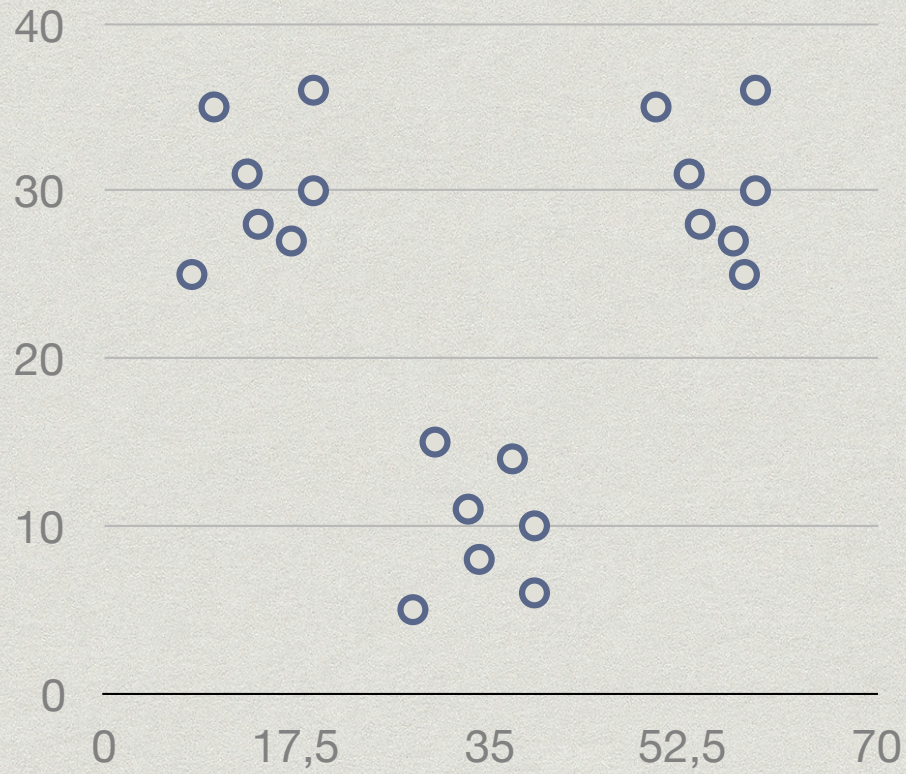
CLUSTERING

ALESSANDRO PANCONESI, SAPIENZA

What is Clustering?

- A grouping of data objects such that, objects in the same group are similar (or close) while objects in different groups are dissimilar (or far apart)



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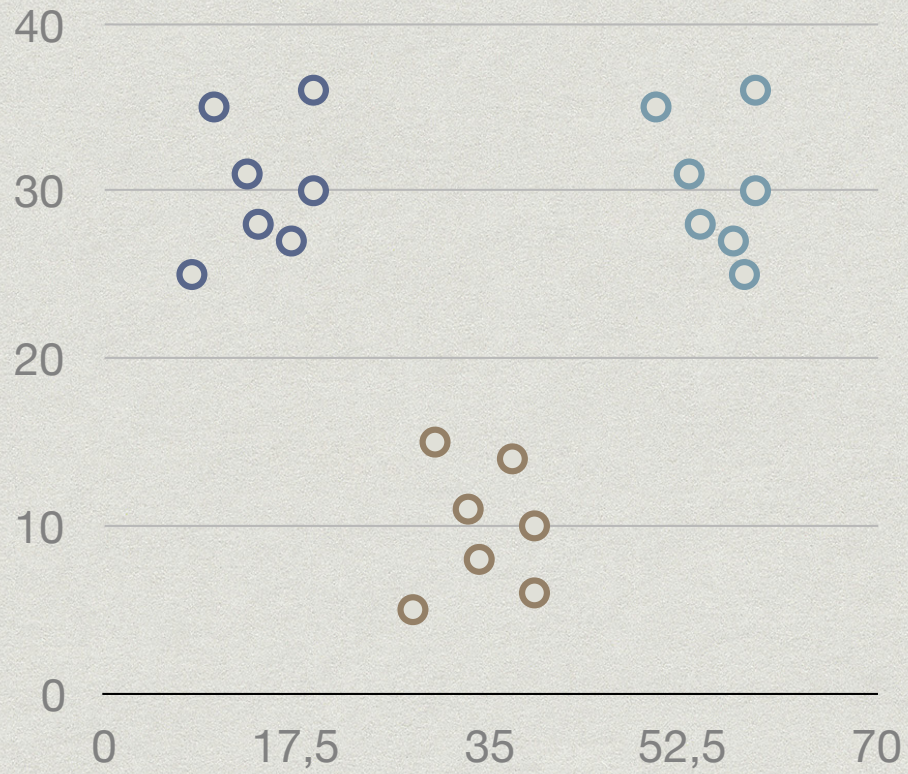
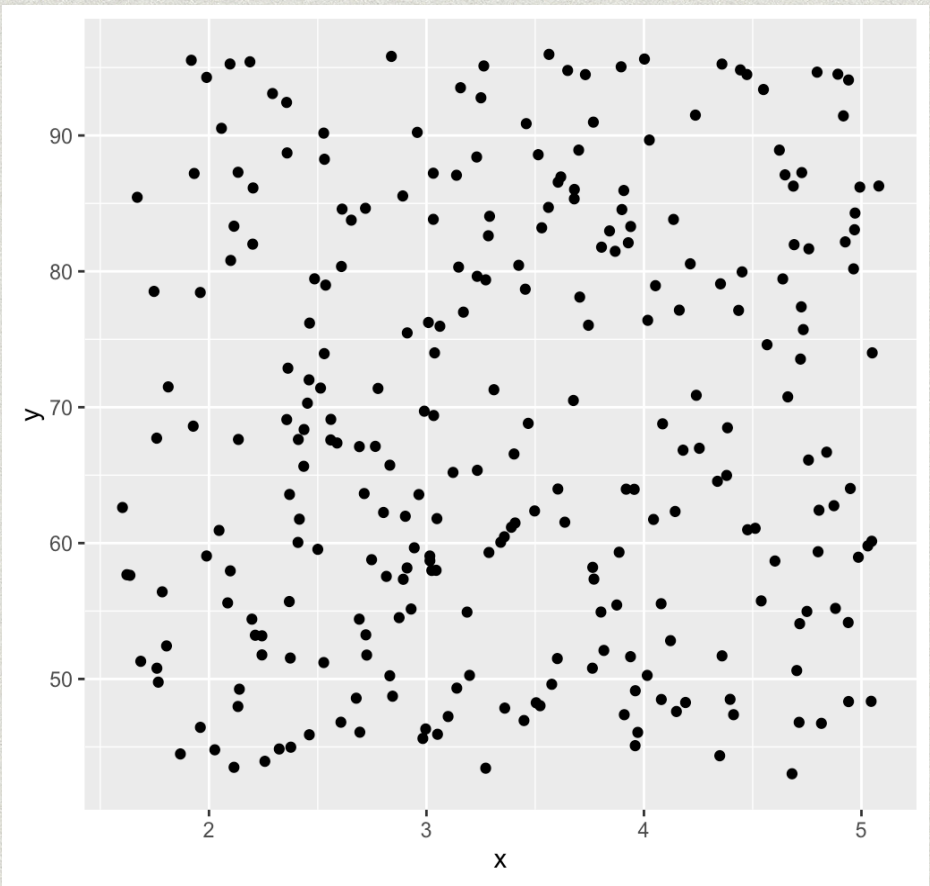


What is Clustering?

- Clustering is an intuitively appealing idea, but it is far from being well-defined, or for that matter, well-definable



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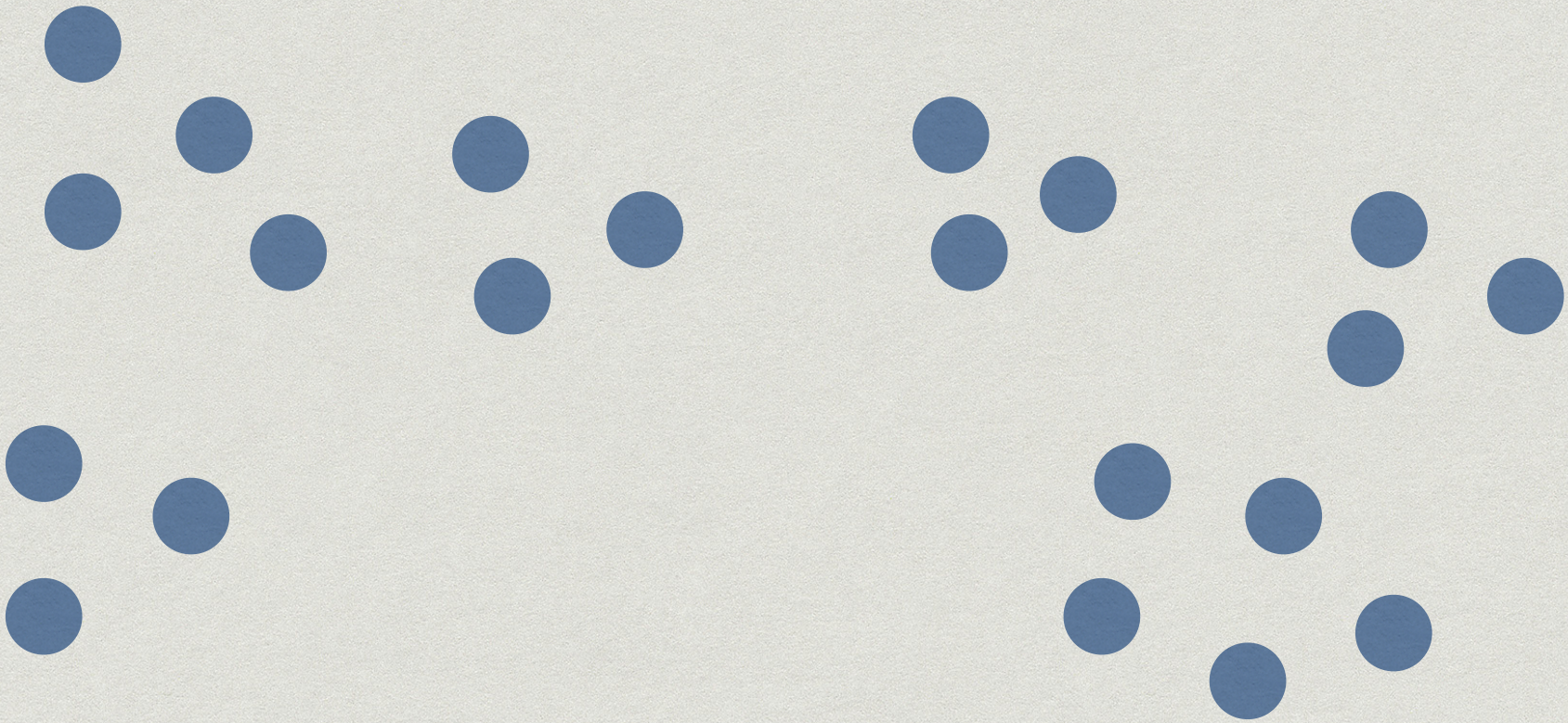
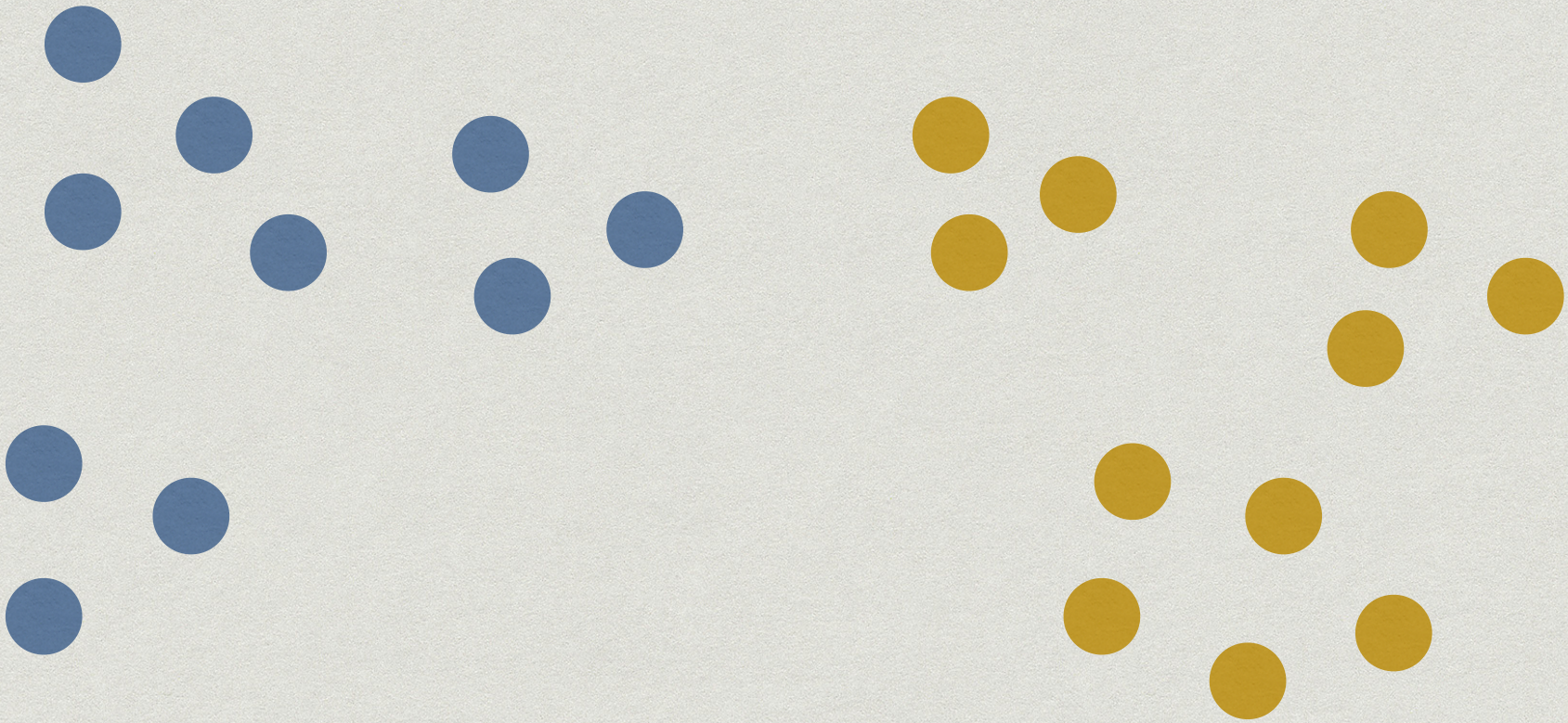


What is Clustering?

Two clusters?



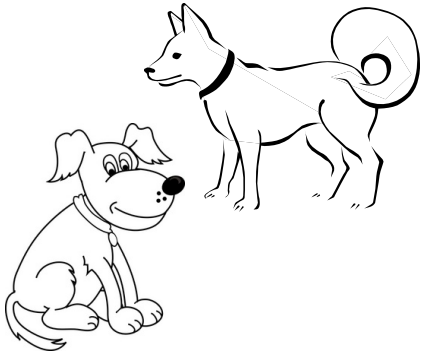
What is Clustering?

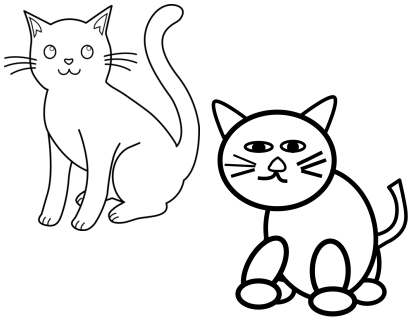
Four clusters?

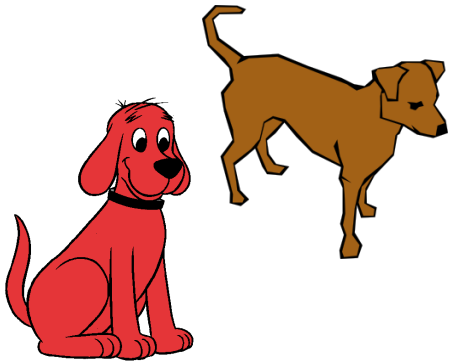
What is Clustering?

Six clusters?

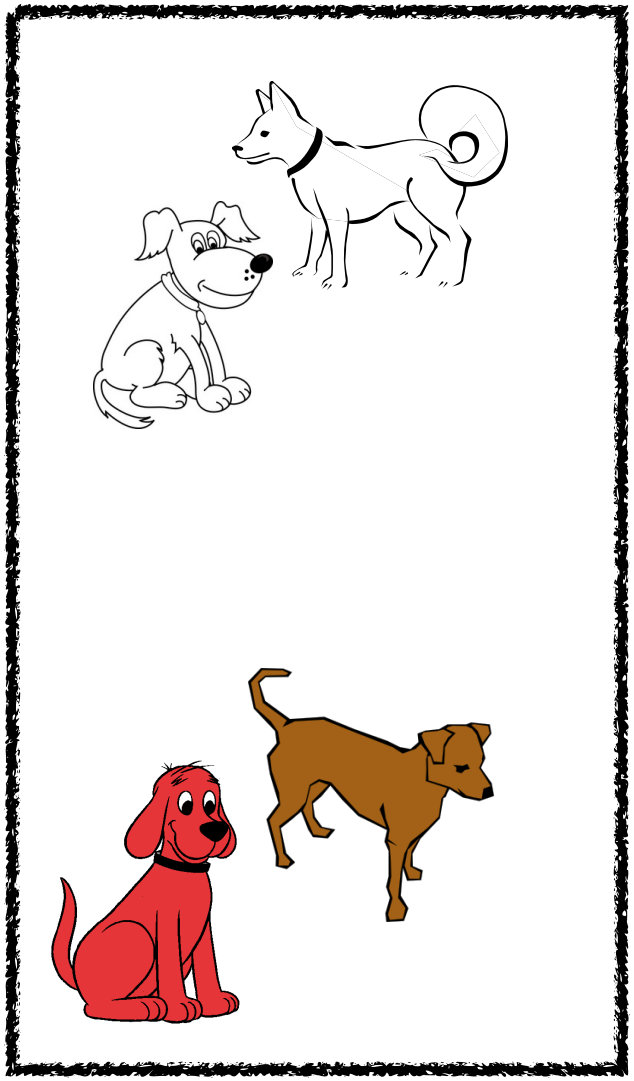
What's similar?

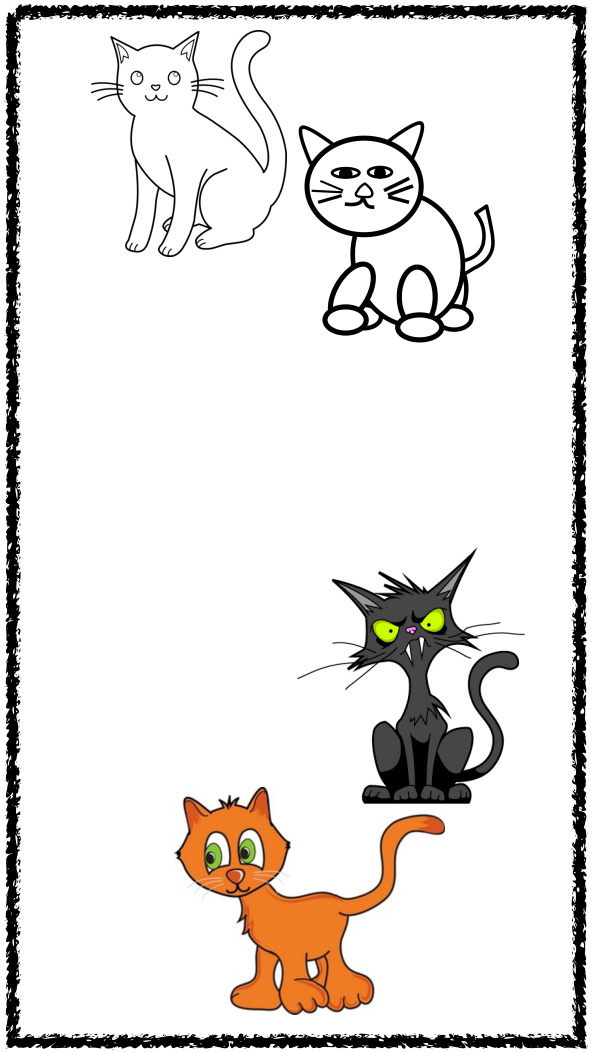






What's similar?





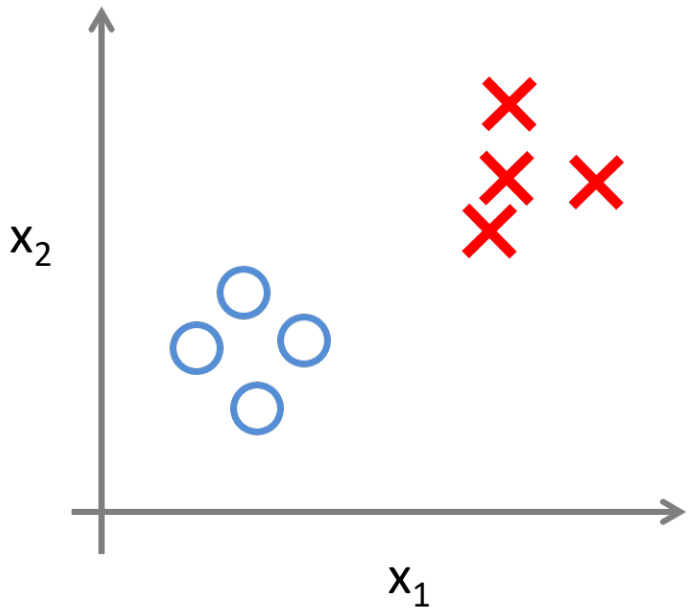
What's similar?

What is clustering?

- Still, clustering is extremely useful
- …with a huge array of applications in all sorts of data analysis

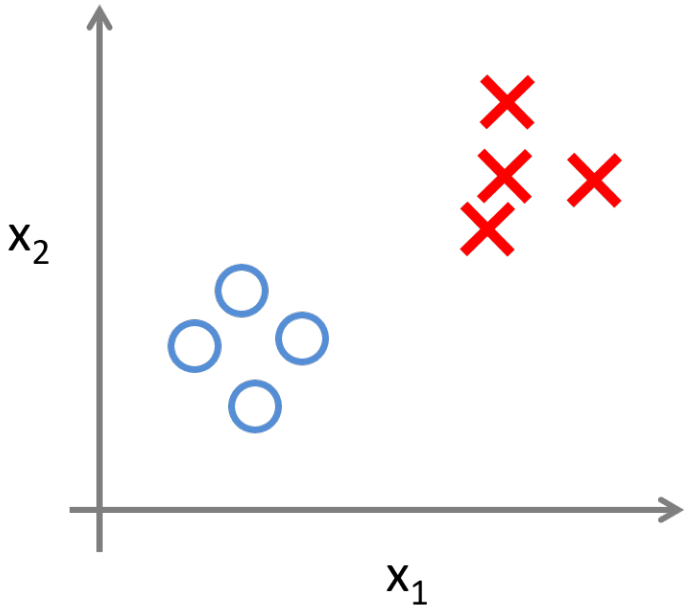
Supervised vs. Unsupervised

Supervised Learning

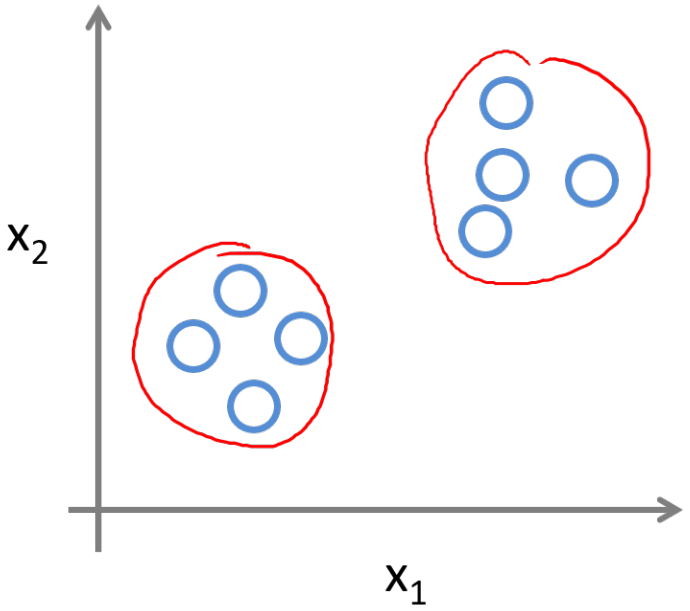


Supervised vs. Unsupervised

Supervised Learning



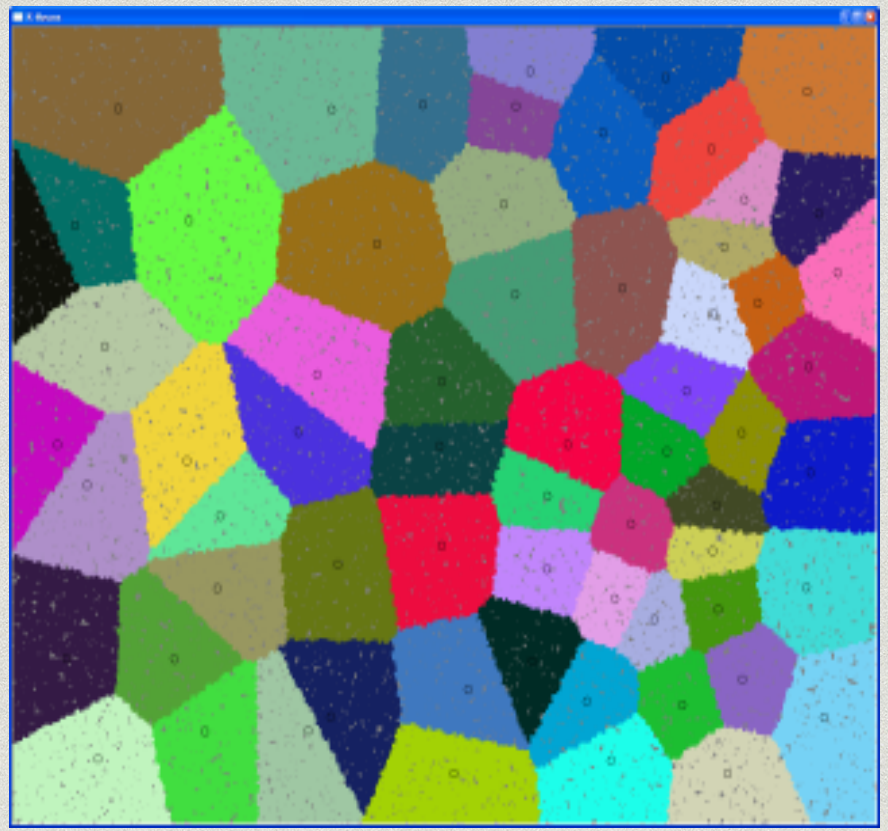
Unsupervised Learning



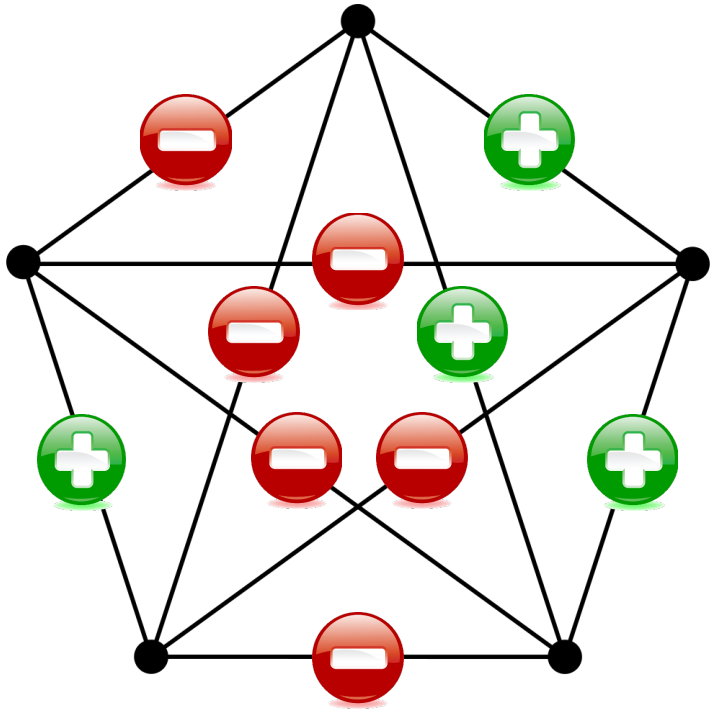
THE CLUSTERING ZOO

The Clustering Zoo

- There are dozens of different notions of “clustering”
- Here, we will consider only clusterings that partition the input data (a graph or points in space)



Correlation Clustering



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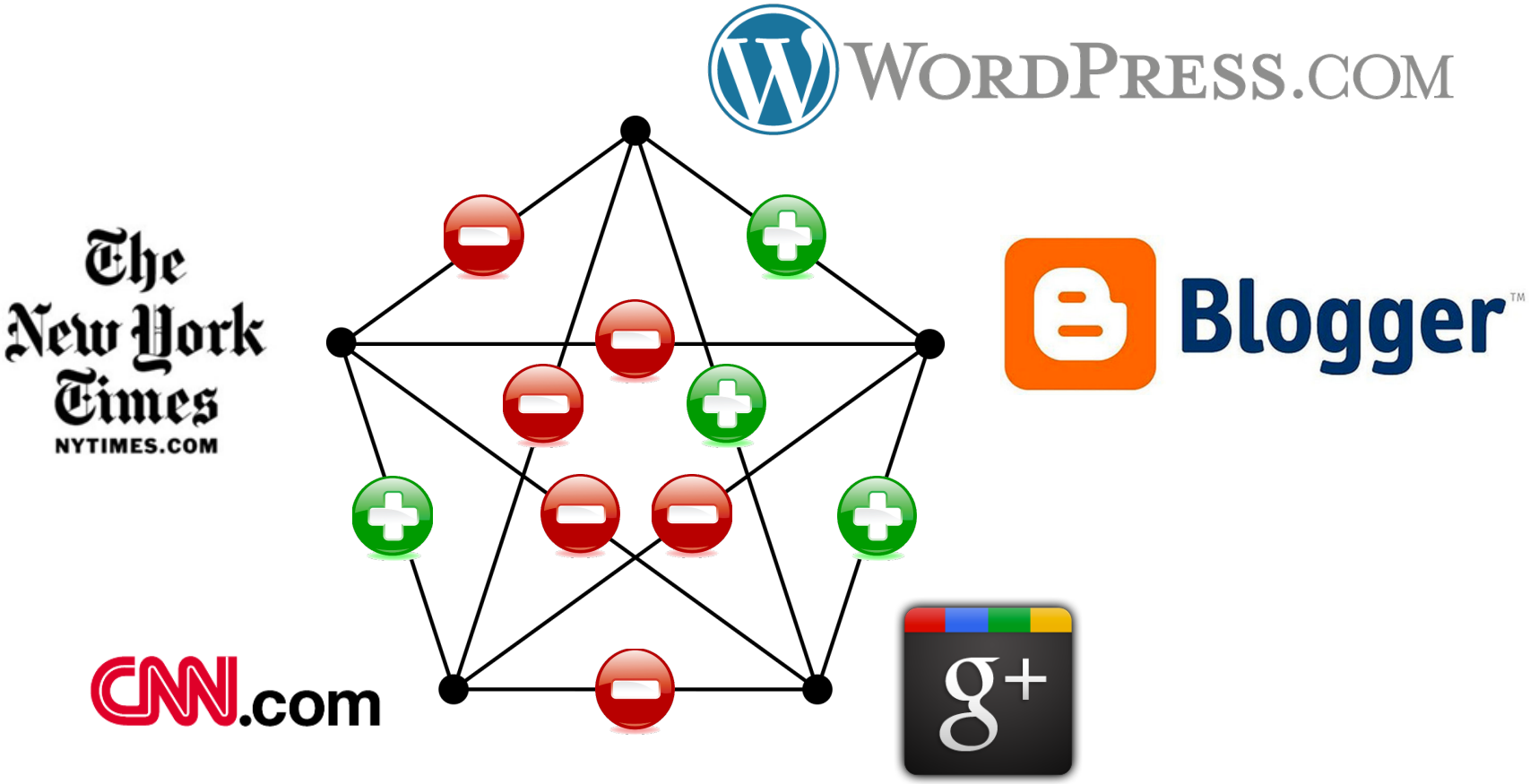

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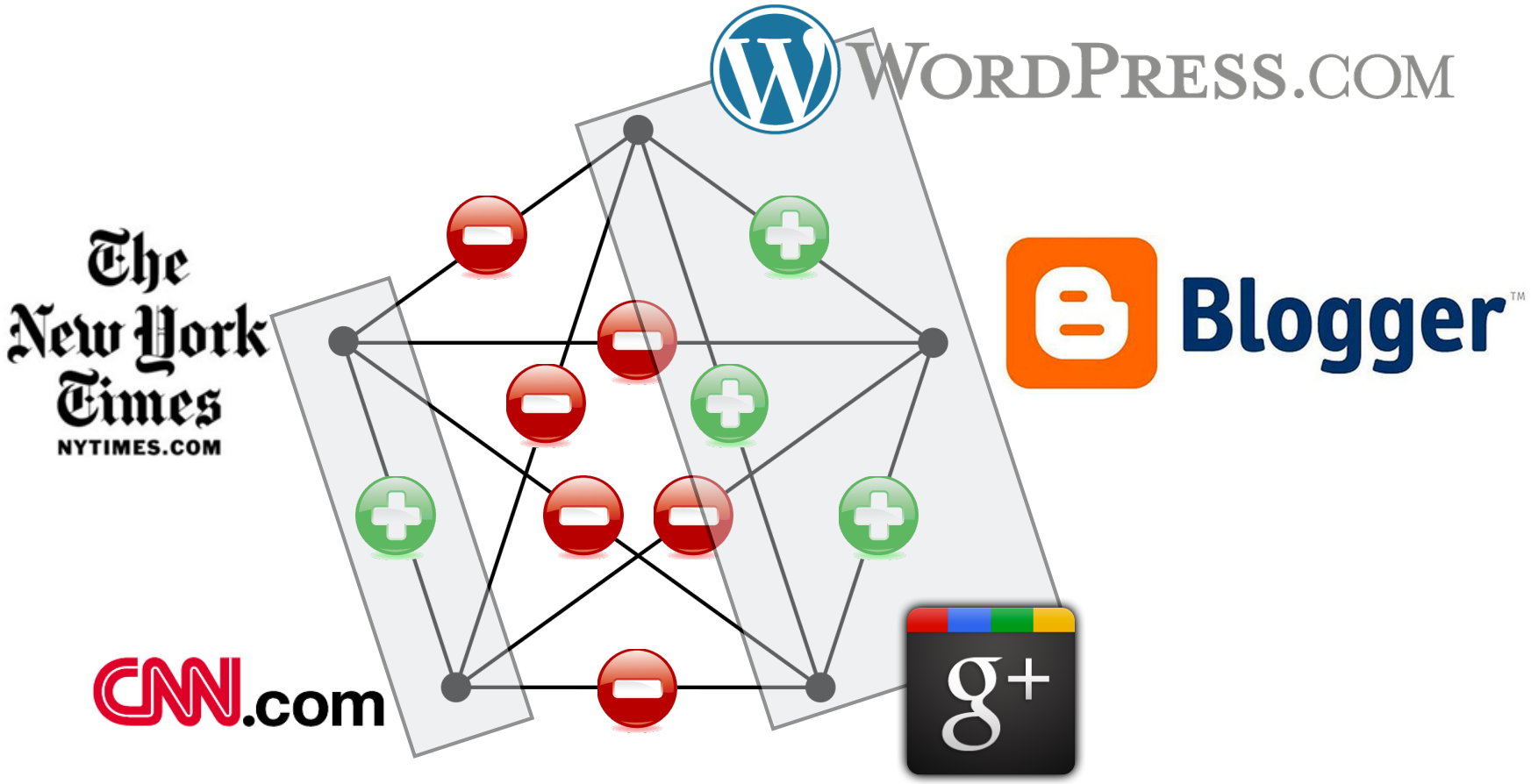

Correlation Clustering

The goal is to partition the elements in
disjoint clusters
so as to **minimize** the number of **mistakes**

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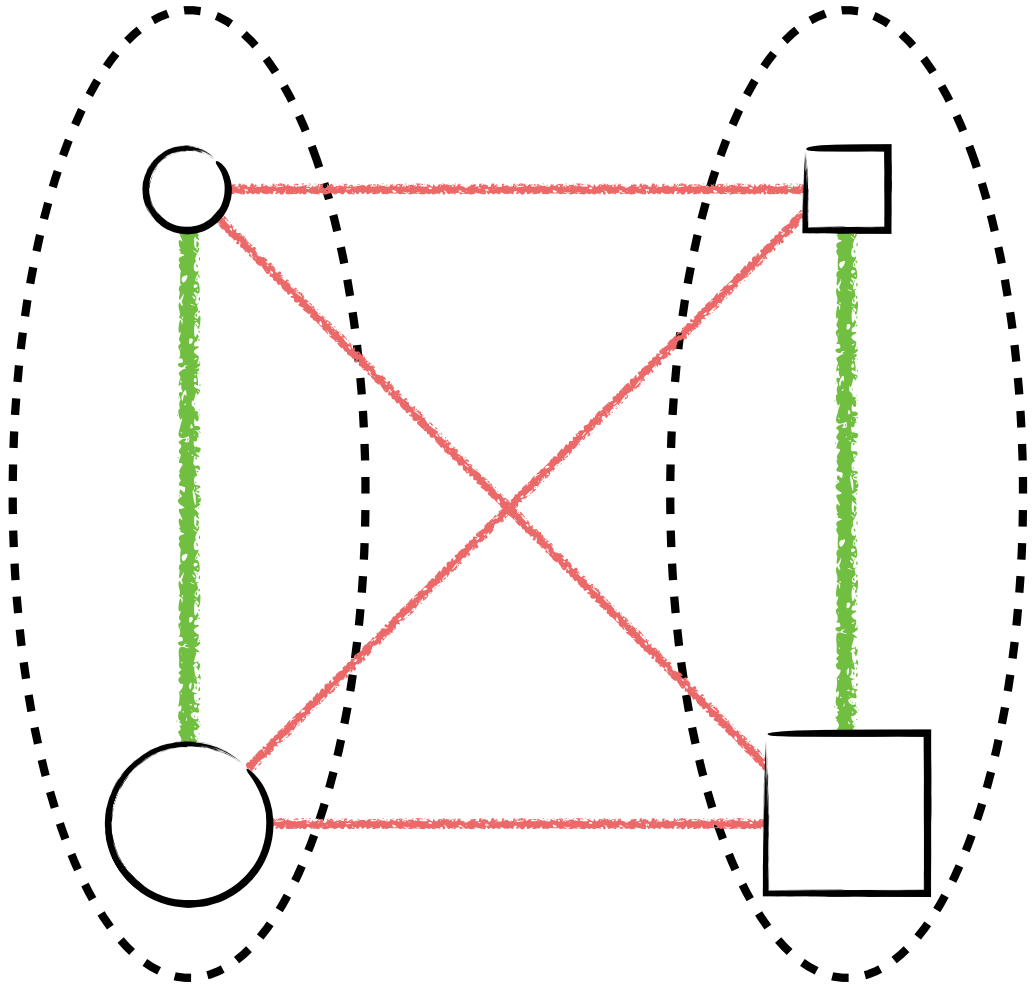
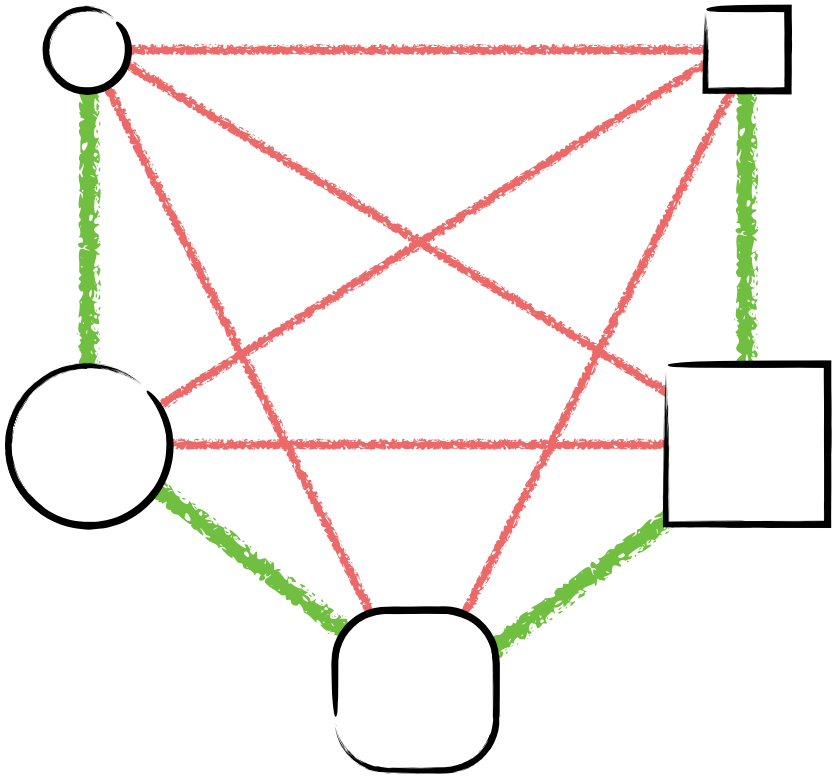
The **number of clusters**
is not decided a priori

Correlation Clustering



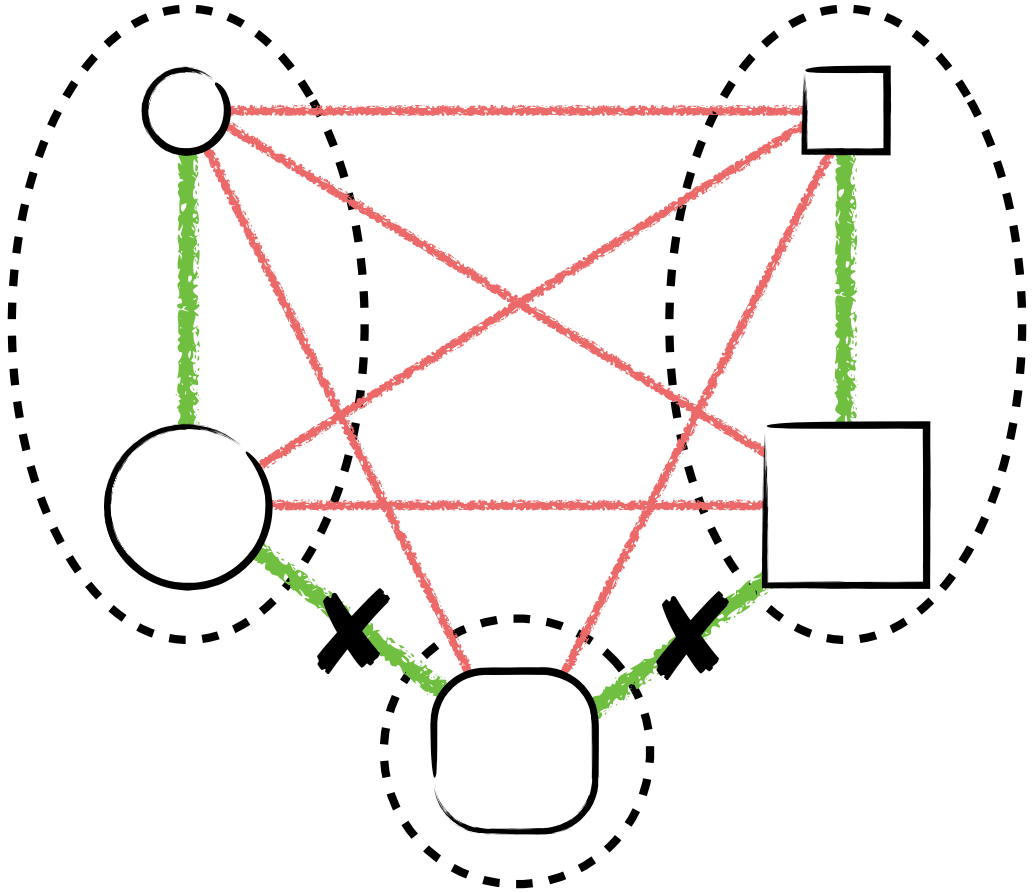
"Perfect clustering"
(0 mistakes)

Correlation Clustering



In this instance you cannot have zero mistakes

Correlation Clustering



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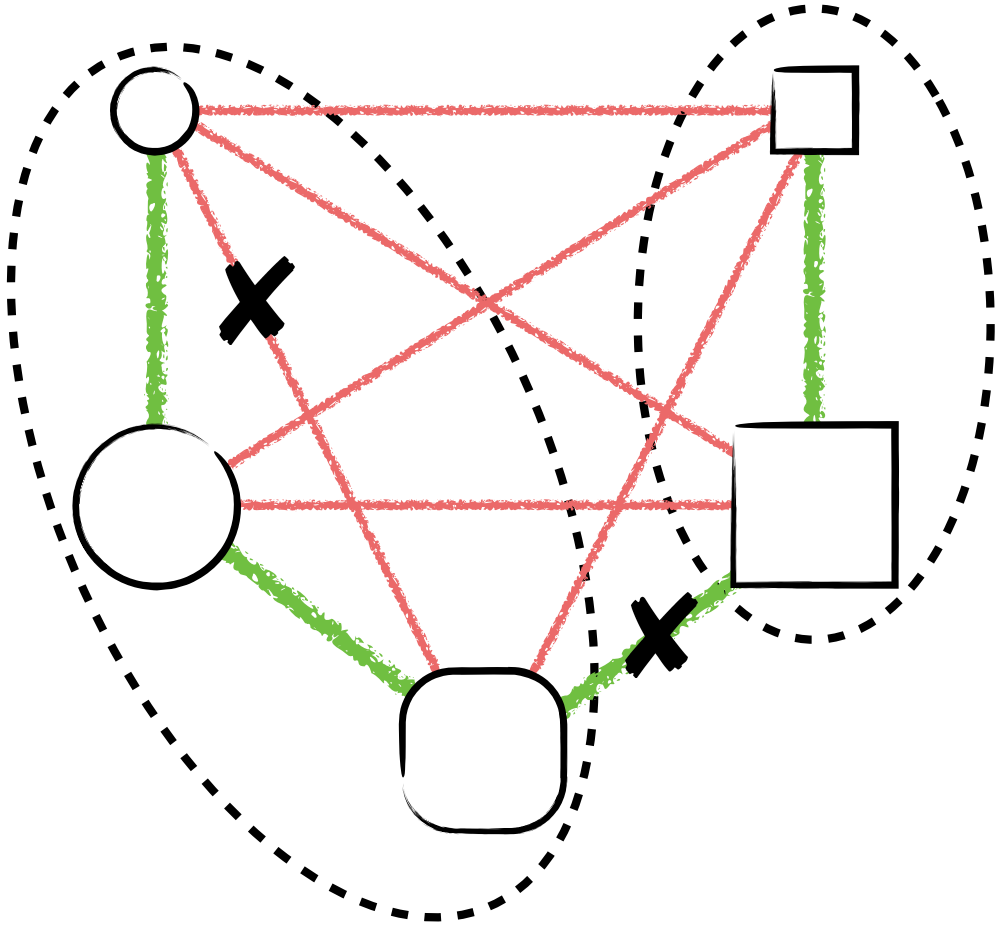

In this instance you cannot have zero mistakes

k-means Clustering

- We are given a set S of n points in R^d
- Assume k is also given
- Find k points $c_1,..,c_k$, called centers (or means) such that the following cost is minimised

$$\text{cost}(c_1, \ldots, c_k) := \sum_{i=1}^{n} \min_j d(x_i, c_j)^2$$

k-means Clustering

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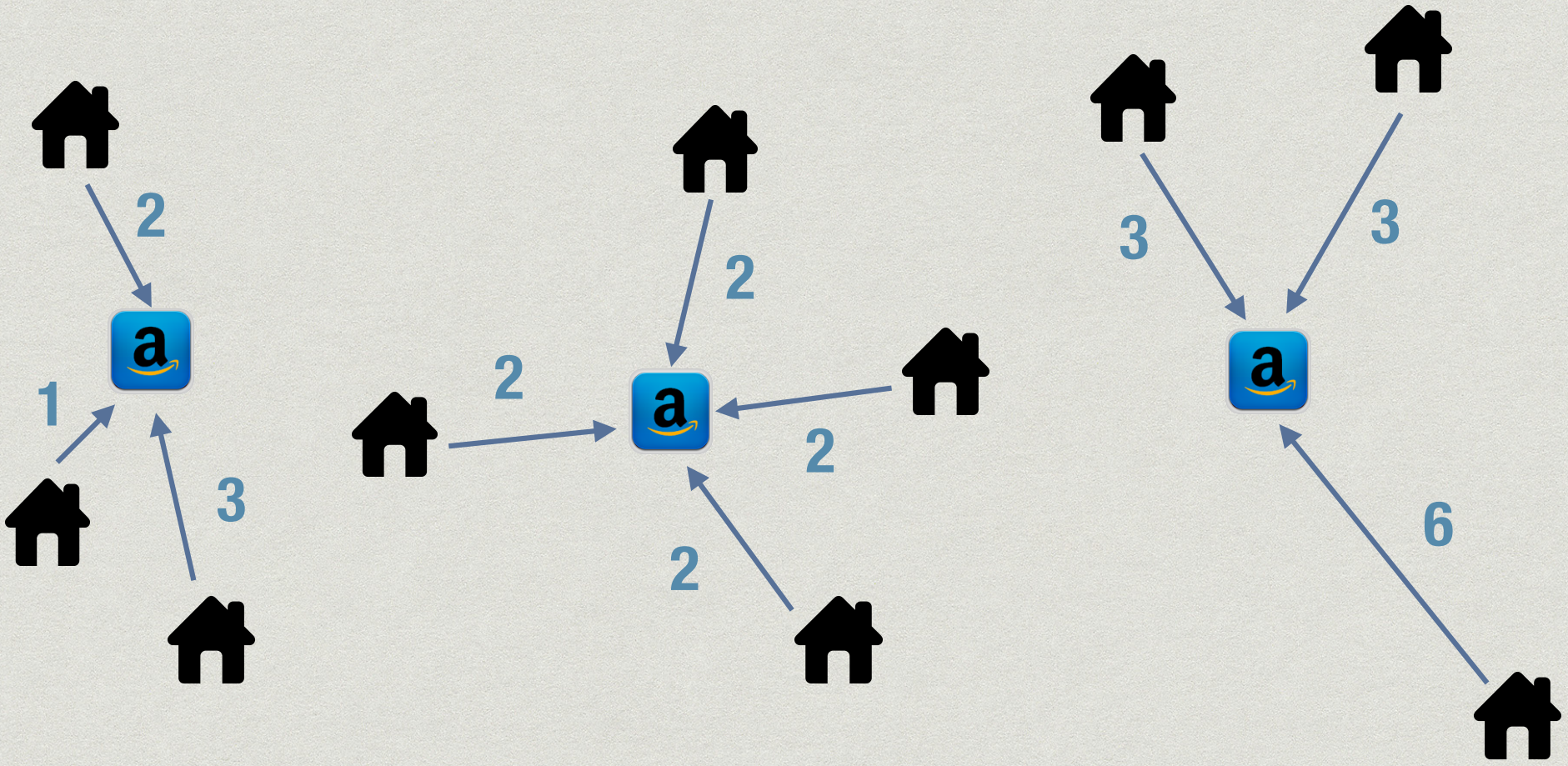


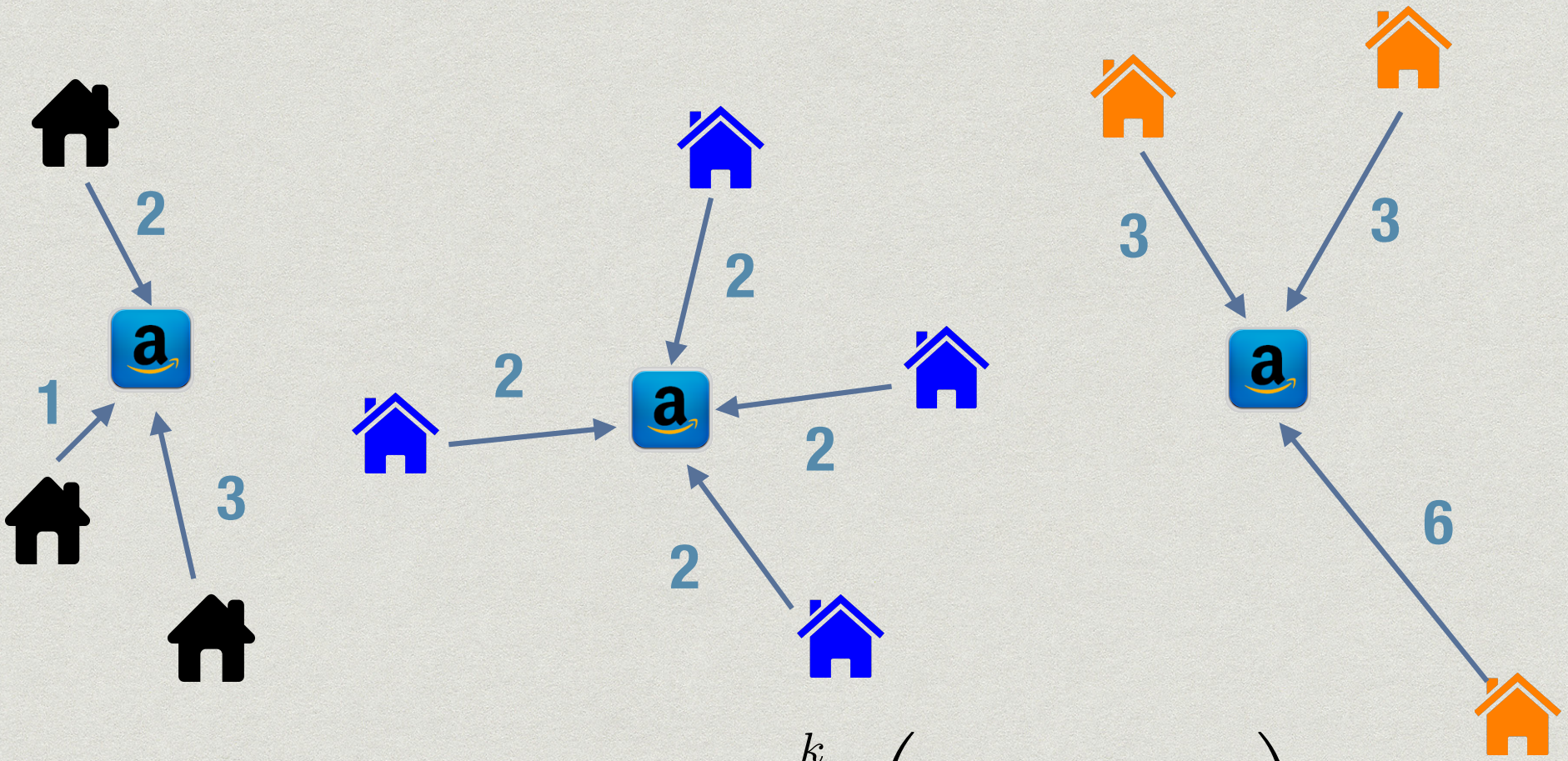
$$cost(c_1, c_2, c_3) = 84$$

k-means Clustering

- Equivalently, given a set S of n points in R^d and an integer k…
- find $c_1,..,c_k$ and partition S into $S_1,..,S_k$ by assigning each x in S_i to c_i, in such a way the following cost is minimised

$$\text{cost}(c_1, \ldots, c_k) := \sum_{i=1}^{k} \left(\sum_{x \in S_i} d(x, c_i)^2 \right)$$

k-means Clustering



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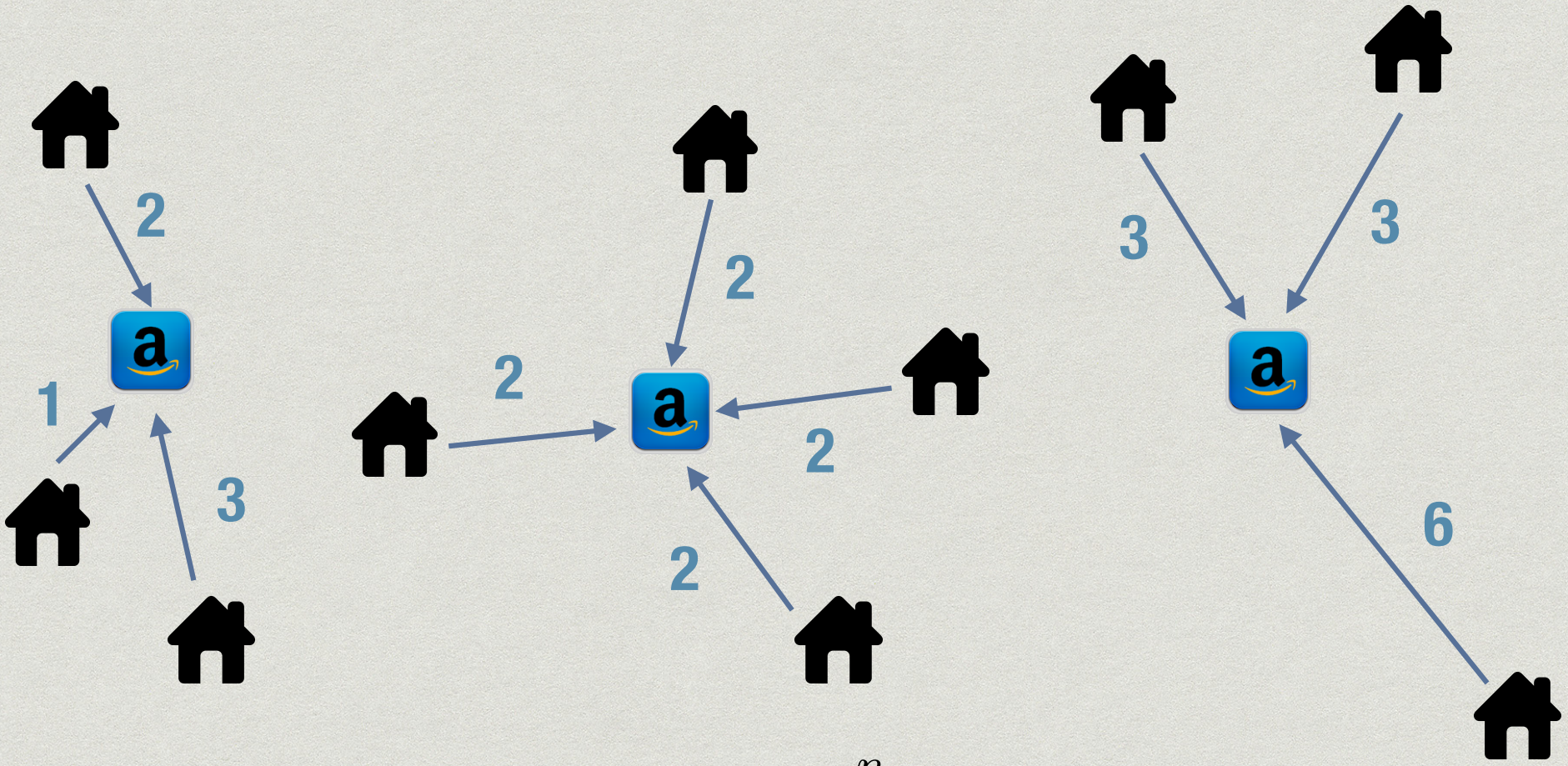

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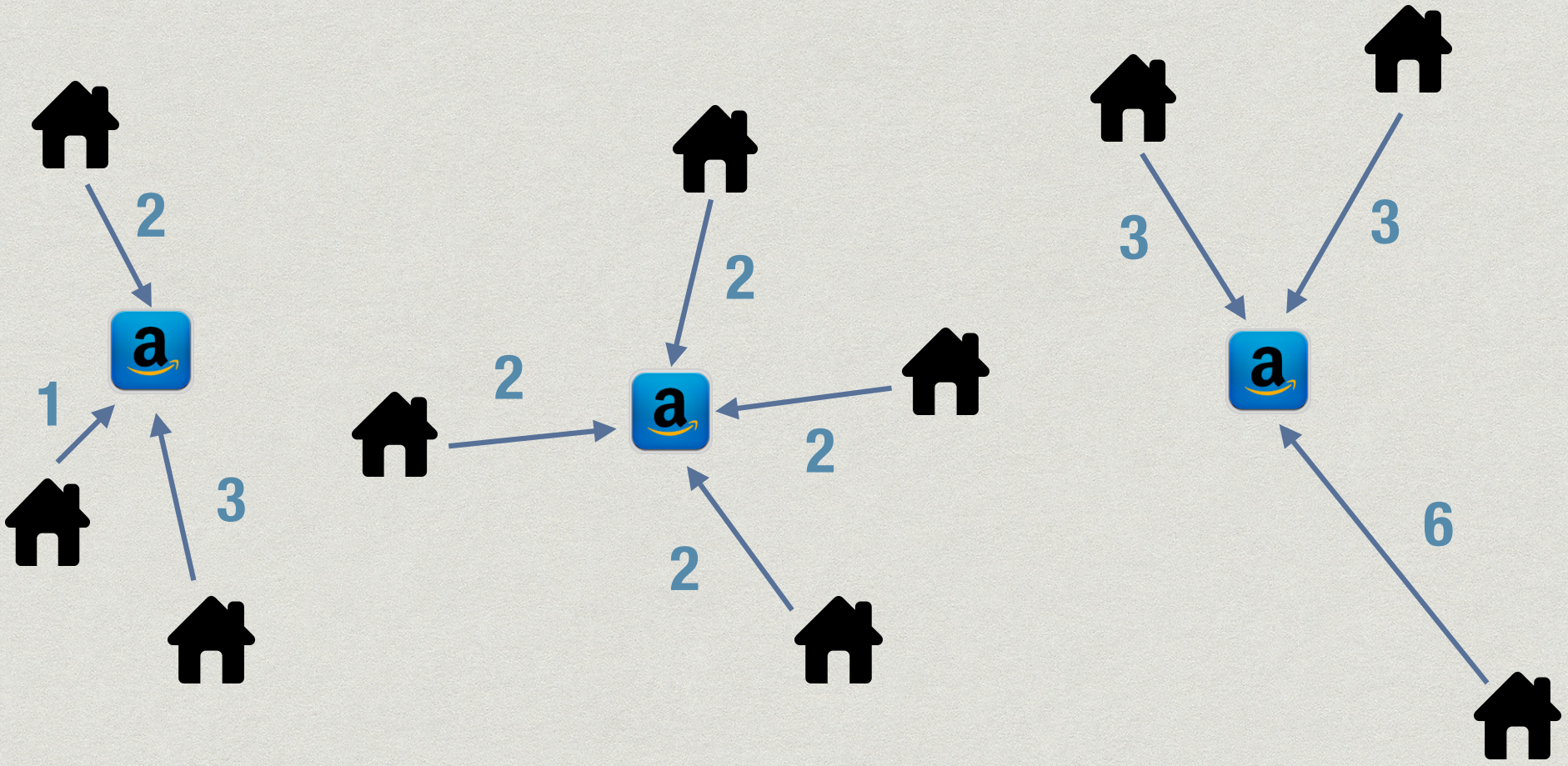


$$cost(c_1, c_2, c_3) = 26$$

k-median Clustering

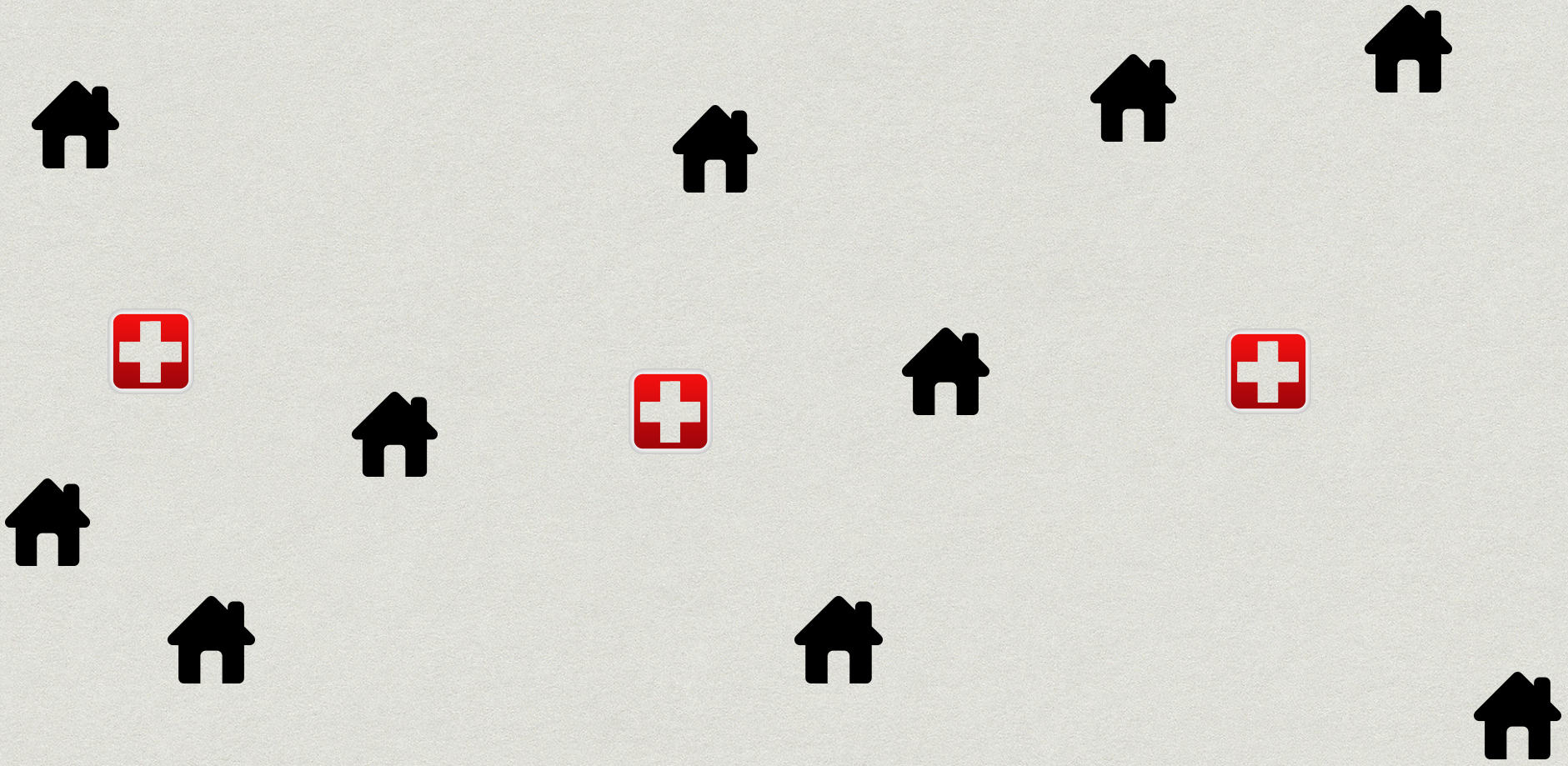
- Same input as in k-means clustering, but objective function becomes

$$\text{cost}(c_1, \ldots, c_k) := \sum_{i=1}^{n} \min_j d(x_i, c_j)$$

k-center Clustering

$$\text{cost}(c_1, \ldots, c_k) := \max_{x \in S} \min_{j} d(x, c_i)$$

k-center Clustering



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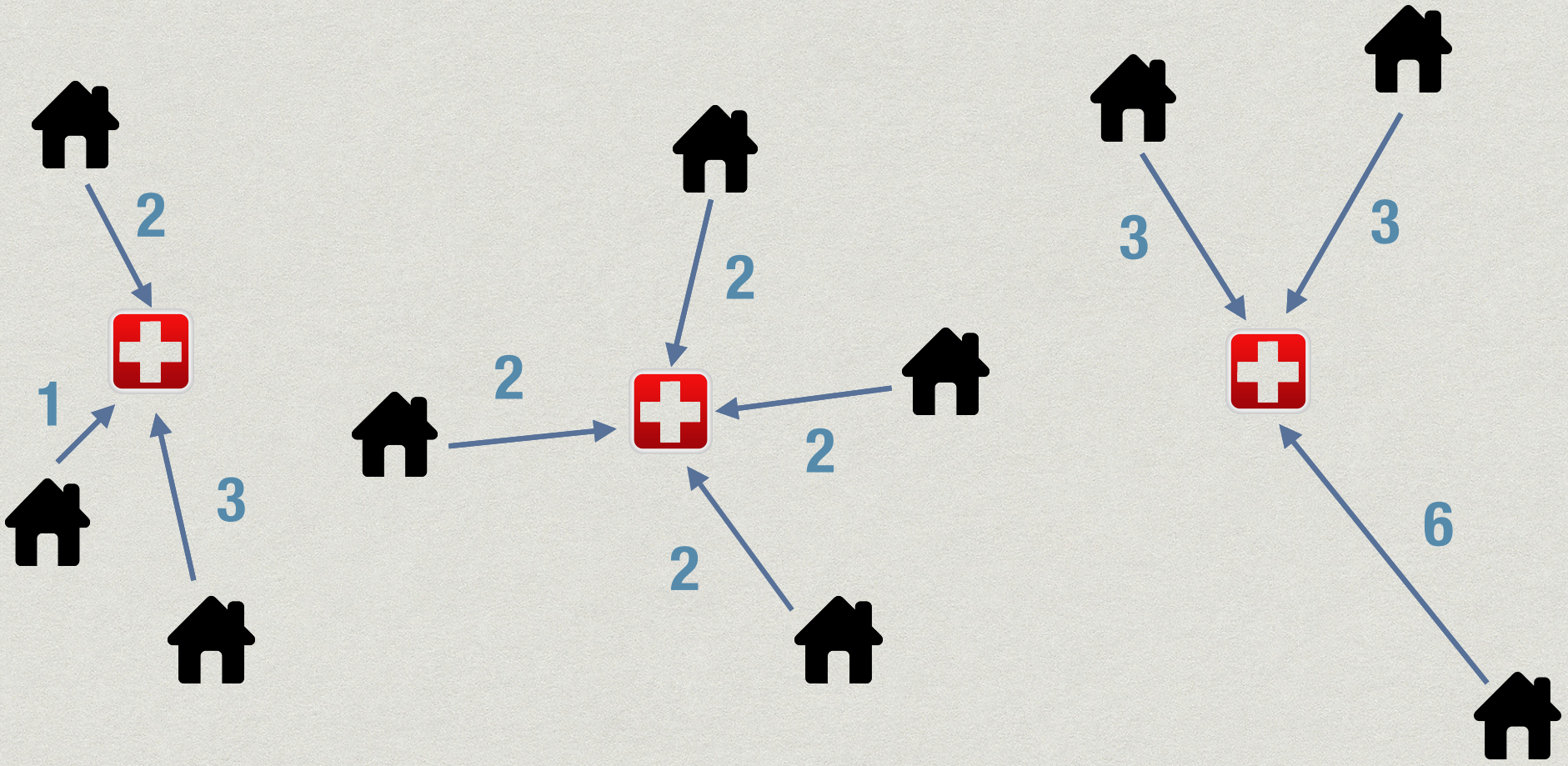

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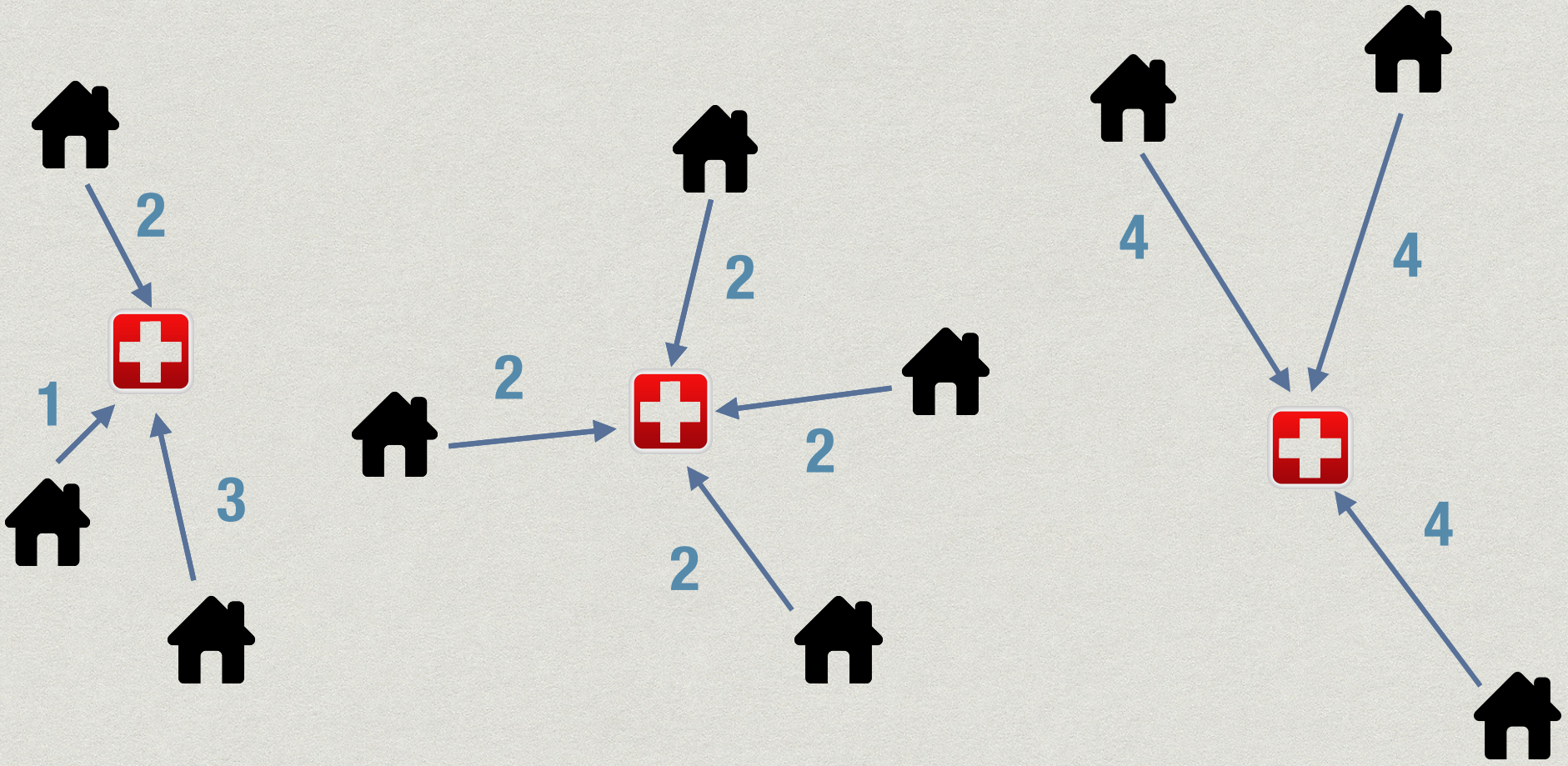

$$\text{cost}(c_1, \ldots, c_k) := \max_{x \in S} \min_{j} d(x, c_i)$$

k-center Clustering

- We want to build k facilities (say hospitals) in such a way that no point in S is too penalised, i.e. we want to minimise the maximum distance between every point and its closest center

$$\text{cost}(c_1, \ldots, c_k) := \max_{x \in S} \min_{j} d(x, c_i)$$

Algorithms for clustering

K-Means / Lloyds' Algorithm

- We are given *n* vectors on *d* dimensions;
  we aim to select *k* clusters

- Choose *k* vectors arbitrarily (eg uniformly at random) as *centroids*

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- Until *stability:*
  - create an empty cluster for each centroid;
  - add each vector to the cluster of the closest centroid;
  - for each cluster, compute its new centroid (the mean of its vectors).

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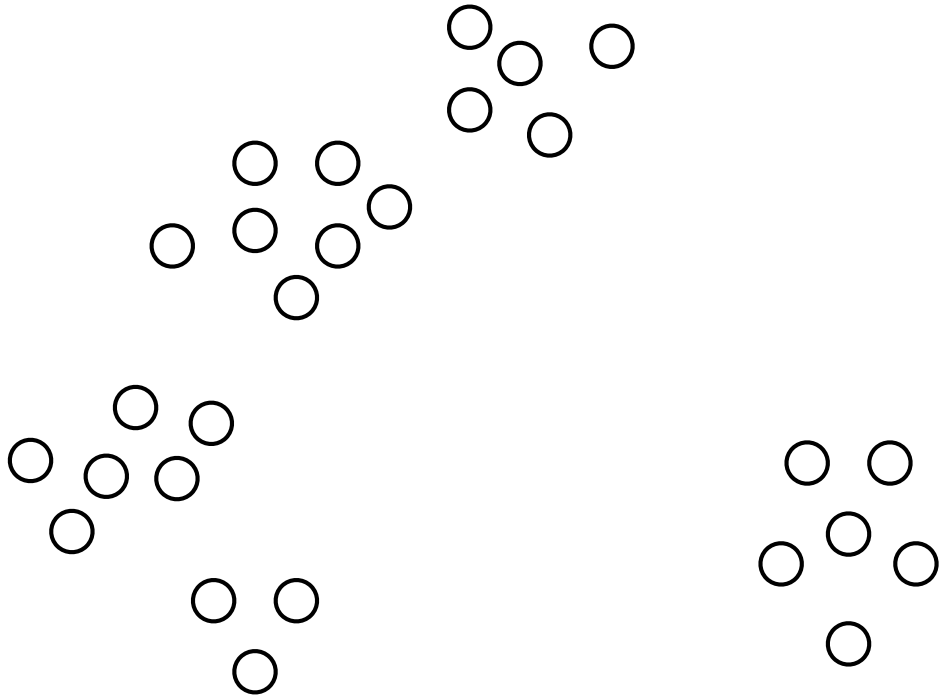
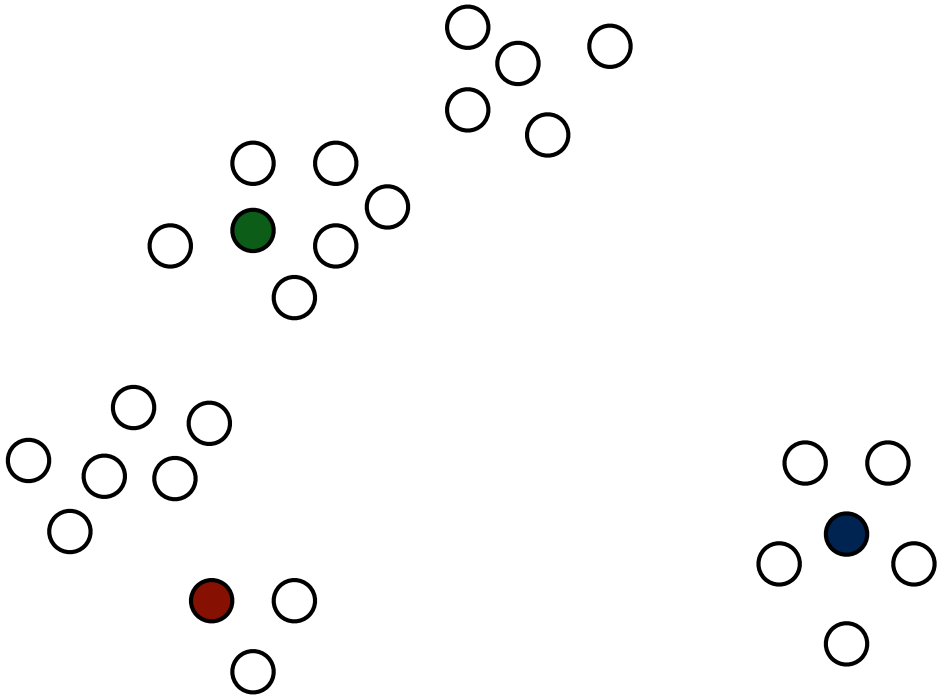
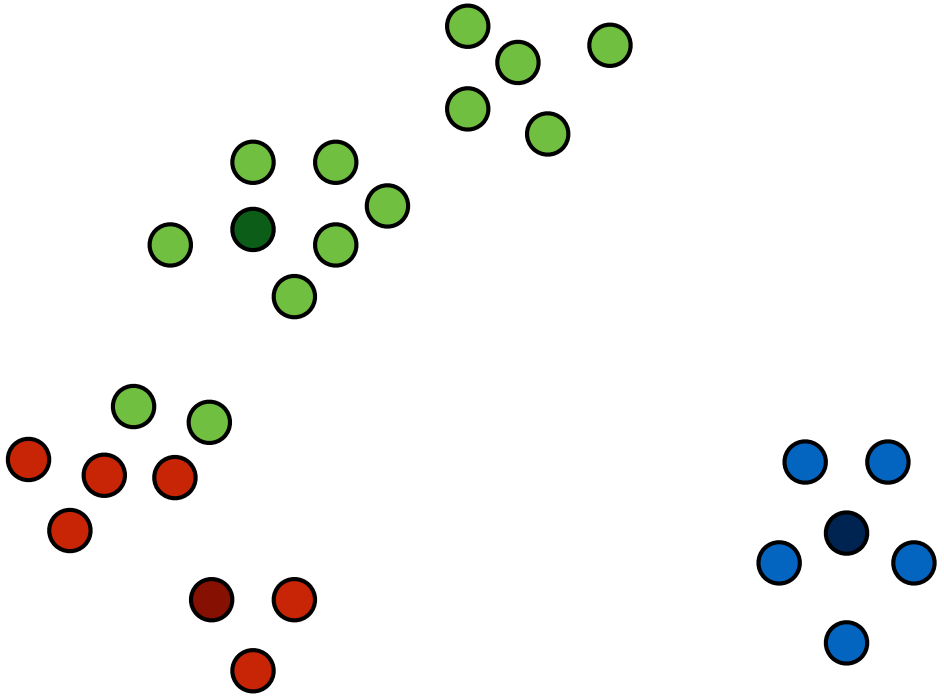
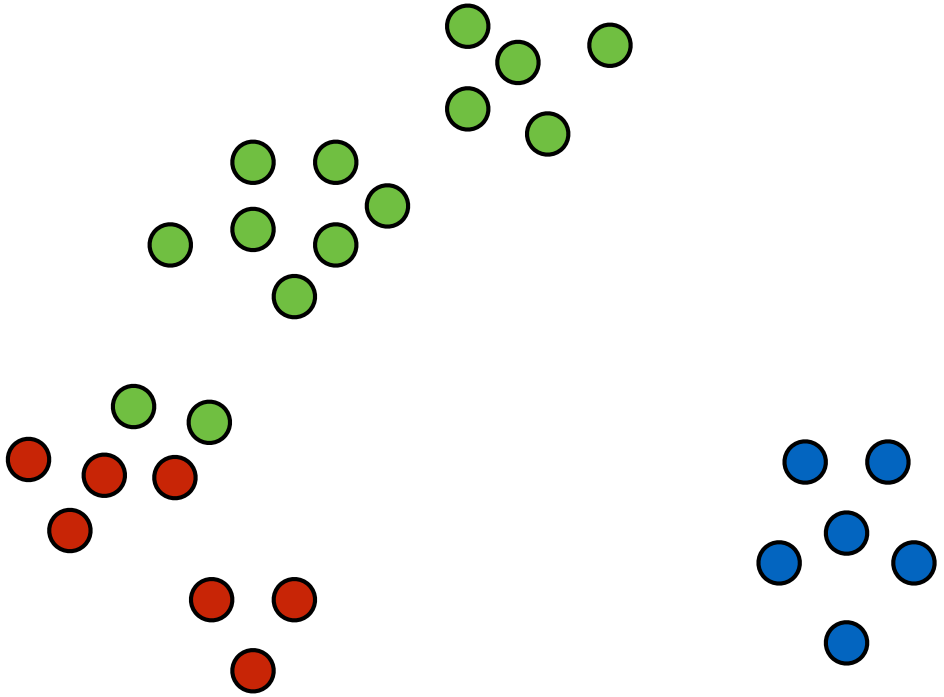
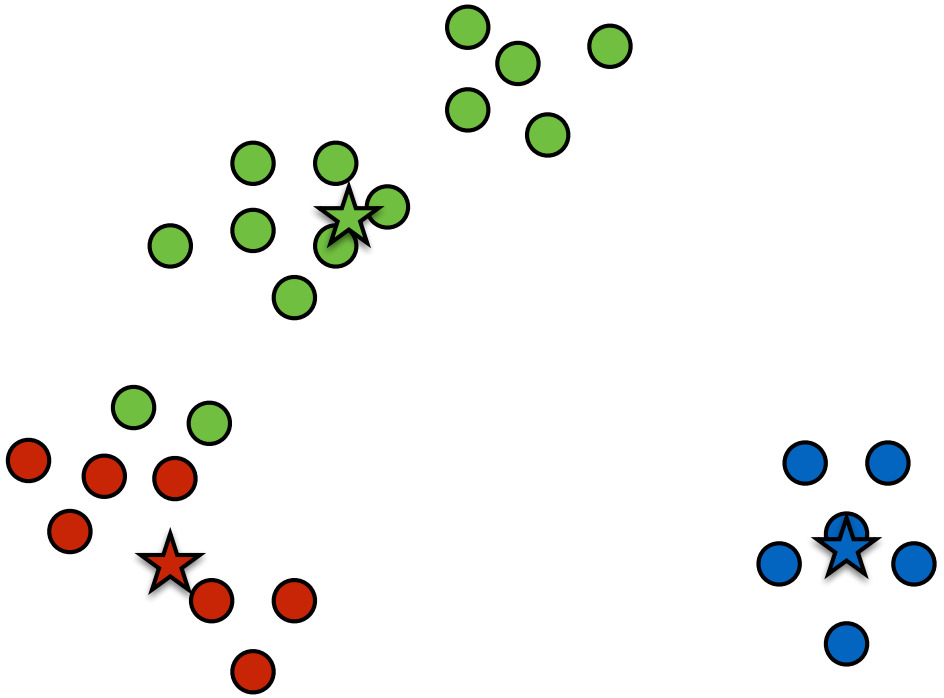
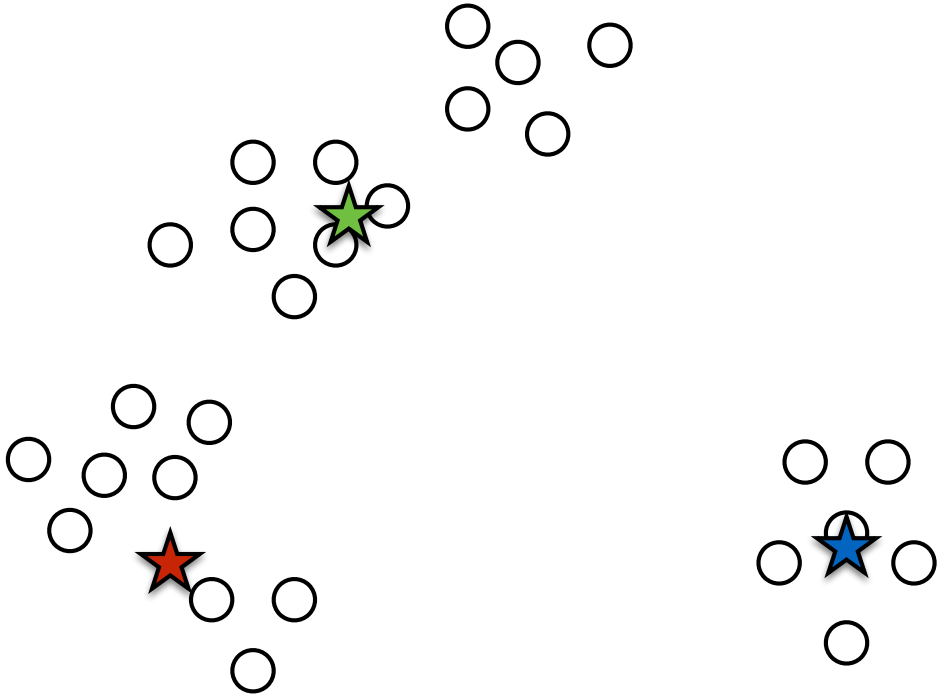


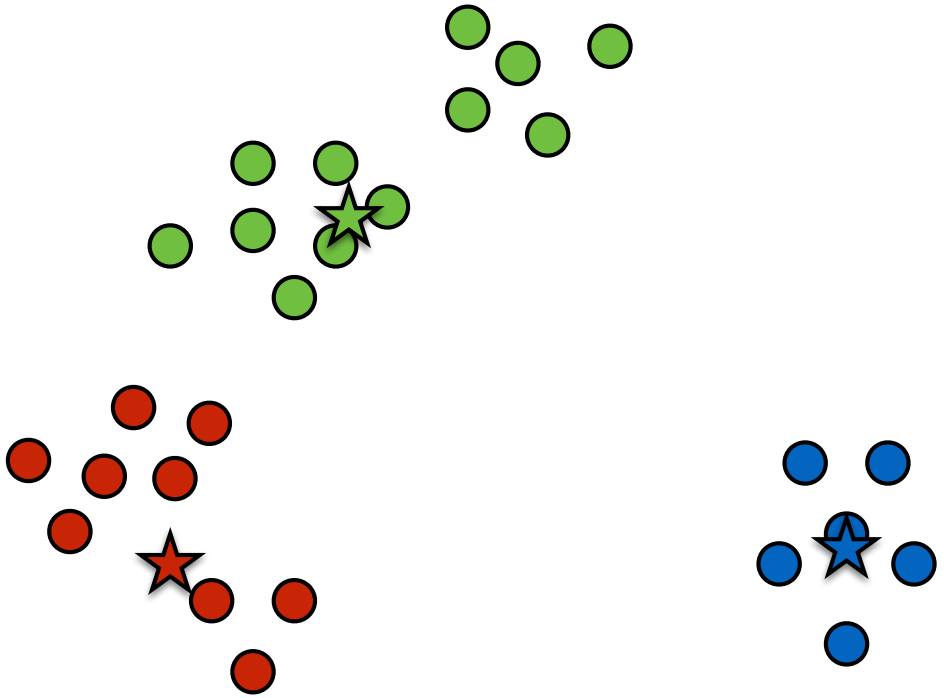


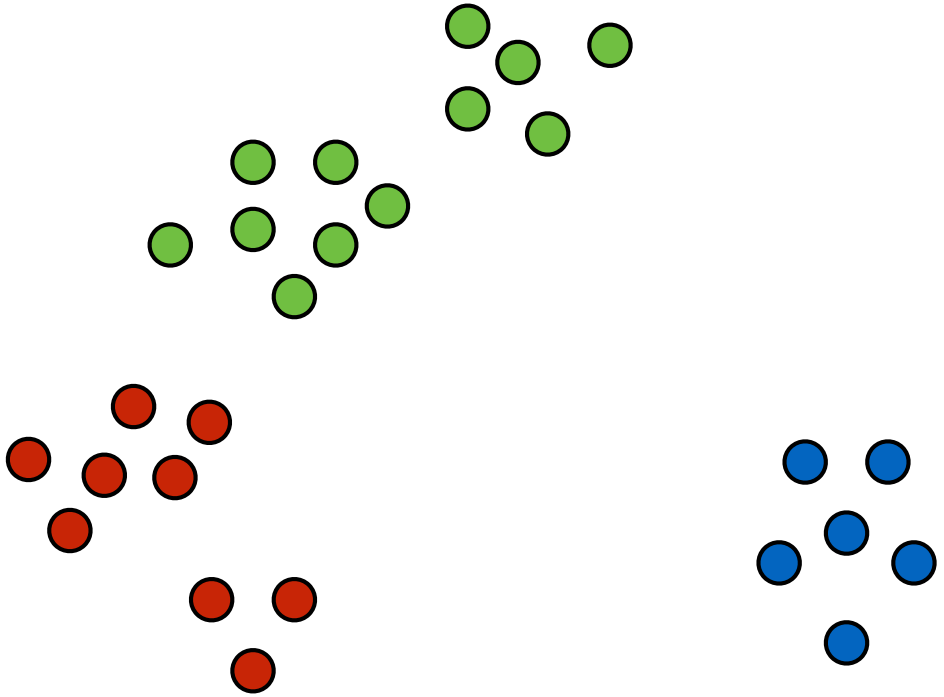


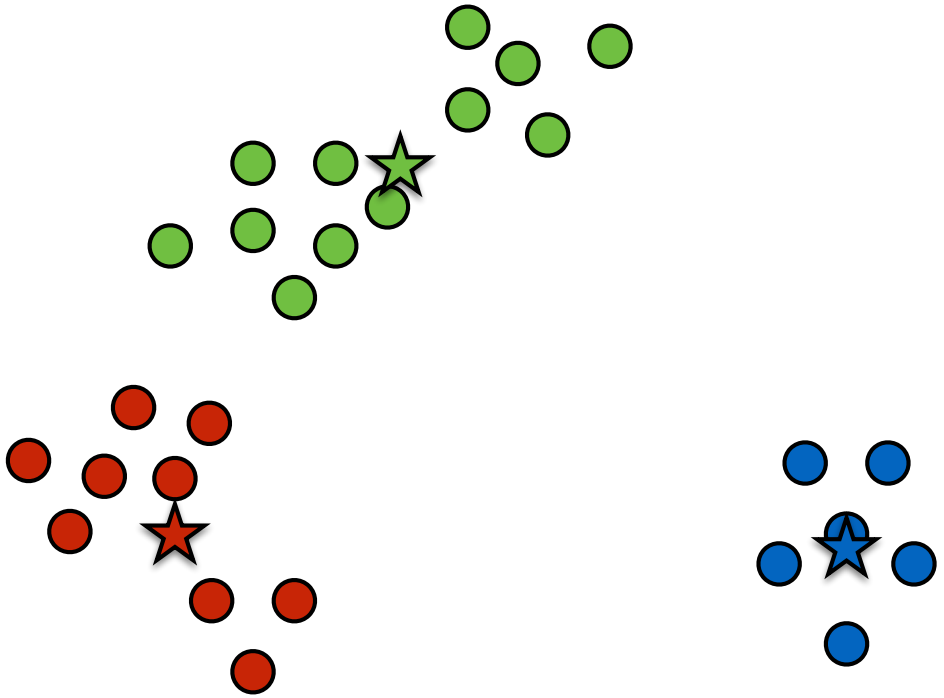


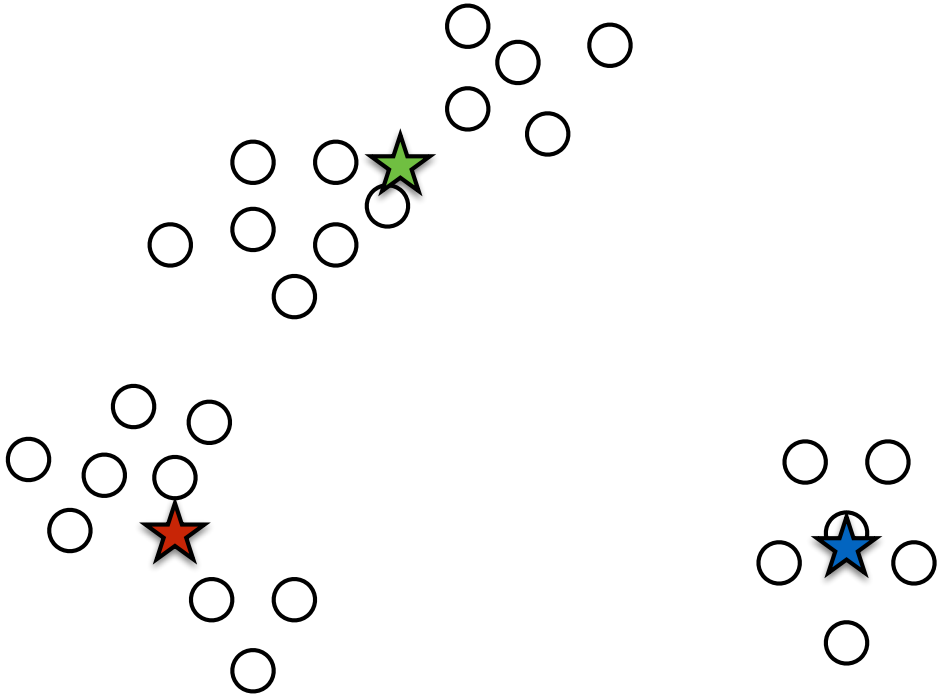


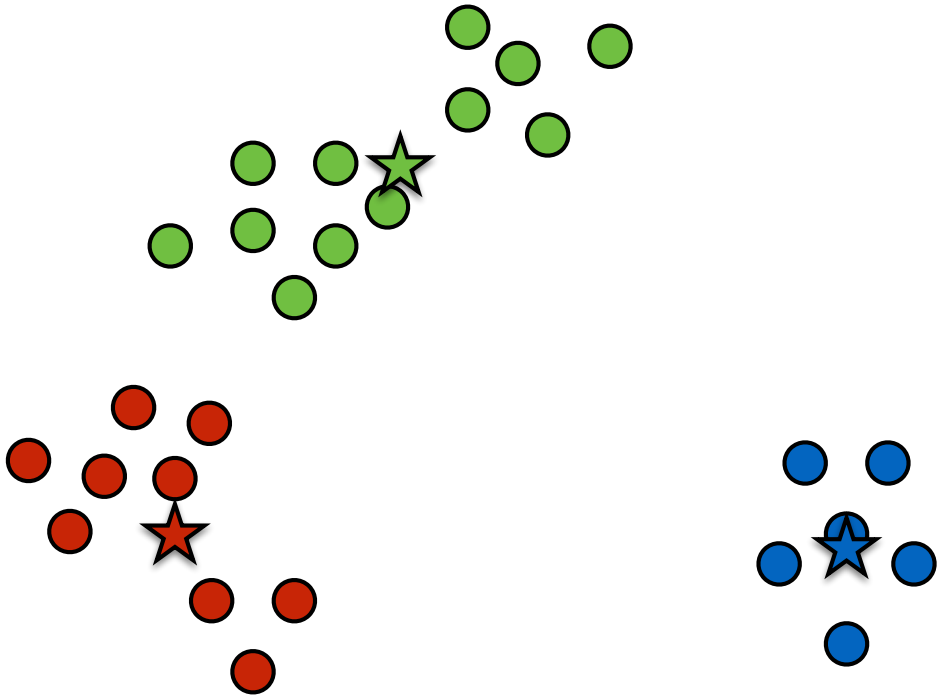












The clustering is finally stable

K-Means/Lloyd's Algorithm

- Does the algorithm computes the optimal k-means clustering? NO!
- Does it come close to it? NO! It can be arbitrarily bad
- Is the algorithm efficient? No! It can take **exponential time**
- What does it do? It computes a local minimum
- Why do people use it? Good question

K-Means Clustering

- Ok, Lloyd's algorithm does not compute the optimum..
- ..is there an **efficient** algorithm that does? No, and in fact, it **may not exist**

TIME IS OF THE ESSENCE

Time is of the essence

	N=50	N=100	N=1000	$N = 10^6$	$N = 10^9$
N	~0	~0	~0	0.001 sec	1 sec
N^2	~0	~0	0.001 sec	16 min	31 years
2^N	13 days	2871 U	$>10^{283}$ U	!	!
3^N	227,643 centuries	$> 10^{21}$ U	!	!	!
N!	$> 10^{46}$ U	$> 10^{140}$ U	!	!	!

computer speed = 1 billion operations per second

U is the Age of the Universe

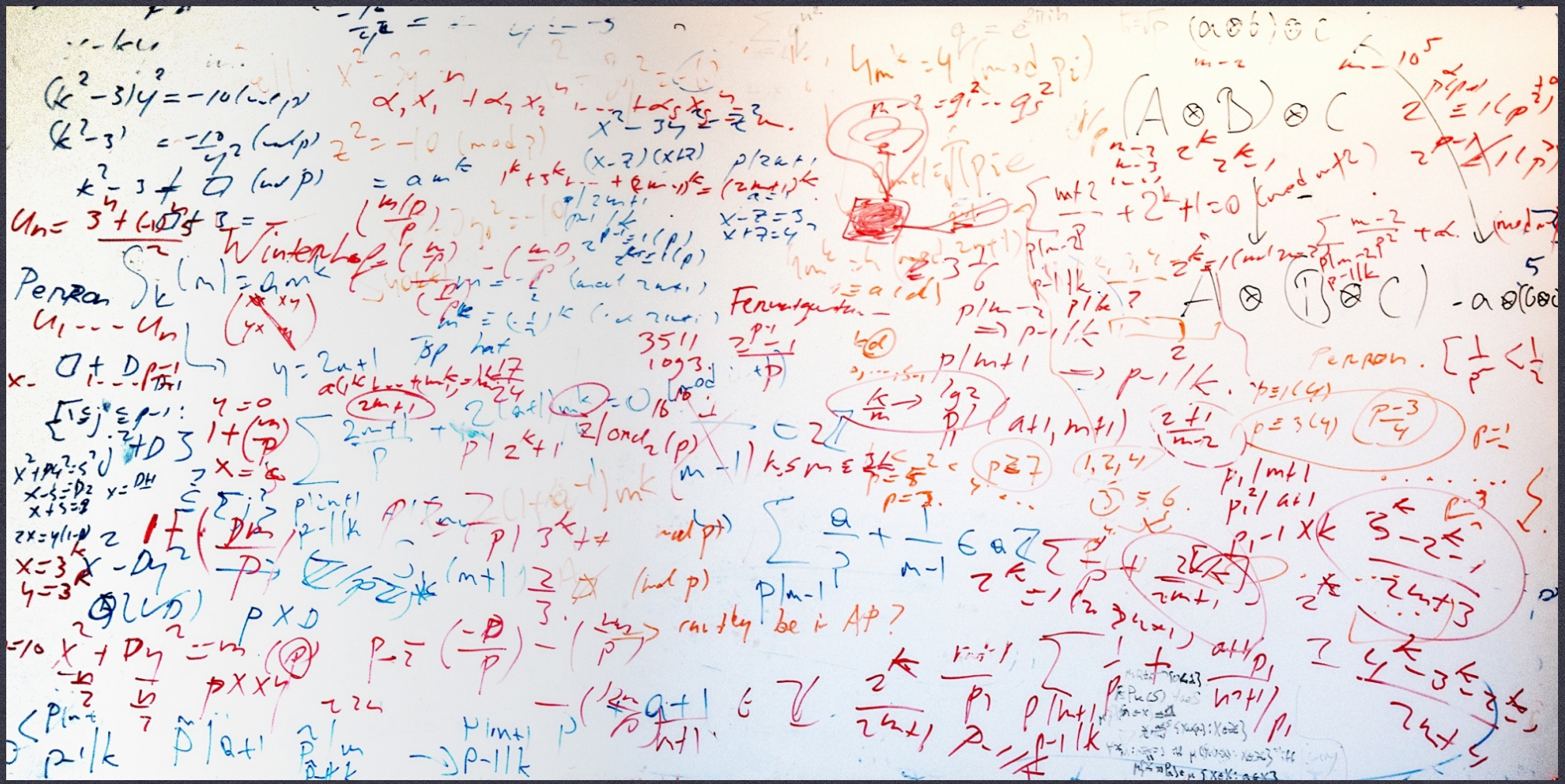
Time is of the essence

	N=50	N=100	N=1000	$N = 10^6$	$N = 10^9$
N	~0	~0	~0	~0	0.001 sec
N^2	~0	~0	~0	~0	11 days
2^N	18 minutes	2.8 U	$>10^{280}$ U	!	!
3^N	226 centuries	$> 10^{18}$ U	!	!	!
N!	$> 10^{43}$ U	$> 10^{137}$ U	!	!	!

computer speed improves one thousand times
U is the Age of the Universe

Moral of the story

- No technological improvement will ever make an exponential-time algorithm practical



BACK TO THE BOARD