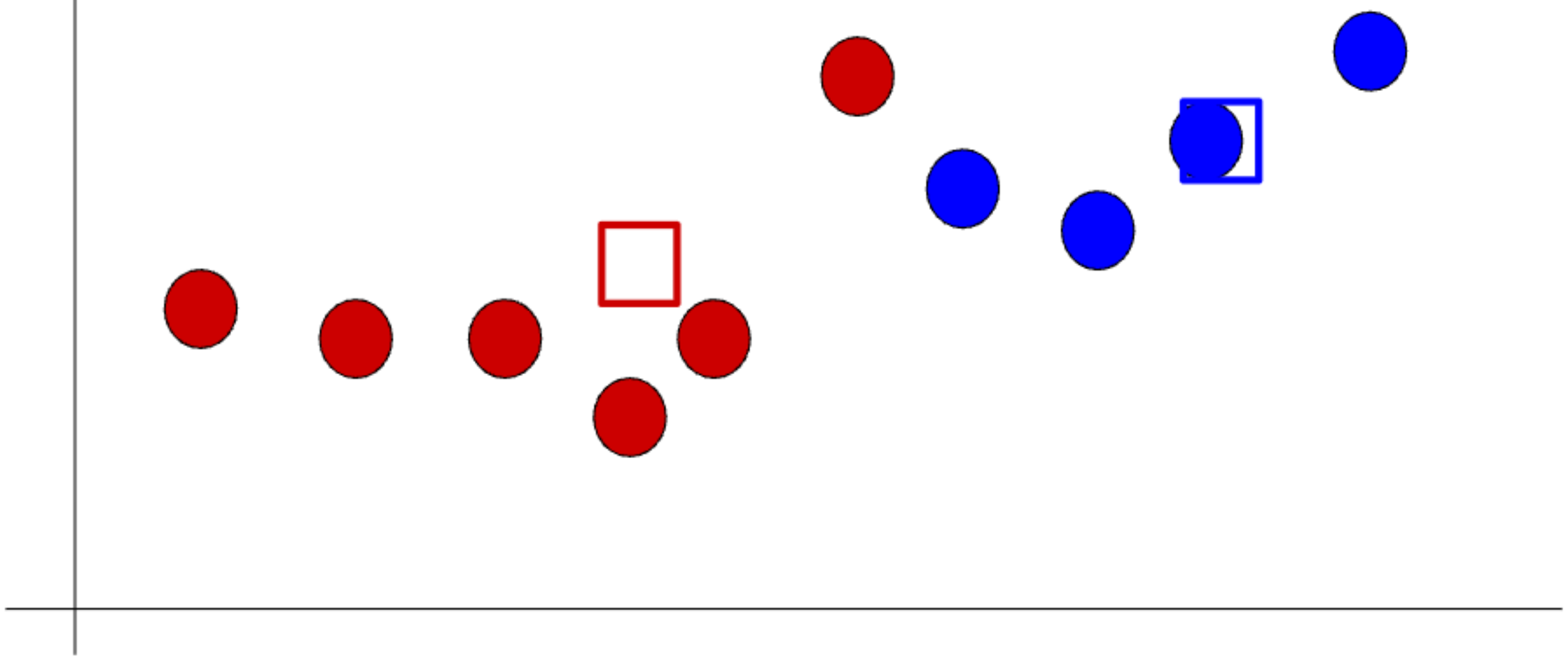
k-means: second round

Centroids are updated: real centroid of the assigned samples.



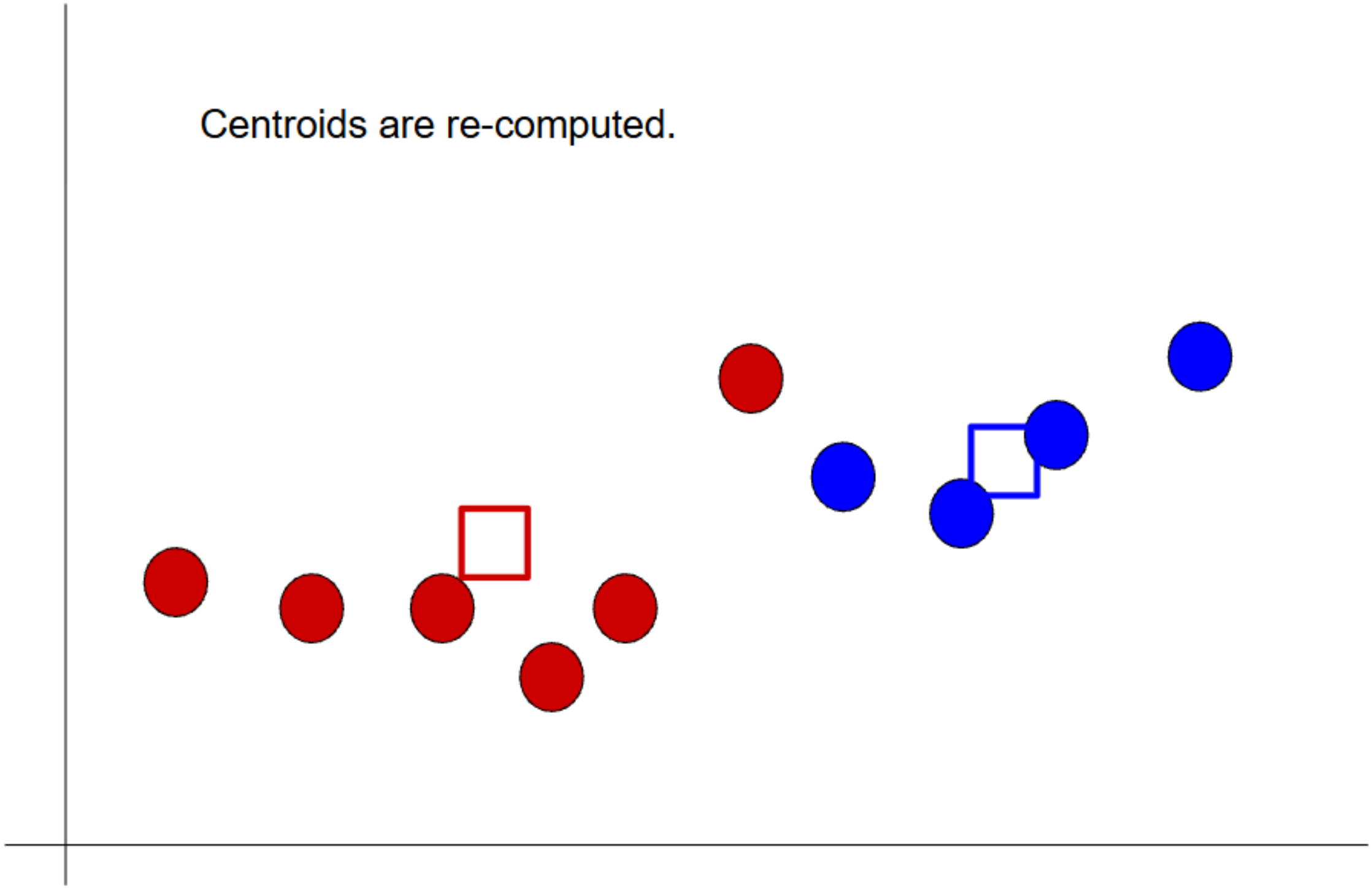
k-means: second round

Samples are re-assigned on the basis of the new centroids.



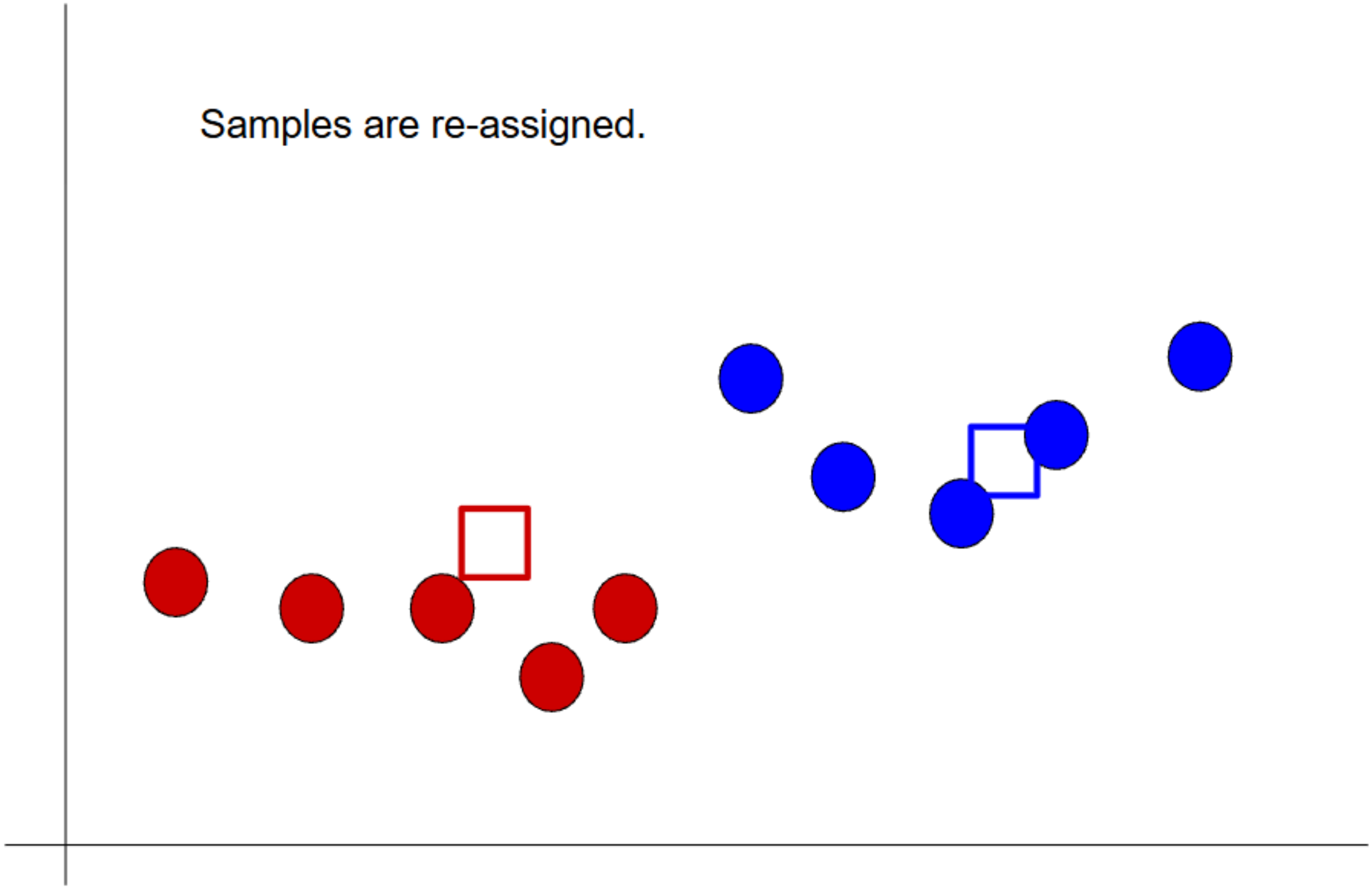
k-means: third round

Centroids are re-computed.



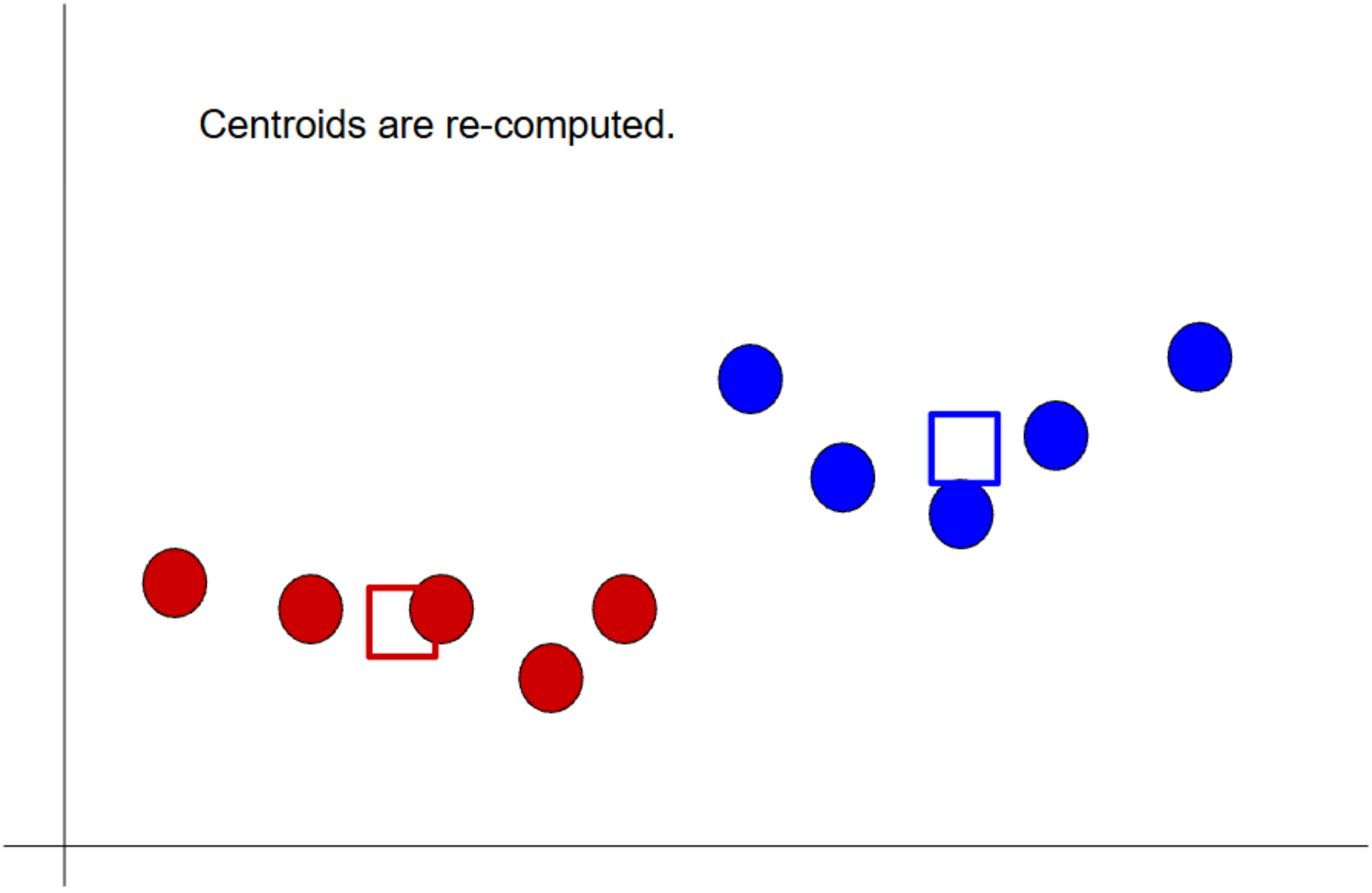
k-means: third round

Samples are re-assigned.



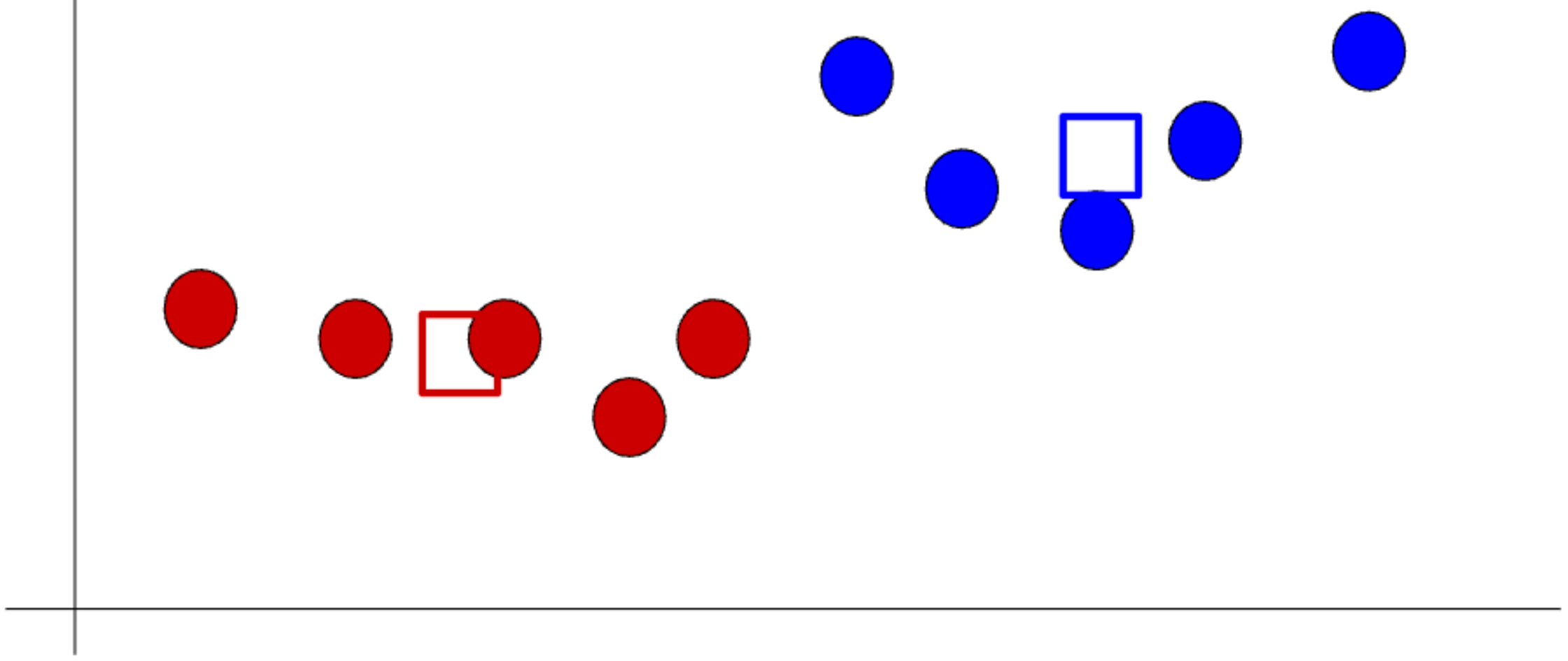
k-means: fourth round

Centroids are re-computed.



k-means: fourth and last round

No sample is re-assigned!
STOP THE ITERATION



Picking first k points

- The way how we choose the k points can make the k-means algorithm to **converge faster**.
  - The assignment loop (internal loop) is linear on the number of points for each cluster… but number of rounds (external loop) is unknown!
  - Usually rounds << m but the worst case reaches 2^m rounds: **exponential time**
- Good way to choose first points is to pick **dispersed** set of points:
  - pick first point at random.
  - pick as next point the one with the **largest minimum distance** from the already selected points.
  - repeat until we have k points.

Largest minimum distance?

- Let's say we already selected *s* centroids *c* and we want to pick up the next one among the *m* points *p*

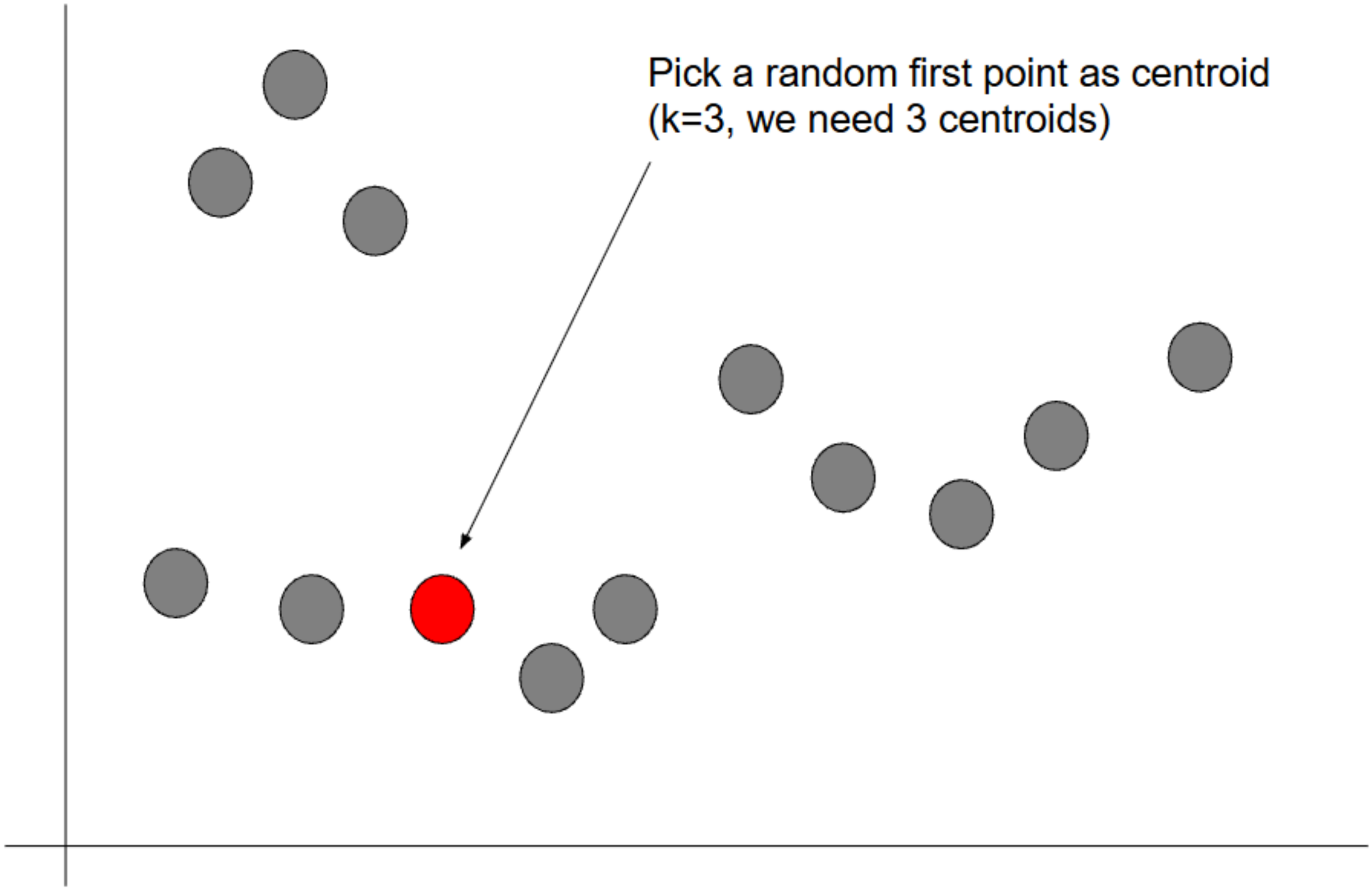
$$\mathbf{max}(\mathbf{min}(d(p_1,c_1),\ldots,d(p_1,c_s)) , \ldots , \mathbf{min}(d(p_m,c_1),\ldots,d(p_m,c_s)))$$

- When we have selected only 1 centroid, picking the next is easy, because the above becomes:

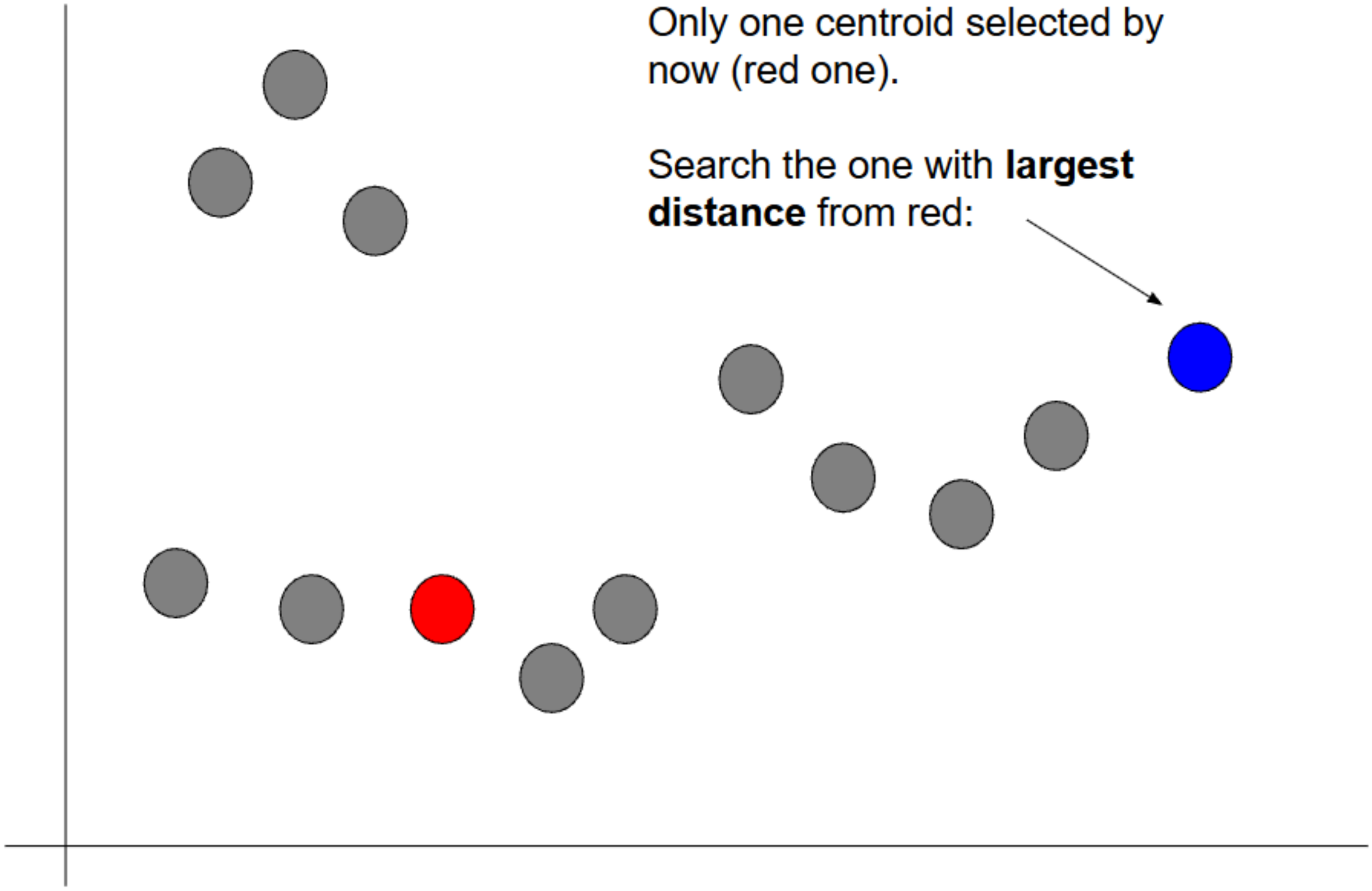
$$\mathbf{max}(d(p_1,c_1),\ldots,d(p_m,c_1))$$

- When we have 2 or more centroids already, for each point we
  - first search the nearest centroid (minimum)
  - then use that value to pick the point farther from any centroid (largest)

Example on picking points 1/3



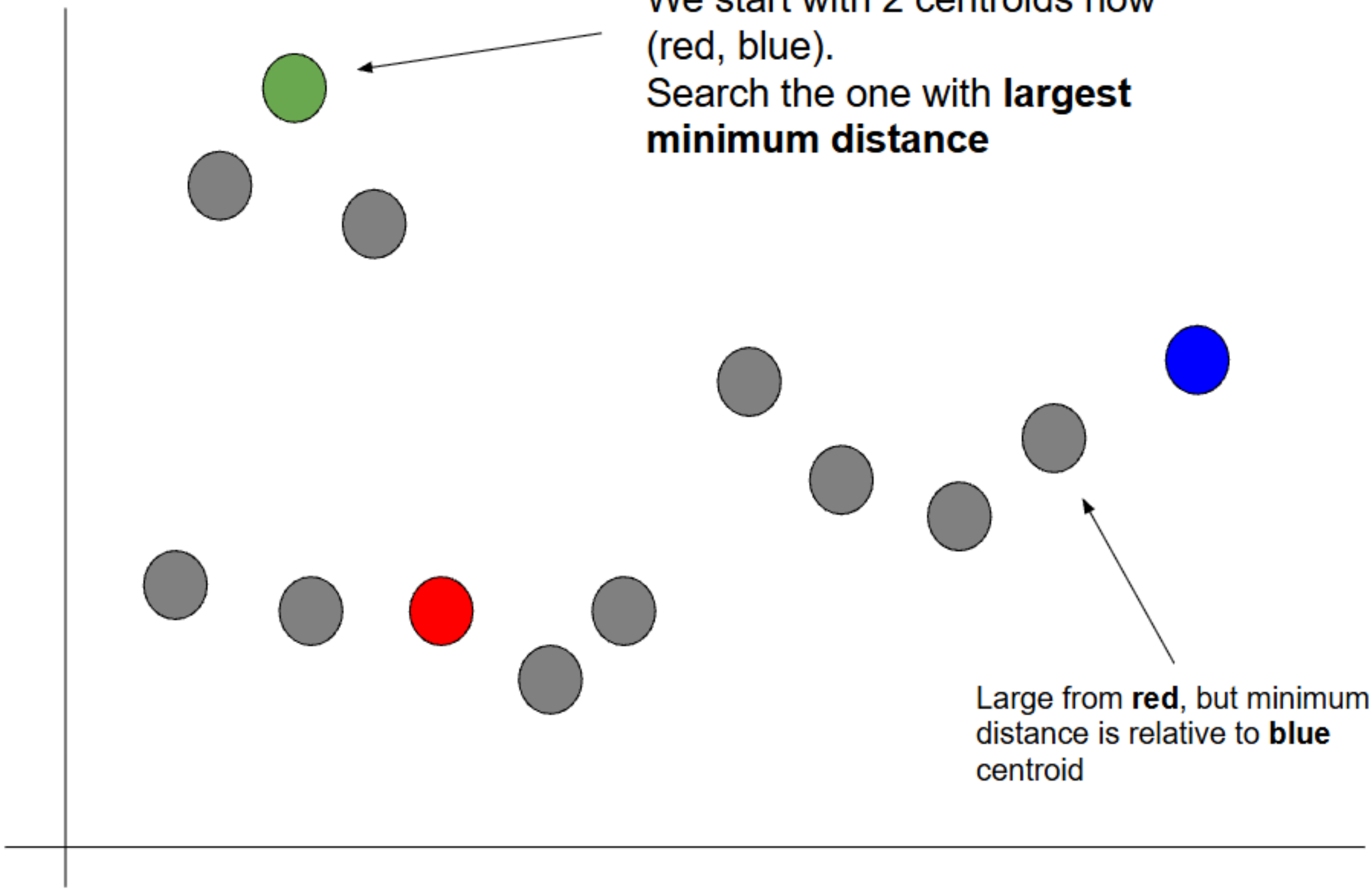
Example on picking points 2/3



Only one centroid selected by now (red one).

Search the one with **largest distance** from red:

Example on picking points 3/3

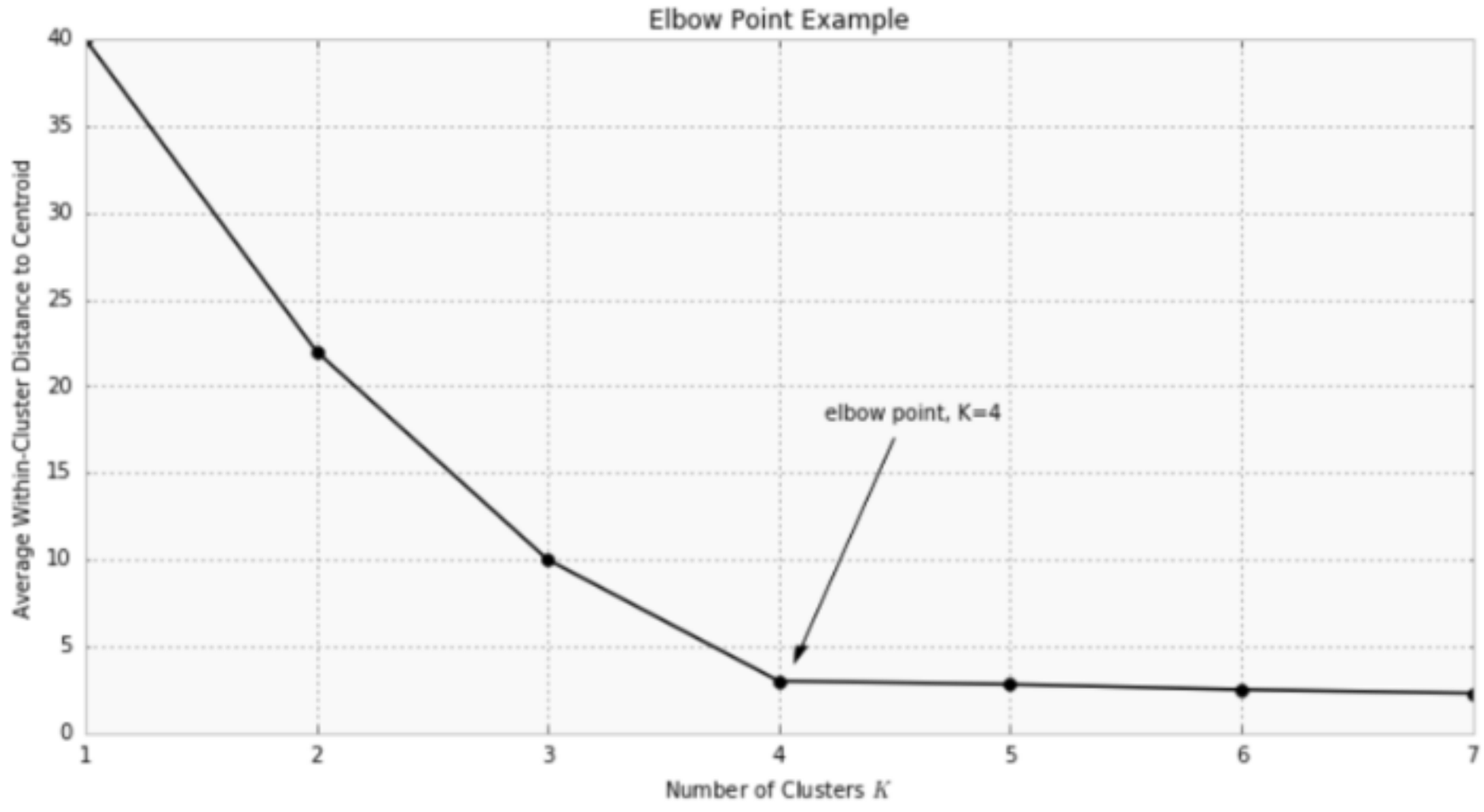


Choosing k

- Choosing into how many clusters we should group the documents depends on the task, there's no good automatic way.
- However, some measures can help:
  - usually the average distance of all documents from the cluster centroid is used.
  - k-means is then ran over different values of k.
    - increasing k **will always** decrease the average distance.
      - We should stop when the improvement begin to be small: **elbow point**

Elbow method

- The elbow method is a visual method to roughly find the best value for k.
- When the line chart looks like an arm, then the "elbow" on the arm is the value of k that is the best.



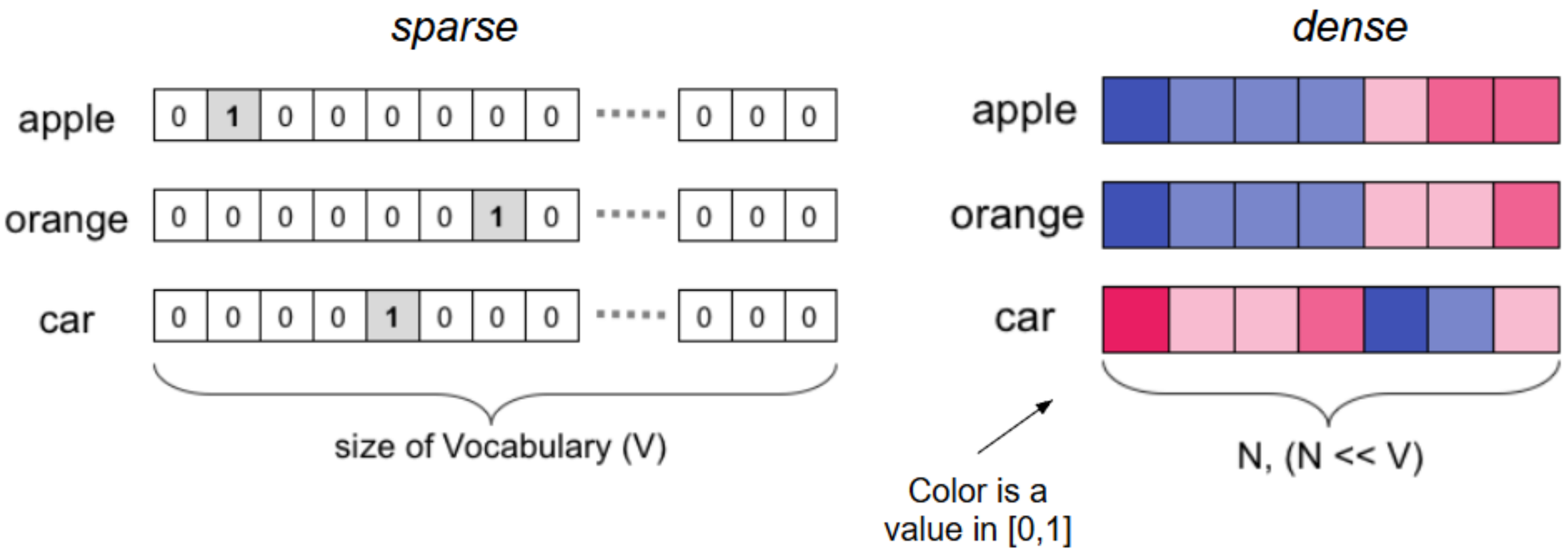
Learning a better representation

- In supervised and unsupervised methods we used a **vector representation** for any object:
  - the similarity of the vectors implied the similarity of the objects
  - in the 2D examples, only two features were used to describe them and their distance on the plane was used to compute similarity.

- Traditionally, a boolean model is used to represent categorical features, like words:
  - a word can be either present or absent (**sparse** representation)
  - there is no notion of similarity between words in this representation.
- In the last decade, unsupervised methods has been proposed to **compute deeper representations of words (word embeddings)**
  - Their **dense** vectors place the word in a position dependent on its meaning.

Sparse vs Dense representation

- Traditional: **sparse high dimensional** vectors
  - atomic representations: word is represented by an index in a V-dim vector (e.g. one-hot vectors, bag of words)
  - V is the dimension of the dictionary, elements are active one-at-a-time
- Word Embeddings: **dense low dimensional** vectors
  - meaningful representations, word vectors represent words and their meaning. Similar vectors = similar words.

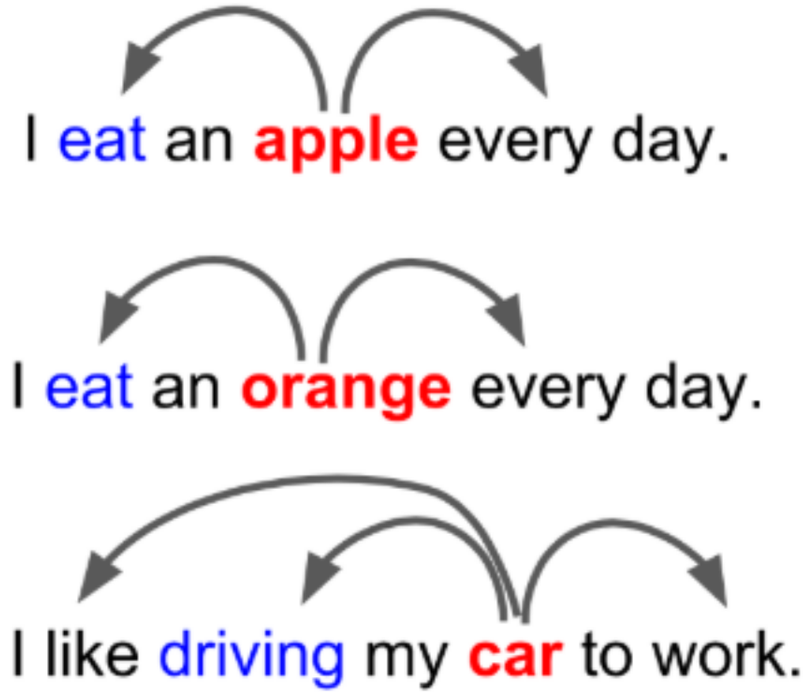


Word embeddings

- Unsupervised techniques:
  - like text clustering and association rules.
  - the goal can be less clear, because it's more a *representation*, it's a mean for other goals.
  - a better representation can be then used for supervised learning.
- Word embeddings are **vector representations of words** computed using *optimization* techniques where:
  - each word is associated with a real valued vector in n-dimensional space (usually n=50-1000)
  - word vectors are similar when words are similar
  - word2vec, GloVE and fastText
- The vector space of word embeddings shows **linguistic regularities.**

Learning word embeddings

- Word embeddings are based on **Distributional Hypothesis**:
  - *"words that are used and occur in the same contexts tend to support similar meanings"*
- We learn **contextual** representations from **corpora:**



Optimization problem

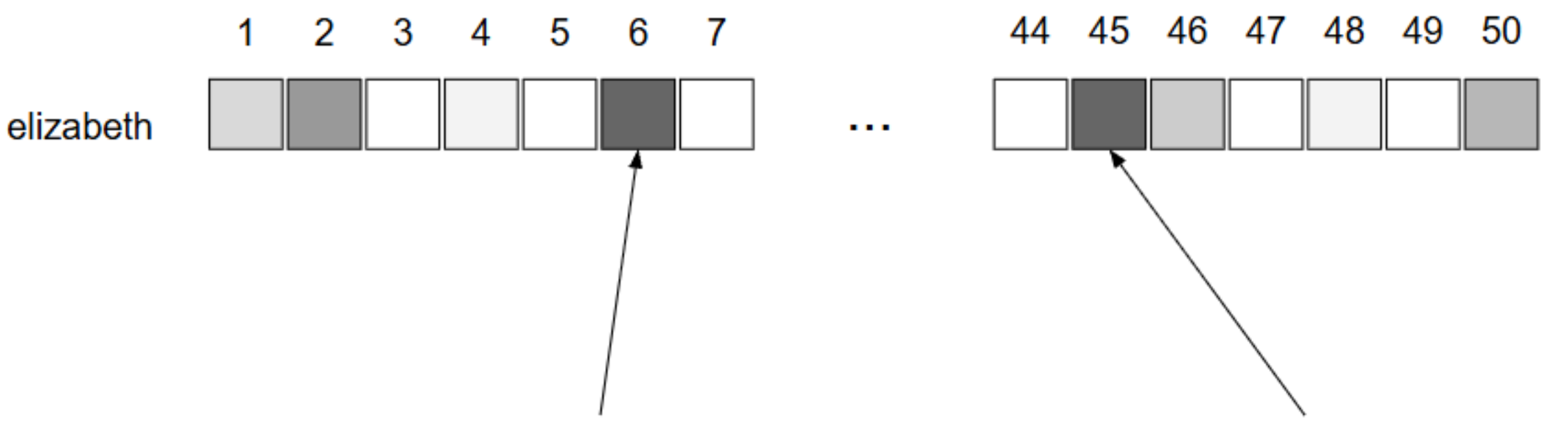
- The learning algorithm of word embeddings solve an *optimization problem*, the same kind we have seen in logistic regression.
- It uses two basic notions:
  - **distance** between vectors (as seen in IR section with vector space model)
  - appearance in the same **context** (2 words before and 2 words after are usually considered the context of a target word)
- The optimization problem of word embedding has two objectives:
  - **Minimize** the distance between vectors of words that appear frequently in the same context (*argmin*)
  - **Maximize** the distance between vectors of words that never appear in the same context (*argmax*)

Why word embeddings?

- Word embeddings learn linguistic properties of words, linked to their semantic, from huge corpora like:
  - Wikipedia
  - Google News
- With respect to sparse representation (like bag-of-words), word embeddings carry on some **semantic** knowledge in the representation
- Using word embeddings to represent natural language text has brought higher accuracy in many areas of text mining and information retrieval.

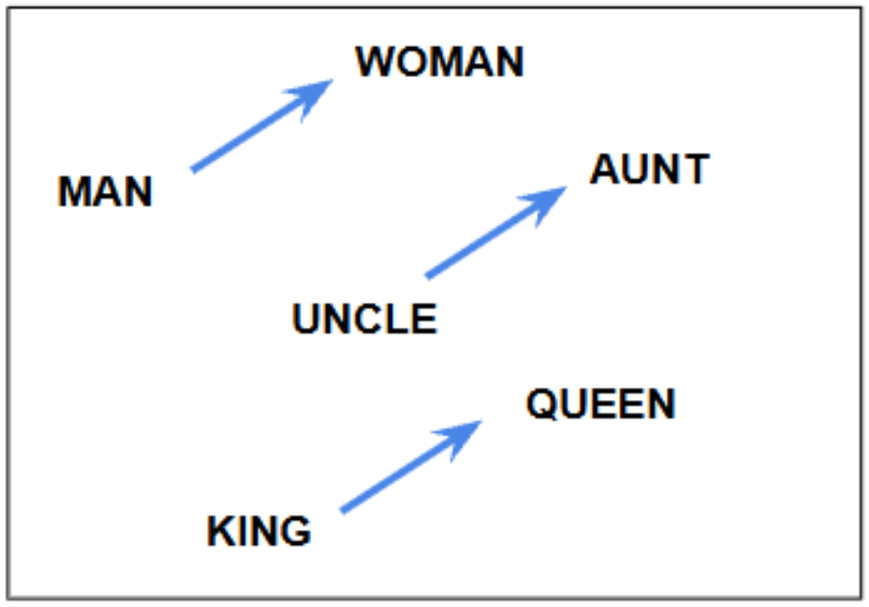
Vector elements

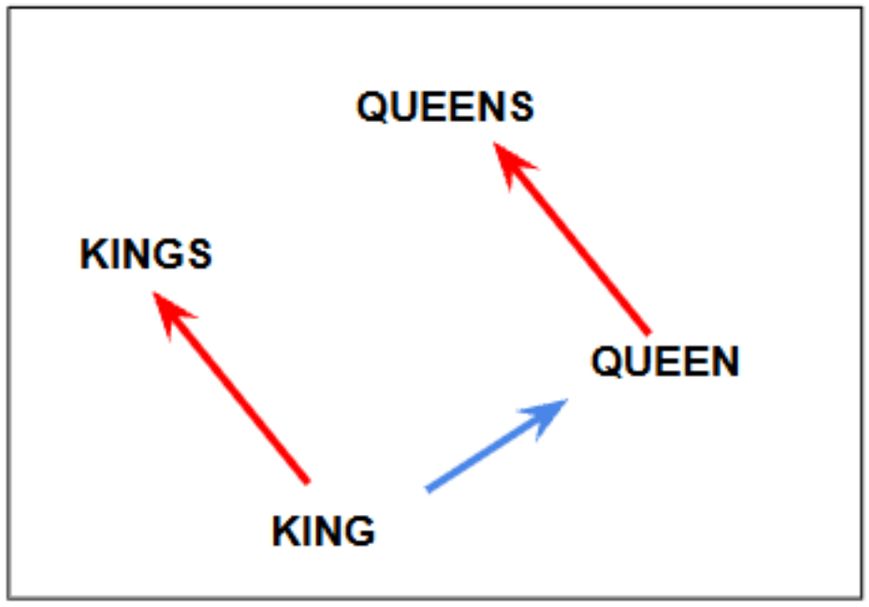
- Word vectors are filled so that words that are used in the same context are close together in the vector space.
- The meaning of each element of a word vector is not clear a priori.
- However, they have shown to capture abstract concepts!



Linguistic regularities

- We can do nearest neighbor search around result of vector operation “king - man + woman” and obtain “queen”.
- We observe both **semantic** and **syntactic** regularities.





Direction of gender notion

Direction of number notion

Linguistic regularities: evaluation

- To evaluate a word embedding, a dataset of 20K “questions” exists of this kind:

Athens: Greece	Oslo: _____
Angola: kwanza	Iran: _____
brother: sister	grandson: _____
possibly: impossibly	ethical: _____
walking: walked	swimming: _____

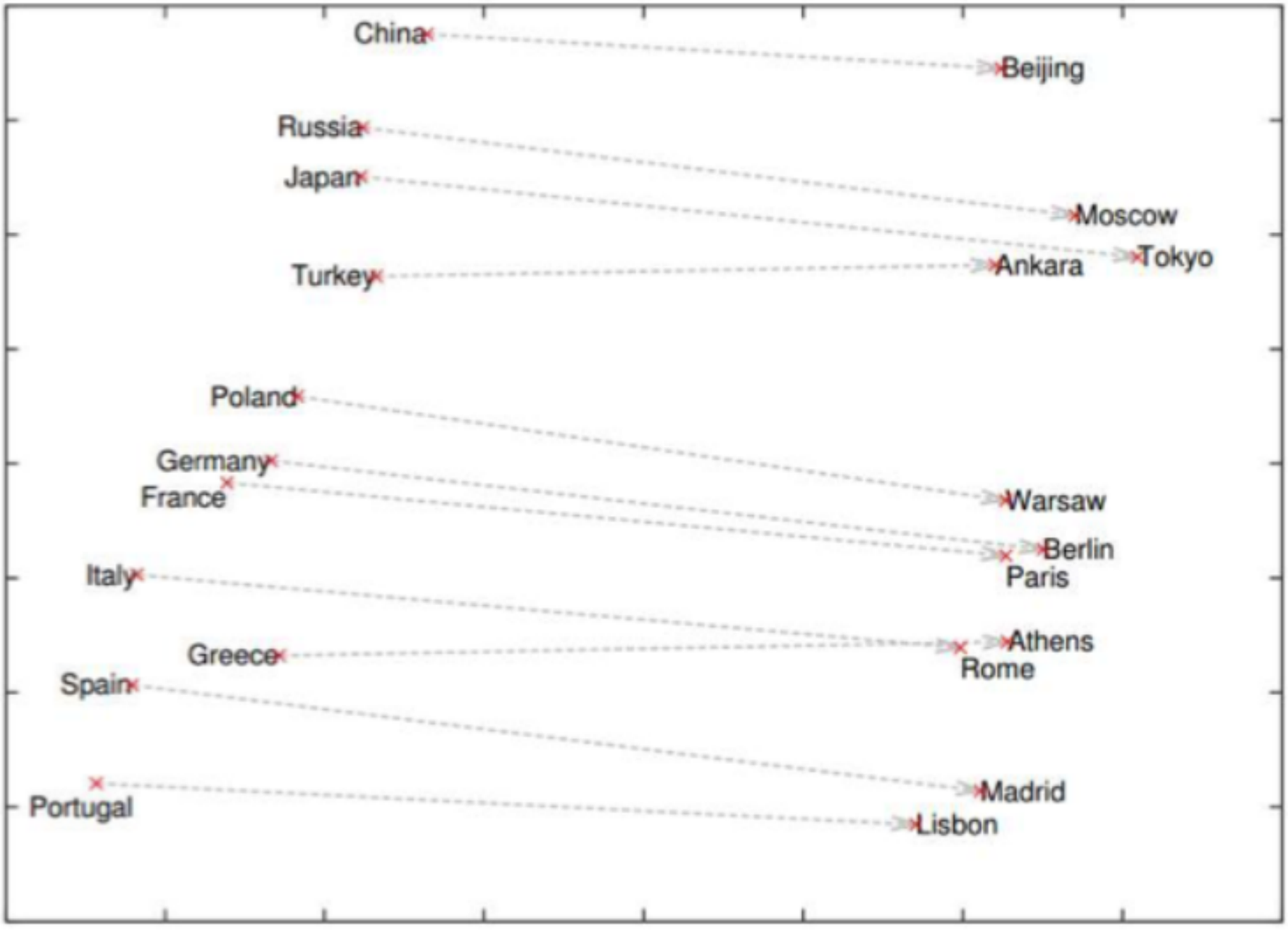
- When trained on the union of Wikipedia and Google News, word2vec reach 91% of correct answers for the 20K questions.

More analogies

- The following are obtained using Word2Vec

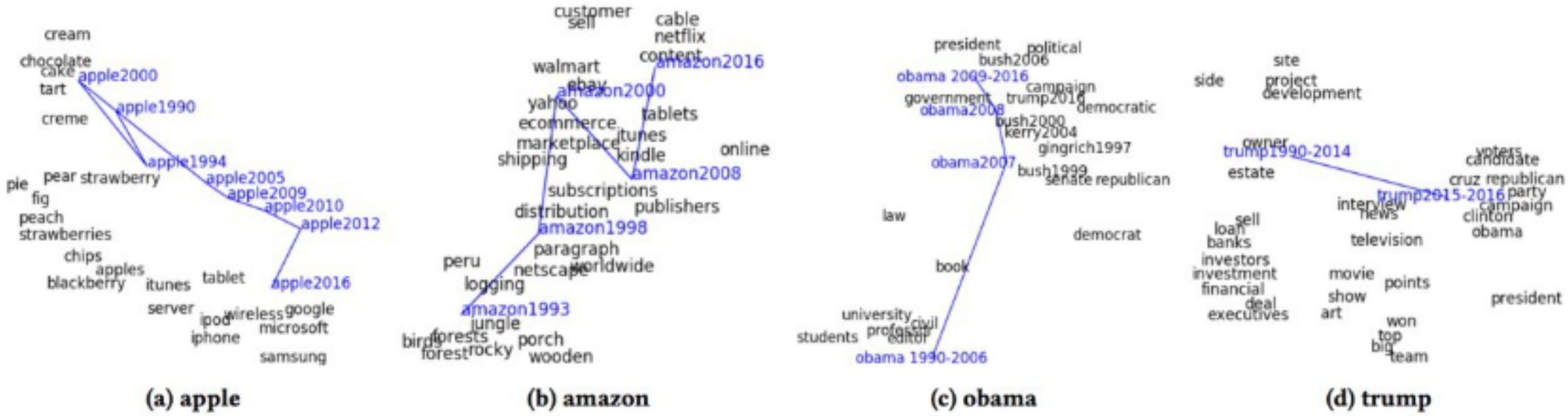
Expression	*Nearest token*
Paris - France + Italy	Rome
bigger - big + cold	colder
sushi - Japan + Germany	bratwurst
Cu - copper + gold	Au
Windows - Microsoft + Google	Android
Montreal Canadiens - Montreal + Toronto	Toronto Maple Leafs

2D Visualization



Shift over time

- Recent studies show how recomputing word embedding depending on creation time captures shifts in the word meaning/perception.

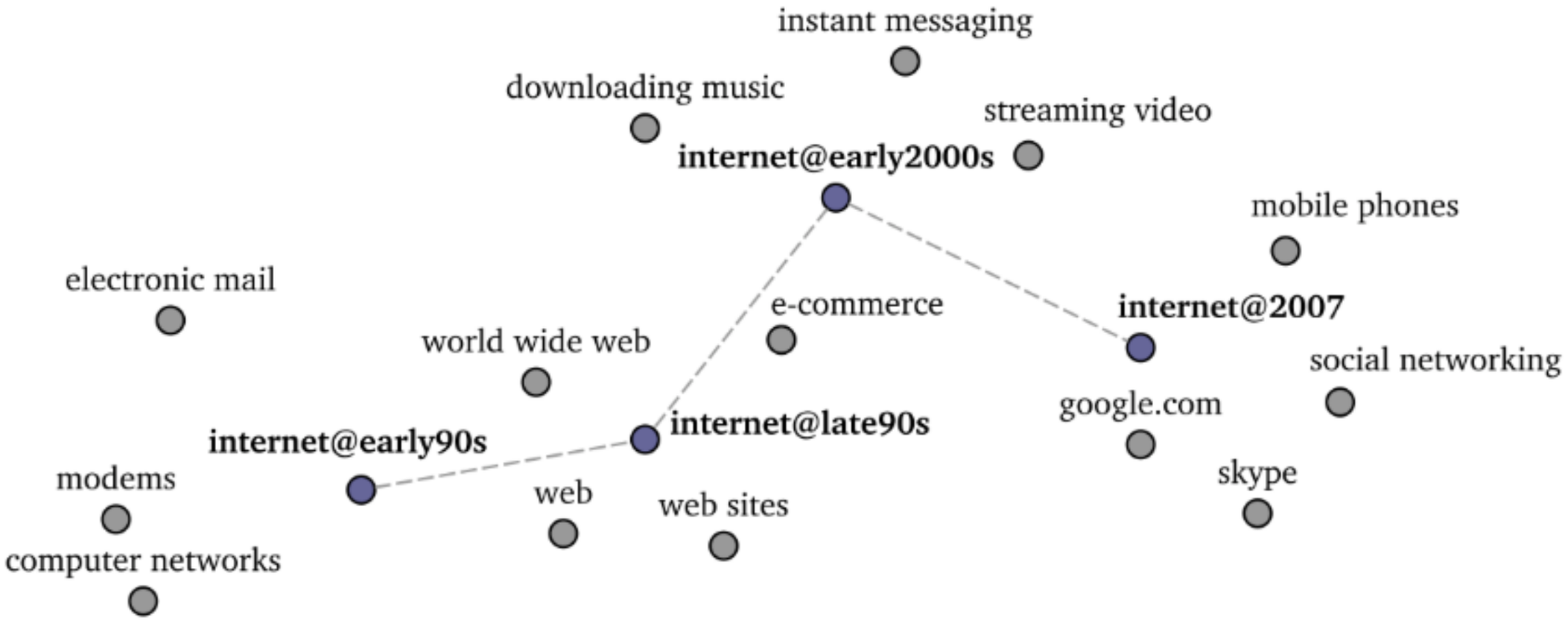


(a) apple (b) amazon (c) obama (d) trump

- Hamilton, W. L., Leskovec, J., & Jurafsky, D. (2016). Diachronic Word Embeddings Reveal Statistical Laws of Semantic Change. In Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (pp. 1489–1501).
- Bamler, R., & Mandt, S. (2017). Dynamic Word Embeddings via Skip-Gram Filtering. In Proceedings of ICML 2017.
- Szymanski, T. (2017). Temporal Word Analogies : Identifying Lexical Replacement with Diachronic Word Embeddings. In Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics (pp. 448–453).

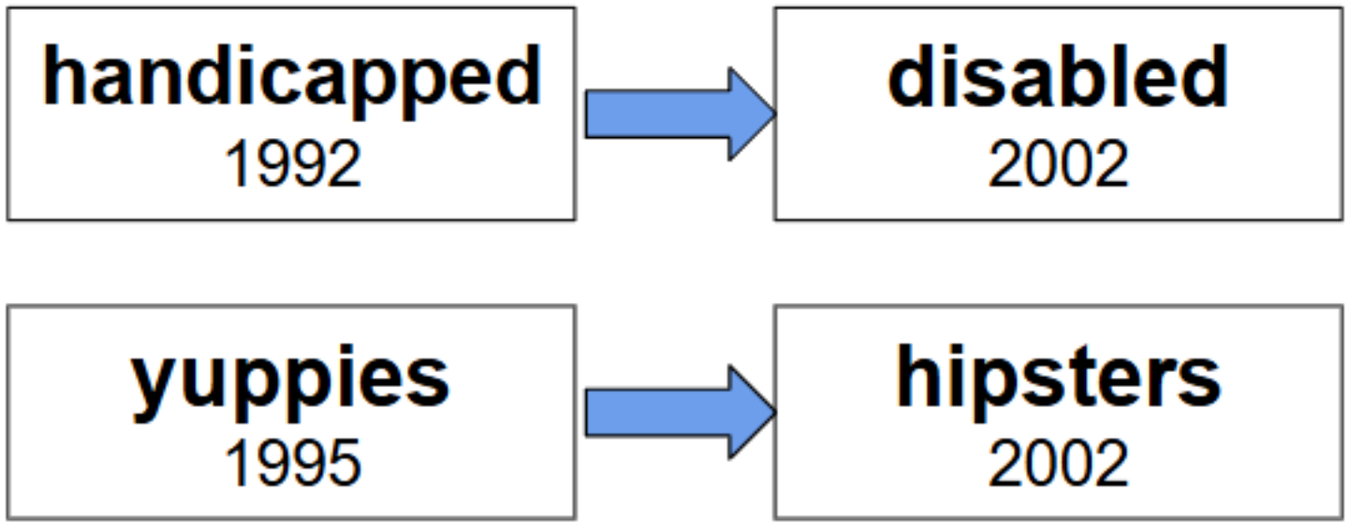
Problem: Semantic Evolution

- Large corpora usually **span across several years**, and even **decades.**
- **Language changes** over time reflecting the cultural and social evolution.
- **Problem**: Current word embeddings models are static and they can't capture dynamics in semantics.

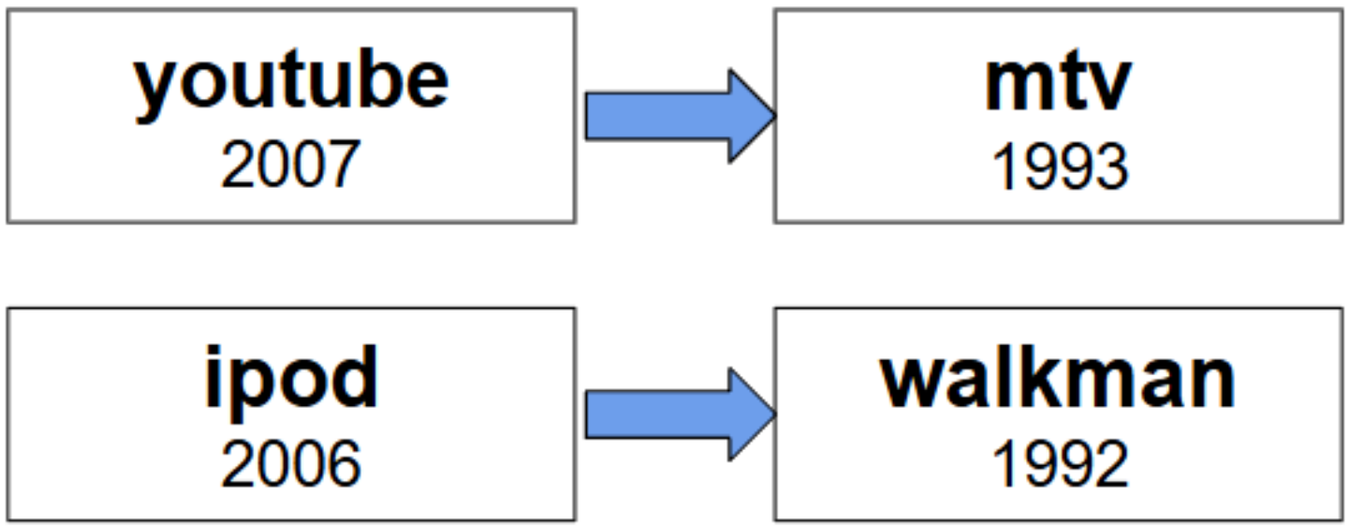


Temporal analogies (1/2)

- Temporal Analogies towards the **Future**

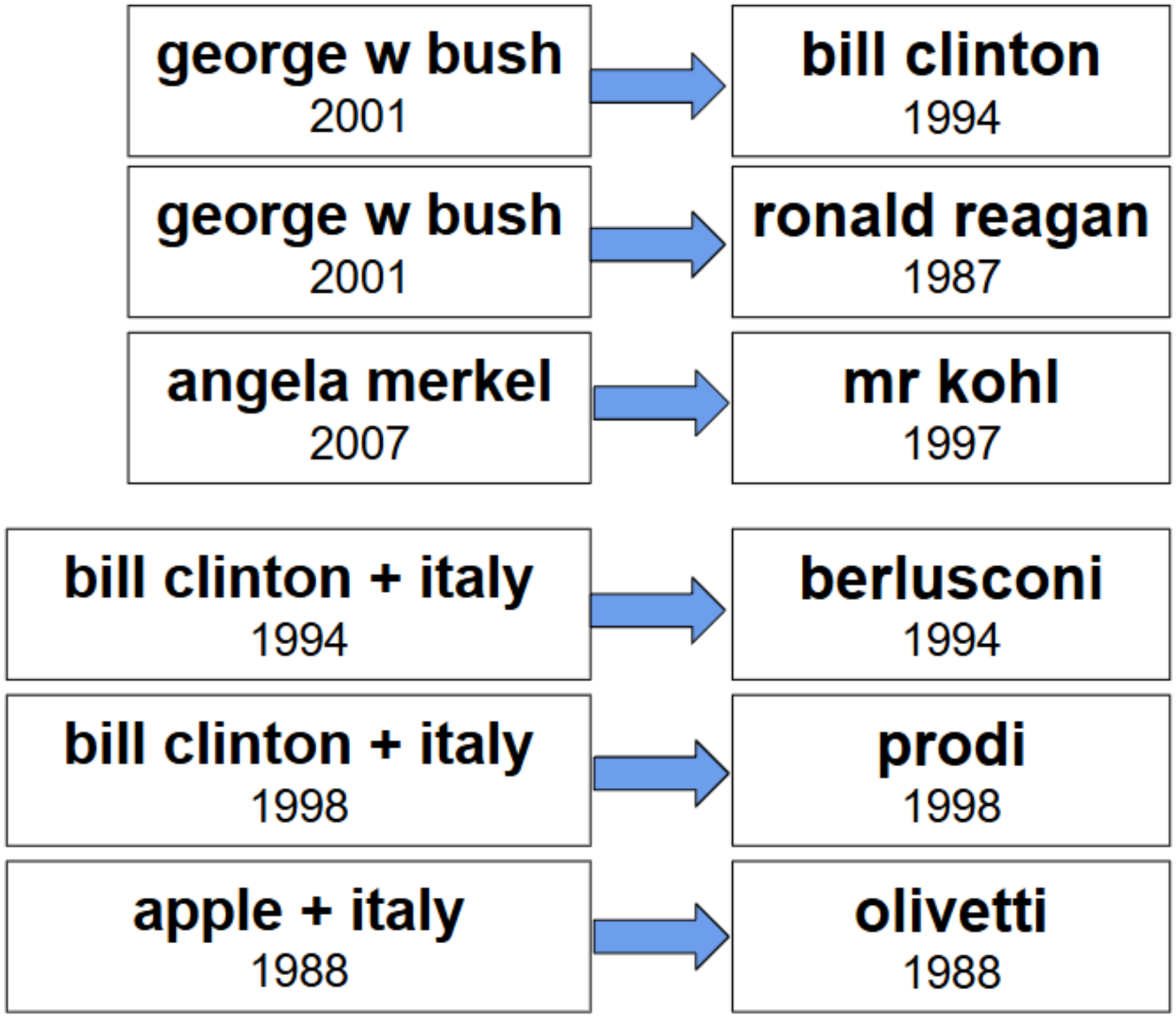


- Temporal Analogies towards the **Past**

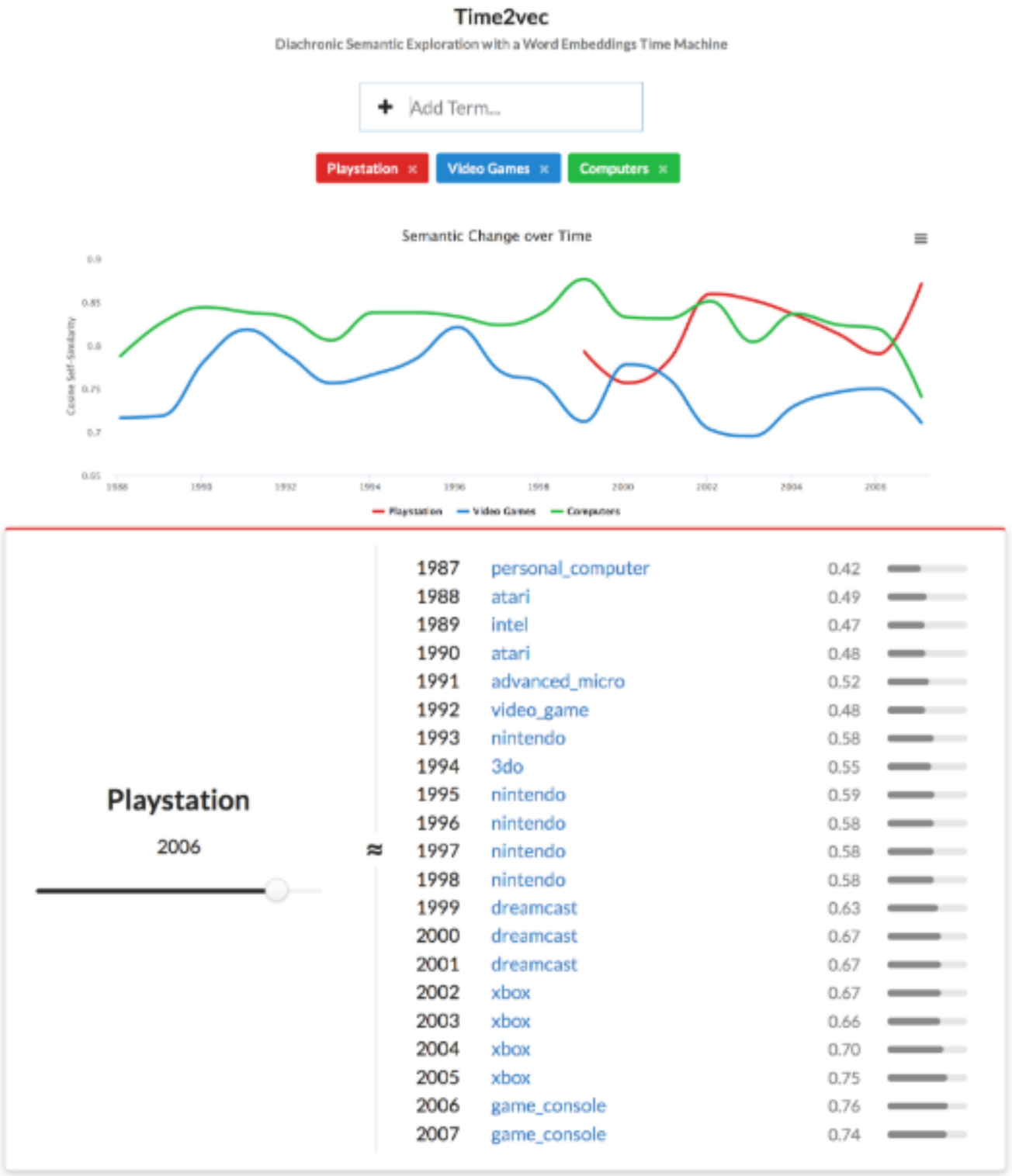


Temporal analogies (2/2)

- Temporal Equivalences



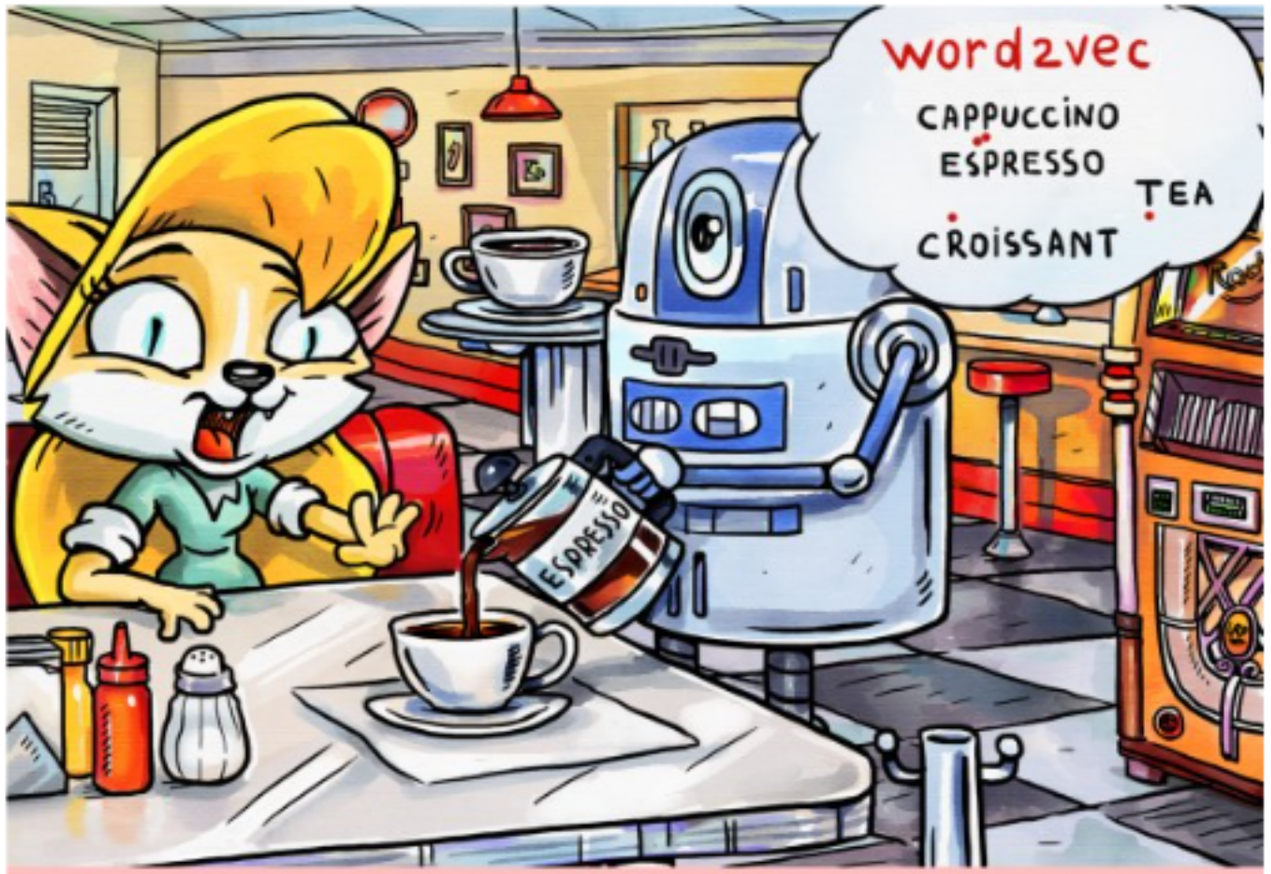
Time2Vec: web application



http://smartdata.cs.unibo.it/time2vec/

Current issues

- Sometimes words can be similar because strictly related and used in the same context, however can be very far in their meaning.
  - E.g.: **antonyms** such as bad and good, crucial for sentiment analysis.



- Espresso? But I ordered a cappuccino!
- Don't worry, the cosine distance between them is so small that they are almost the same thing.

PRACTICE DEMO

-

BEGIN

Used software: Jupyter, Sci-kit Learn
Find them in the Anaconda package here: https://www.anaconda.com/

Where to get word embeddings

- Word embeddings algorithms for Python are publicly available:
  - **fastText**: https://github.com/facebookresearch/fastText
  - **word2vec**: https://radimrehurek.com/gensim/
  - **GloVe**: https://github.com/stanfordnlp/GloVe
- You can use the gensim library for word2vec to load other trained word embeddings models
- Instead of training word embeddings yourself (takes time!), you can find **pre-trained** word embeddings online, e.g. for fastText:
  - https://github.com/facebookresearch/fastText/blob/master/pretrained-vectors.md

Jupyter Demo: fastText

We will load a pre-trained word embedding, learned from Wikipedia English and try out some algebraic operations

```
In [34]: from gensim.models import KeyedVectors
```

```
In [5]: model = KeyedVectors.load_word2vec_format('wiki.en.vec')
```

```
In [6]: model.wv.most_similar(positive=['woman', 'king'], negative=['man'])
```

```
Out[6]: [(u'queen', 0.6606324315071106),
         (u'princess', 0.5824028253555298),
         (u'regnant', 0.5788114666938782),
         (u'princesses', 0.5610353946685791),
         (u'consort', 0.5389299988746643),
         (u'regnants', 0.5266367197036743),
         (u'queenmother', 0.5214954614639282),
         (u'monarch', 0.5059499144554138),
         (u'\u2018princess', 0.5048949718475342),
         (u'parmaprincess', 0.5012947916984558)]
```

```
In [18]: model.wv.most_similar(positive=['paris', 'italy'], negative=['france'])[0]
```

```
Out[18]: (u'rome', 0.7258368134498596)
```

```
In [27]: model.wv.most_similar(positive=['obama','good'], negative=['bush'])[0]
```

```
Out[27]: (u'decent', 0.6170227527618408)
```

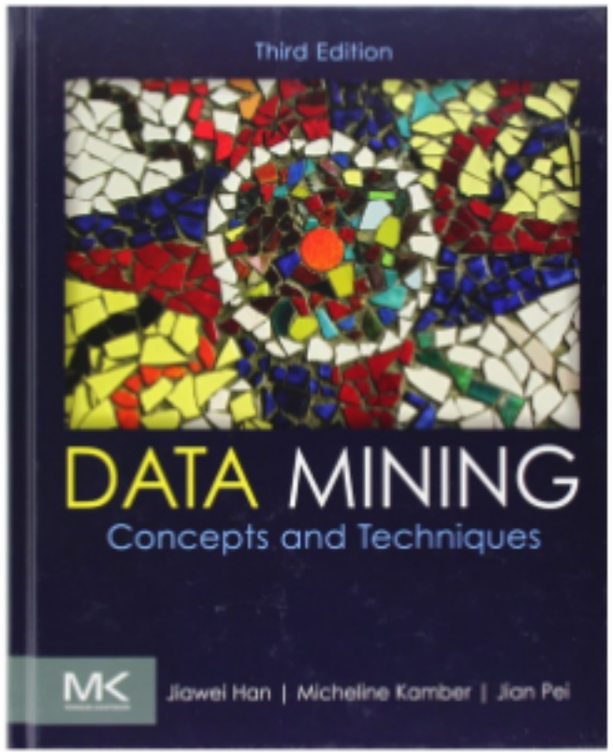
PRACTICE DEMO

-

END

References

Data Mining
Concepts and Techniques
Authors: Jiawei Han, Micheline Kamber, Jian Pei.



Representations for Language:
From Word Embeddings to
Sentence Meanings
Authors: Christopher Manning - Stanford University

Links for CBD projects

Google Form to add your project:

https://goo.gl/forms/Vq2fizYBBk4WYhly1

Google Spreadsheet with added projects:

https://goo.gl/WgSrrN