Supervised Learning and Clustering

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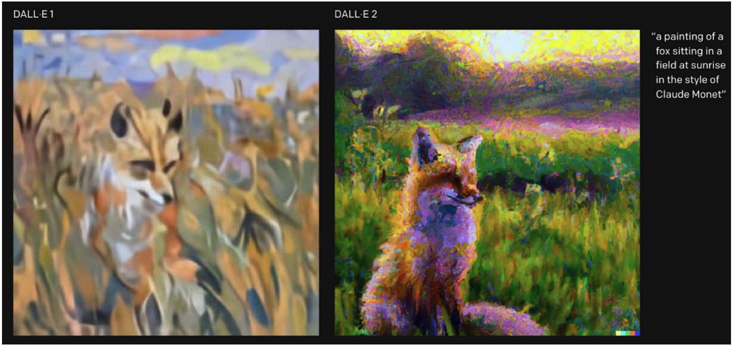
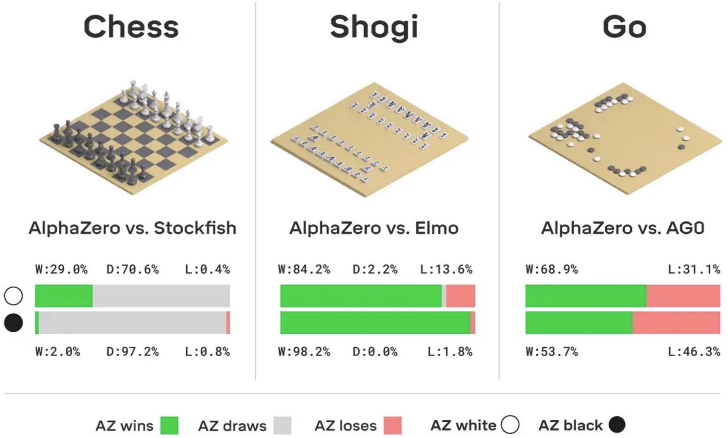
Section 1: What is machine learning?

A computer program is said to learn
from experience **E**
with respect to a task **T**
and performance measure **P**,
if its performance at task **T**, as measured in **P**, improves with
experience **E**.

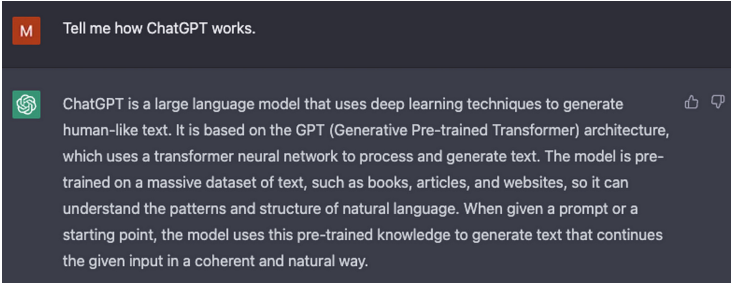
What can machine learning do?



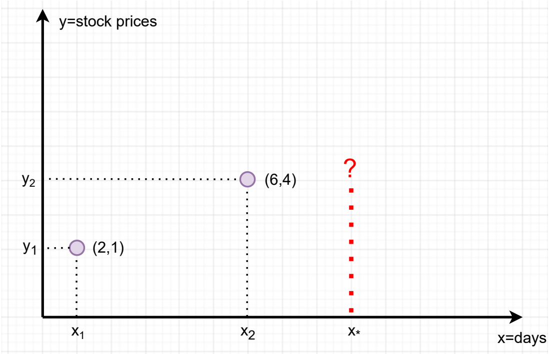
What can machine learning do?



What can machine learning do?



Stock price prediction

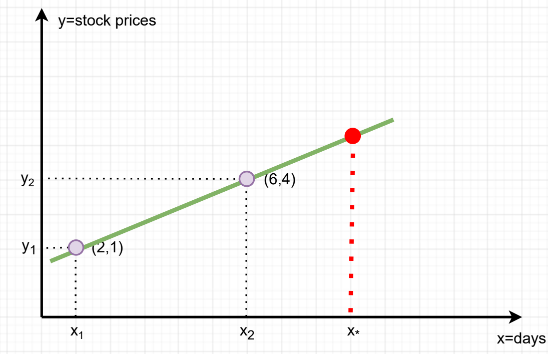


We are given the following two observations:

- The stock price at day number 2 is 1 DKK.
- The stock price at day number 6 is 4 DKK.

How can we predict the price at an arbitrary day x_* in the future?

How far do we get with high school math?

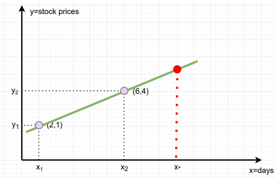


- Find the equation of the line passing through the two points

$$y - y_1 = \frac{y_2 - y_1}{x_2 - x_1}(x - x_1) \rightarrow y - 1 = \frac{4-1}{6-2}(x - 2) \rightarrow y = 0.75x - 0.5$$

- Treat the line as a predictor function: $f(x) = 0.75x - 0.5$

Which recipe did we follow?



- Collect a **data set**, i.e. a set of observations

$$S = \{(2,1), (6,4)\}$$

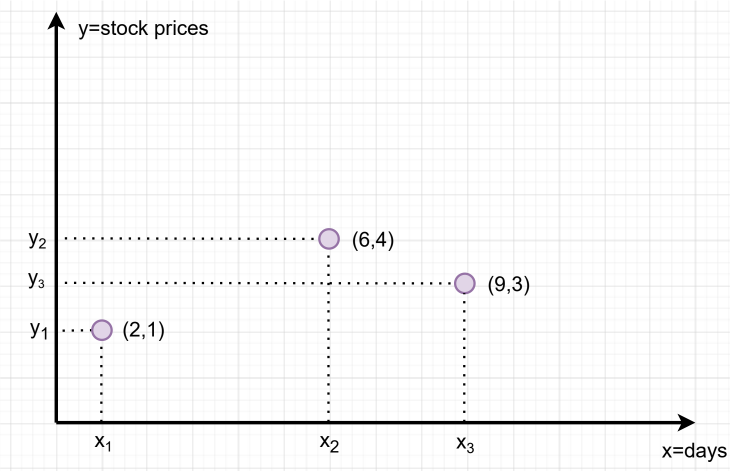
- Assume a **model** about how the system works: **a line**
- **Fit** the model to data, i.e. **learn**: Find the equation of the line passing through the two points

$$y - y_1 = \frac{y_2 - y_1}{x_2 - x_1}(x - x_1) \rightarrow y - 1 = \frac{4-1}{6-2}(x-2)$$
$$\rightarrow y = 0.75x - 0.5$$

- Use $f(x) = 0.75x - 0.5$ to make new predictions, i.e. **generalize**.

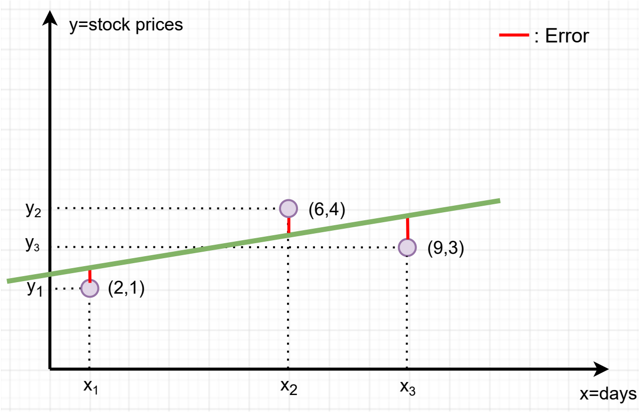
What if we have a third observation?

Now machine learning starts.



There is no line that can go through all the three data points!

How about finding the **best** line $y = ax + b$?



- For each choice of a, b, we will have a different line. Which one is the best? Best in terms of what?
- **Hint:** Whichever line we choose, the model will make an **error**. Quantify the error first, minimize the error next.

Error

Since it does not matter if our prediction y_* was above or below the target value y, it is reasonable to define the error as:

$$e(y, y_*) = (\underbrace{y_*}_{\text{predicted}} - \underbrace{y}_{\text{observed}})^2$$

What is the geometric shape of the function that has y_* on the x-axis and $e(y, y_*)$ on the y-axis?

Loss

Each time our model makes a prediction, it will incur some error. The sum of these errors gives us the **loss** of our model (a line defined by a slope a and an intercept b) on the data set S[1]:

$$
\begin{aligned}
L(a,b,S) &= \frac{1}{3}\sum_{i=1}^{3} e(f(x_i,a,b)-y_i) \\
&= \frac{1}{3}\sum_{i=1}^{3} (f(x_i,a,b)-y_i)^2 \\
&= \frac{1}{3}(2a+b-1)+\frac{1}{3}(6a+b-4)+\frac{1}{3}(9a+b-3) \\
&= \sum_{i=1}^{3} \frac{1}{3}(ax_i+b-y_i)^2
\end{aligned}
$$

[1] Remember: $S=\{(x_1,y_1)=(2,1),(x_2,y_2)=(6,4),(x_3,y_3)=(9,3)\}$

Learning: Choosing the best of three lines

Let

$$\mathcal{H} := \{(a_1, b_1), (a_2, b_2), (a_3, b_3)\}$$

be all the options we have. How would you choose the best one?

Learning: Choosing the best of three lines

Evaluate the loss with each option

$$L(a_1, b_1, S) := \frac{1}{3}(2a_1 + b_1 - 1) + \frac{1}{3}(6a_1 + b_1 - 4) + \frac{1}{3}(9a_1 + b_1 - 3)$$
$$L(a_2, b_2, S) := \frac{1}{3}(2a_2 + b_2 - 1) + \frac{1}{3}(6a_2 + b_2 - 4) + \frac{1}{3}(9a_3 + b_3 - 3)$$
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and choose the line that gives the smallest loss. In formal terms, choose a_{best}, b_{best} that satisfies

$$L(a_{best}, b_{best}, S) = \min\{L(a_1, b_1, S), L(a_2, b_2, S), L(a_3, b_3, S)\}.$$

Choosing the **arg**ument that **min**imizes a function can be expressed shortly via the $\arg\min$ operation:

$$a_{best}, b_{best} = \arg \min_{(a,b)\in\mathcal{H}} L(a, b, S)$$

Learning: Choosing the best of infinitely many lines

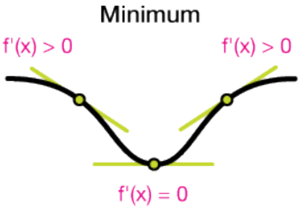
- In fact a, b can be any real number. So we have infinite number of options. How shall we find out the best one?
- Best: a, b that minimizes the loss:

$$a_{best}, b_{best} = \arg\min_{a,b \in \mathbb{R}} L(a, b, S)$$

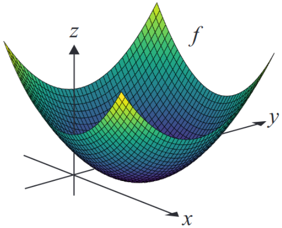
- What is special with the point $L(a_{best}, b_{best}, S)$? **Hint:** How does the loss function **change** in the neighborhood of this point?
  - If there is upward slope, turn back and go down.
  - If there is downward slope, go further ahead.
  - If there is no slope, here it is!

  How can we express the change of a function value with respect to a change in its input values in mathematical terms?

The derivative!



(a) Minima and slopes



(b) 2-dimensional loss

We are looking for values a_{best}, b_{best} that satisfy:

$$L'_a(a = a_{best}, b = b_{best}, S) = 0,$$
$$L'_b(a = a_{best}, b = b_{best}, S) = 0.$$

Recipe for finding a_{best} and b_{best}

1. Set $L'_b(a, b, S) = 0$ and solve for b, which will be an expression of b_{best} in terms of a.
2. Set $L'_a(a, b = b_{best}, S) = 0$ and solve for a, which will be a function of b_{best}. Replace wherever you see b_{best} by the expression found in Step (1).
3. Replace the solution in Step (2) into the expression found in Step (1) to find b_{best}.

Step 1: Find b_{best} in terms of a

$$
\begin{aligned}
0 &= \frac{1}{3}\sum_{i=1}^{3}\left((ax_i + b - y_i)^2\right)'_b && \text{as } (f(x)+g(x))' = f'(x)+g'(x) \\
&= \sum_{i=1}^{3}(ax_i + b - y_i) && \text{as } f(g(x))' = f'(g(x))g'(x) \\
&= 3b - \sum_{i=1}^{3}(y_i - ax_i) && \text{Rearrange terms}
\end{aligned}
$$

Then leaving b alone on one side, we get

$$
b_{best} = \underbrace{\frac{1}{3}\sum_{i=1}^{3} y_i}_{\bar{y}} - a\underbrace{\left(\frac{1}{3}\sum_{i=1}^{3} x_i\right)}_{\bar{x}} = \bar{y} - a\bar{x}
$$

where $\bar{x}$ and $\bar{y}$ are the *center of mass* of the data.

Step 2: Solve for a_{best}

$$
\begin{aligned}
0 &= \frac{1}{3}\sum_{i=1}^{3}\left((ax_i + b_{best} - y_i)^2\right)'_a \\
&= \frac{1}{3}\sum_{i=1}^{3}\left((ax_i + (\bar{y} - a\bar{x}) - y_i)^2\right)'_a \\
&= \sum_{i=1}^{3}(a(x_i - \bar{x}) - (y_i - \bar{y}))(x_i - \bar{x})
\end{aligned}
$$

Leaving a alone on one side, we get

$$
a_{best} = \frac{\sum_{i=1}^{3}(y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{3}(x_i - \bar{x})^2}
$$

Step 3: Evaluate b_{best}

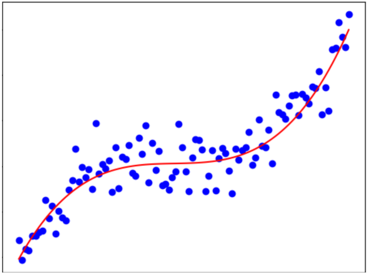
$$
\begin{aligned}
b_{best} &= \bar{y} - a_{best}\bar{x} \\
&= \bar{y} - \left(\frac{\sum_{i=1}^{3} (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{3} (x_i - \bar{x})^2} \right) \bar{x}
\end{aligned}
$$

The best fitting line to data set S is then

$$f(x) = \frac{\sum_{i=1}^{3}(y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{3}(x_i - \bar{x})^2} x + \bar{y} - \left(\frac{\sum_{i=1}^{3}(y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{3}(x_i - \bar{x})^2} \right) \bar{x}$$

We can use this function to predict the output of any x we want.

What if?



- The input-output relationship is nonlinear, i.e. no line-shaped predictor evaluated on the input can even approximate the output.
- We can evaluate the derivatives for arbitrary a, b, but, cannot find a, b values that make the derivatives zero?

Re-express the derivative in a more generic way

$$L'_a(a,b,S) = \frac{2}{3}\sum_{i=1}^{3}\underbrace{(ax_i + b - y_i)}_{f(x_i;a,b)-y_i}\underbrace{x_i}_{(ax_i)'_a}$$

The solution template would be the same if:

- we had not 3 but m data points, i.e. $S = (x_1, y_1), \ldots, (x_m, y_m)$
- our model were not a line but an arbitrary function $f(x;\theta)$
- we computed the derivative of an arbitrary parameter θ of this function

$$L'_\theta(\theta, S) = \frac{2}{m}\sum_{i=1}^{m}(f(x_i;\theta) - y_i)f'_\theta(x_i;\theta)$$

The Gradient Descent Algorithm

- Choose a **learning rate** $\alpha > 0$.
- Initialize θ to an arbitrary value
- **repeat**
  - $\theta \leftarrow \theta - \alpha L'_\theta(\theta, S)$
- **until** θ no longer changes

Making sense of gradient descent

Placing the generic loss derivative calculated in the previous slide into the update rule:

$$\theta \leftarrow \theta - \frac{2\alpha}{m} \sum_{i=1}^{m} (f(x_i; \theta) - y_i) f'_\theta(x_i)$$

In natural language, change parameter θ proportionally to

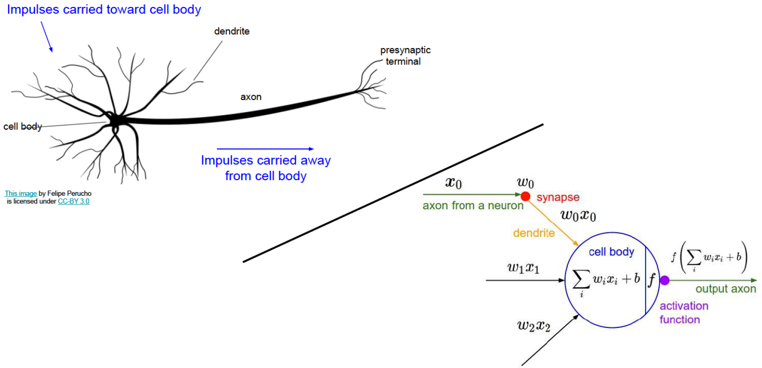
- The signed prediction error of the current model $f(x_i; \theta) - y_i$
- The rate the predictions of the model changes $f'_\theta(x_i)$

This means,

- Make big changes when predictions are bad
- Stop changing when predictions are good

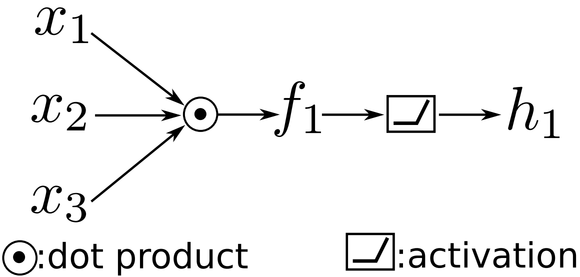
Perceptron: The atom of intelligence

North-West: Biological neuron
South-East: Artificial neuron (perceptron)



The computational graph of a perceptron

Computational graph: block diagram of mathematical operations.



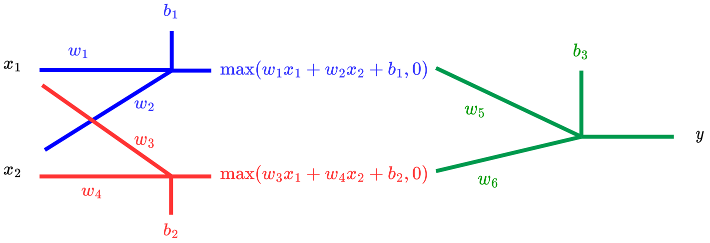
The neuron has weights assigned to each input channel:

- w_1 for x_1, w_2 for x_2, w_3 for x_3, and a bias term b to model the intercept just as in the line fitting example above.

It processes the given input in two steps:

- Linear mapping: $f = \sum_{i_1}^{3} w_i x_i + b$
- Nonlinear activation, for example: $h = \max(0, f)$

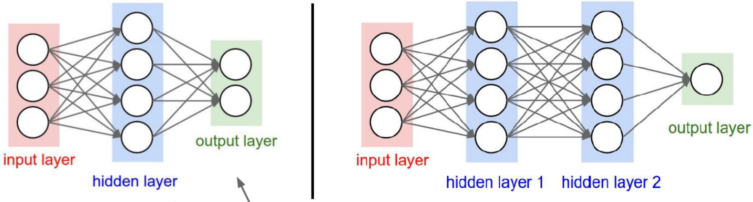
Neural net: A group of connected perceptrons



This neural net will make the following prediction for the input observations (x_1, x_2):

$$f(x_1, x_2) = w_5\Big(\max(w_1x_1 + w_2x_2 + b_1, 0)\Big) + w_6\Big(\max(w_3x_1 + w_4x_2 + b_2, 0)\Big) + b_3$$

The Multi-Layer Perceptron (MLP)



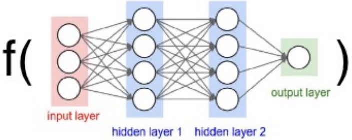
"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"Fully-connected" layers

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

Large Language Models

- The predictor is not a line but a neural network



- The input is not a single value but a long sequence of words:

$$f(\text{her mother would like}) = \text{to}$$

Large Language Models

- The neural net learns to pay more attention to important information in the input sequence:

$$f(\underbrace{\text{her mother}}_{ignore}\ \underbrace{\text{would like}}_{attend}) = \text{to}$$

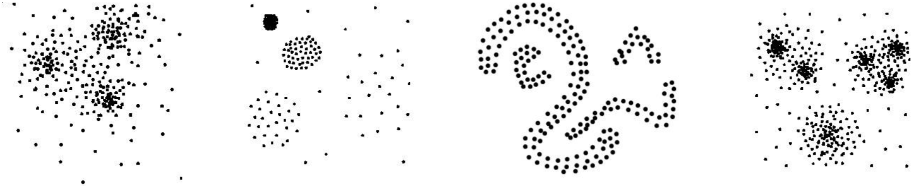
  Attended words influence the output, unattended words are ignored.

- The model generates text progressively by taking its own predictions as input, i.e. **autoregression**:

$$f(\text{her mother would like}) = \text{to}$$
$$f(\text{her mother would like to}) = \text{buy}$$
$$f(\text{her mother would like to buy}) = \text{an}$$
$$f(\text{her mother would like to buy an}) = \text{icecream}$$

Section 2: Purpose of Clustering

- identify a finite number of categories (classes, groups: clusters) in a given dataset
- **similar** objects shall be grouped in the same cluster, **dissimilar** objects in different clusters
- similarity is highly subjective, depending on the application scenario



A Dataset can be Clustered in Different Meaningful Ways

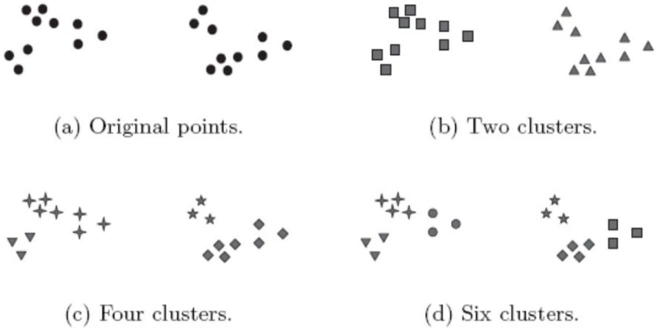
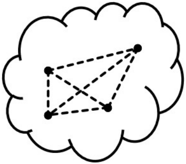


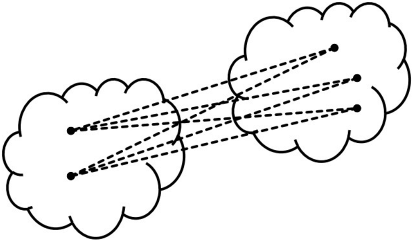
Figure 8.1. Different ways of clustering the same set of points.

Criteria of Quality: Cohesion and Separation

- **cohesion:** how strong are the cluster objects connected (how similar, pairwise, to each other)?
- **separation:** how well is a cluster separated from other clusters?



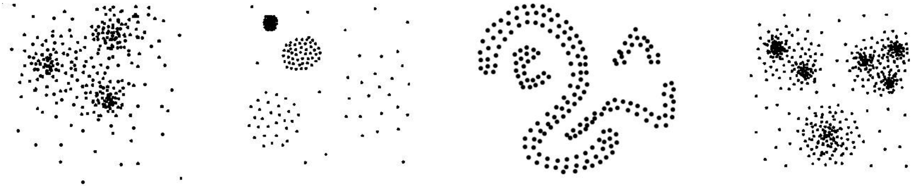
small within cluster distances



large between cluster distances

Optimization of Cohesion

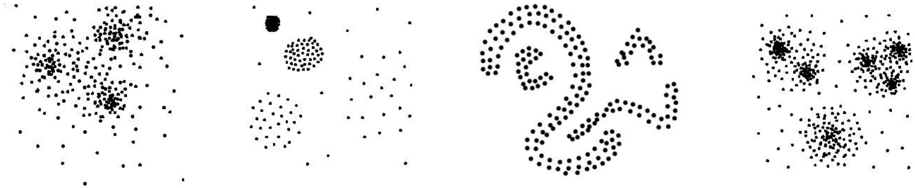
Partitional clustering algorithms partition a dataset into k clusters, typically minimizing some cost function (compactness criterion), i.e., optimizing cohesion.



Assumptions for Partitioning Clustering

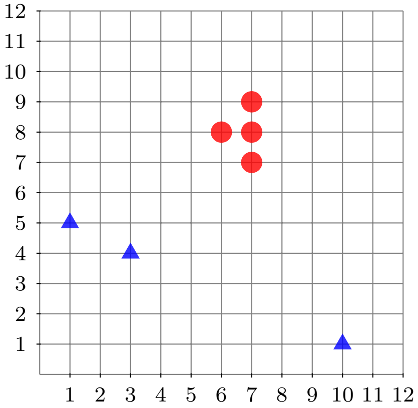
Central assumptions for approaches in this family are typically:

- number k of clusters known (i.e., given as input)
- clusters are characterized by their compactness
- compactness measured by some distance function (e.g., distance of all objects in a cluster from some cluster representative is minimal)
- criterion of compactness typically leads to convex or even spherically shaped clusters



Construction of Central Points: Basics

- data points (objects) are d-dimensional real-valued vectors $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$
- and we measure distances between data point pairs by $||x - y||_2 = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$
- **centroid** μ_C: mean vector of all points in cluster C



$$\mu_{C_i} = \frac{1}{|C_i|} \cdot \sum_{o \in C_i} o$$

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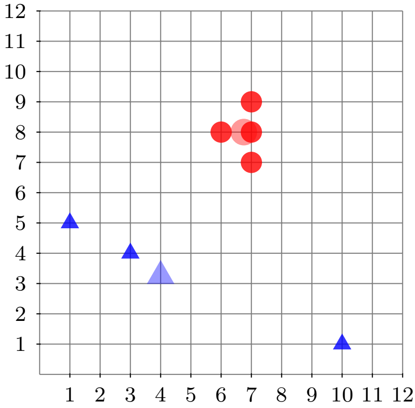


$$\mu_{C_i} = \frac{1}{|C_i|} \cdot \sum_{o \in C_i} o$$

Construction of Central Points: Basics

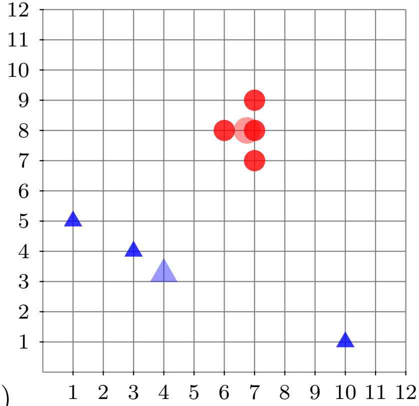
- measure of compactness for a cluster C:

$$TD^2(C) = \sum_{p \in C} ||p - \mu_C||_2^2$$

(a.k.a. SSQ: sum of squares)

- measure of compactness for a clustering

$$TD^2(C_1, C_2, \ldots, C_k) = \sum_{i=1}^{k} TD^2(C_i)$$



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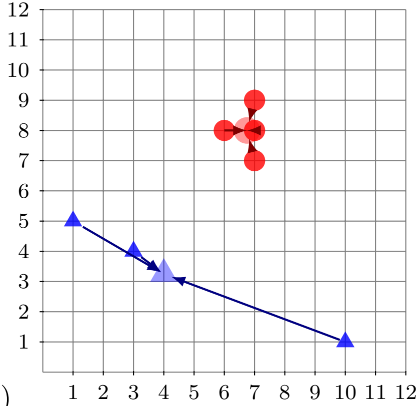
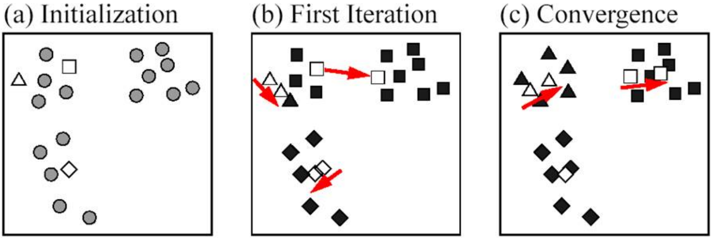


Basic Algorithm

Clustering by Minimization of Variance

- start with k (e.g., randomly selected) points as cluster representatives (or with a random partition into k "clusters")
- repeat:
  - assign each point to the closest representative
  - compute new representatives based on the given partitions (centroid of the assigned points)
- until there is no change in assignment



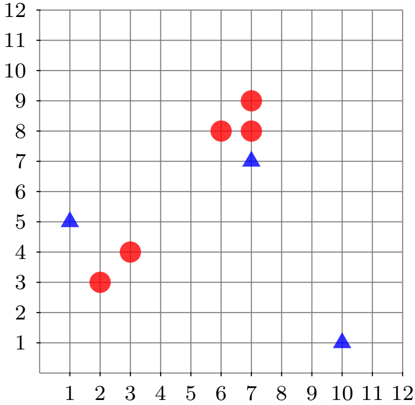
k-means

k-means is a variant of the basic algorithm:

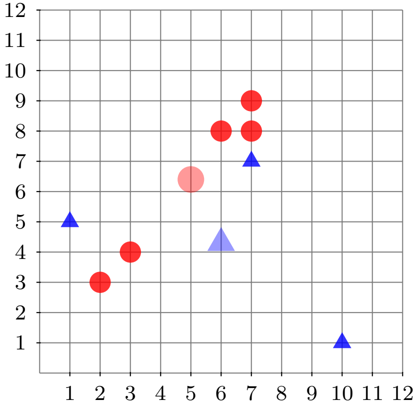
- a centroid is immediately updated when some point changes its assignment
- k-means has very similar properties, but the result now depends on the order of data points in the input file

The name "k-means" is often used indifferently for any variant of the basic algorithm.

k-means Clustering – Lloyd/Forgy Algorithm



k-means Clustering – Lloyd/Forgy Algorithm

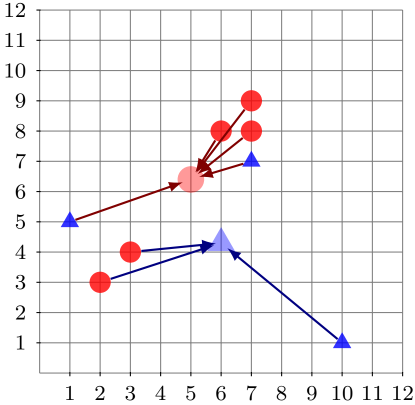


recompute centroids:

$\mu \approx (6.0, 4.3)$

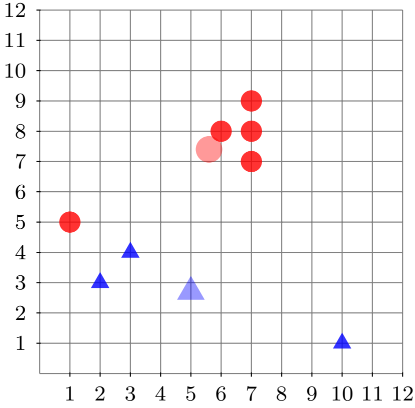
$\mu \approx (5.0, 6.4)$

k-means Clustering – Lloyd/Forgy Algorithm



reassign points

k-means Clustering – Lloyd/Forgy Algorithm

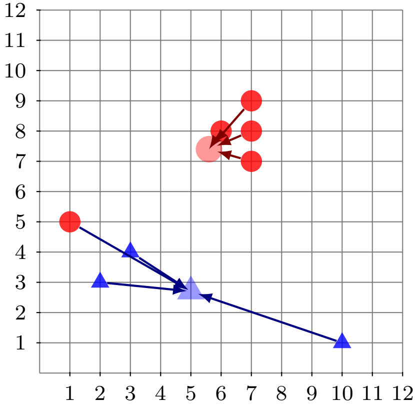


recompute centroids:

$\mu \approx (5.0, 2.7)$

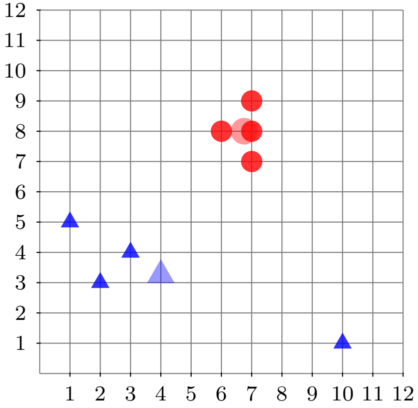
$\mu \approx (5.6, 7.4)$

k-means Clustering – Lloyd/Forgy Algorithm



reassign points

k-means Clustering – Lloyd/Forgy Algorithm

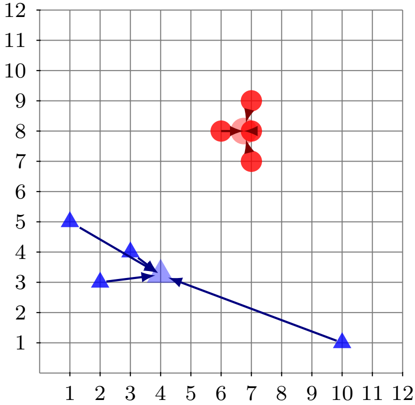


recompute centroids:

$$\mu \approx (4.0, 3.25)$$

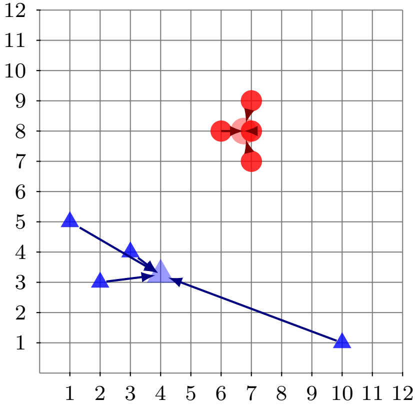
$$\mu \approx (6.75, 8.0)$$

k-means Clustering – Lloyd/Forgy Algorithm



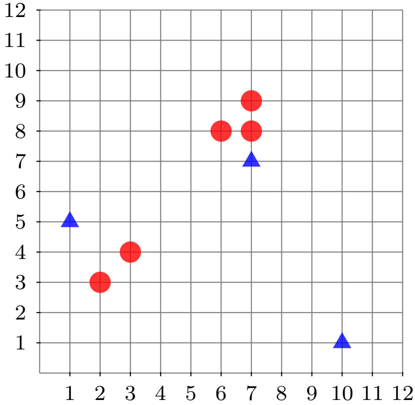
reassign points

k-means Clustering – Lloyd/Forgy Algorithm

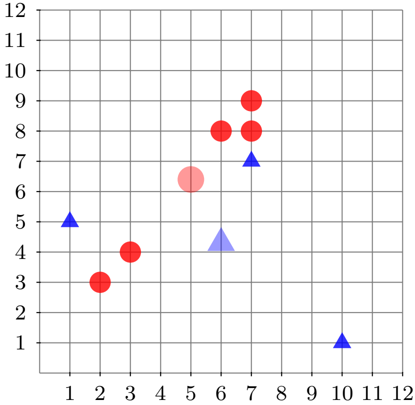


reassign points
no change
convergence!

k-means Clustering – MacQueen Algorithm



k-means Clustering – MacQueen Algorithm

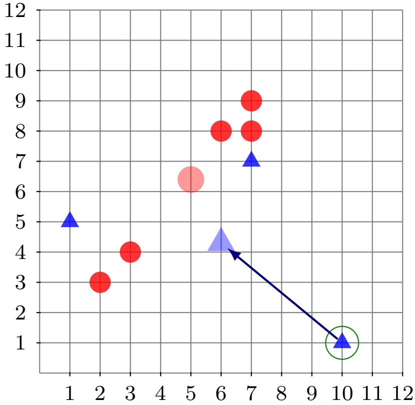


Centroids
(e.g.: from
previous iteration):

$\mu \approx (6.0, 4.3)$

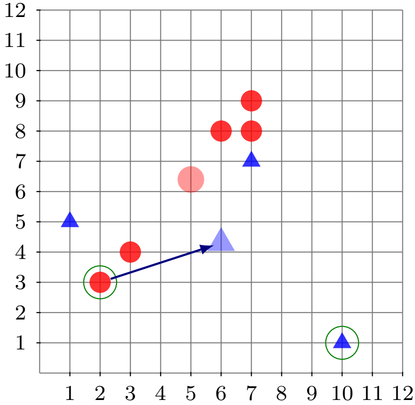
$\mu \approx (5.0, 6.4)$

k-means Clustering – MacQueen Algorithm



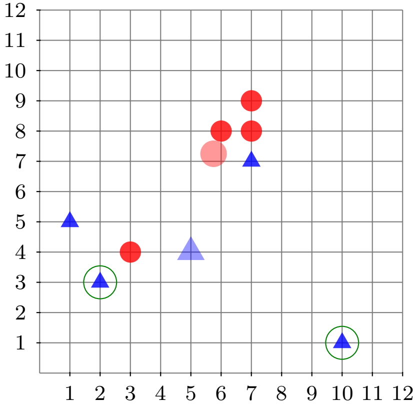
assign first point

k-means Clustering – MacQueen Algorithm



assign second point

k-means Clustering – MacQueen Algorithm

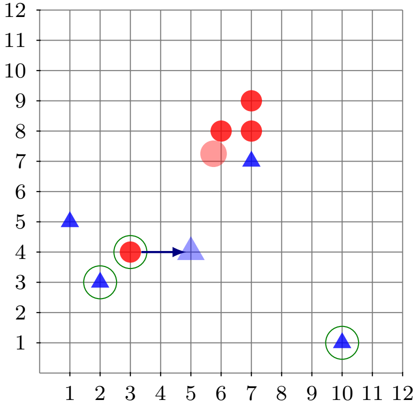


recompute centroids:

$$\mu \approx (5.0, 4.0)$$

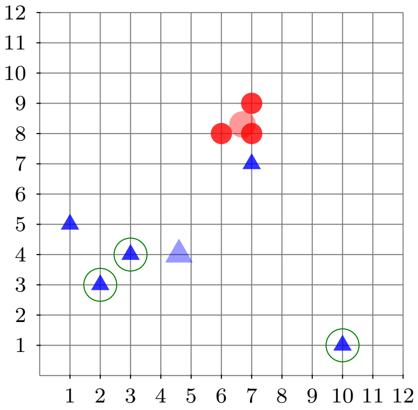
$$\mu \approx (5.75, 7.25)$$

k-means Clustering – MacQueen Algorithm



assign third point

k-means Clustering – MacQueen Algorithm

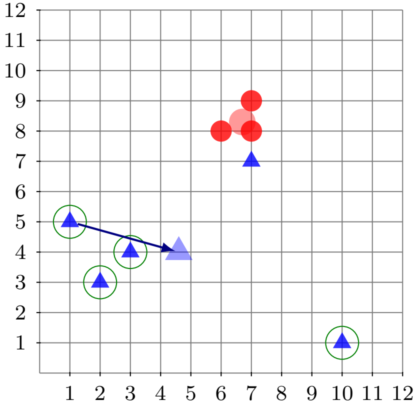


recompute centroids:

$\mu \approx (4.6, 4.0)$

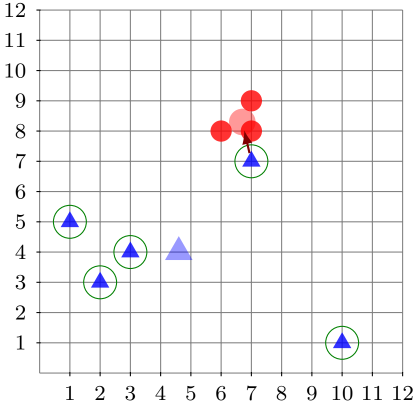
$\mu \approx (6.7, 8.3)$

k-means Clustering – MacQueen Algorithm



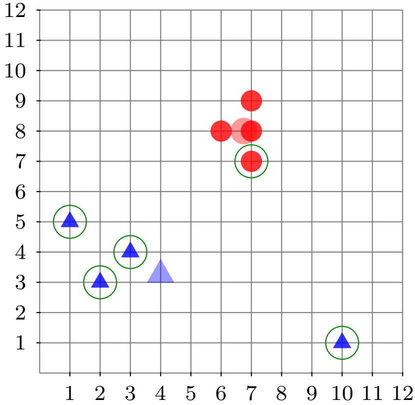
assign fourth point

k-means Clustering – MacQueen Algorithm



assing fifth point

k-means Clustering – MacQueen Algorithm

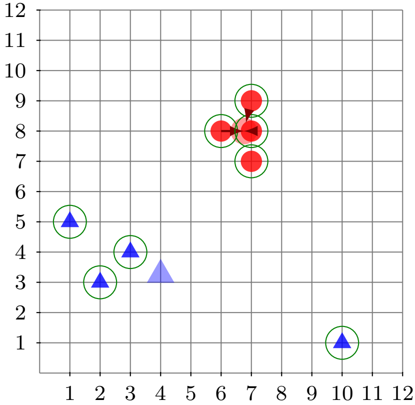


recompute centroids:

$\mu \approx (4.0, 3.25)$

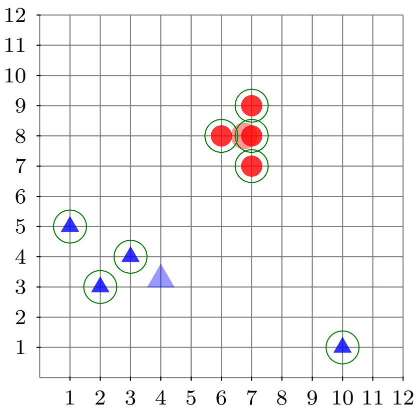
$\mu \approx (6.75, 8.0)$

k-means Clustering – MacQueen Algorithm



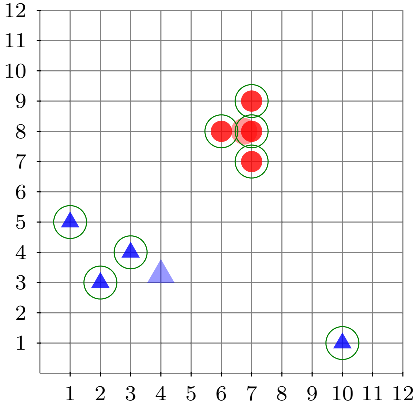
reassign more points

k-means Clustering – MacQueen Algorithm



reassign more points
possibly more iterations

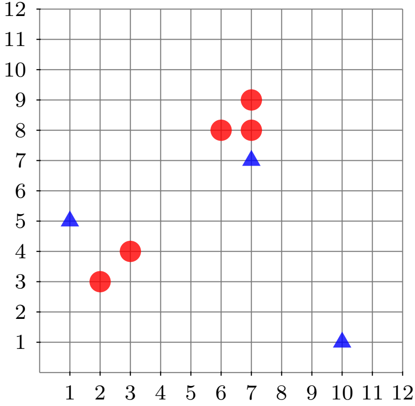
k-means Clustering – MacQueen Algorithm



reassign more points
possibly more iterations
convergence

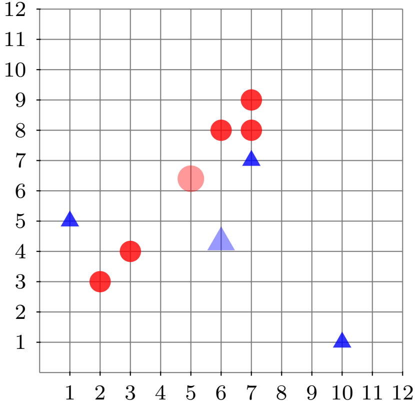
k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



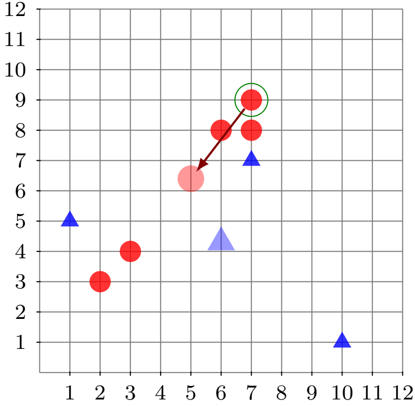
Centroids
(e.g.: from
previous iteration):

$\mu \approx (6.0, 4.3)$

$\mu \approx (5.0, 6.4)$

k-means Clustering – MacQueen Algorithm

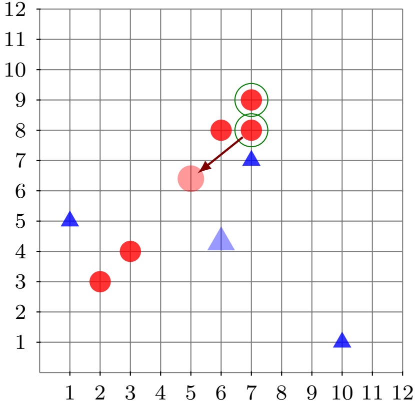
Alternative Run – Different Order



assign first point

k-means Clustering – MacQueen Algorithm

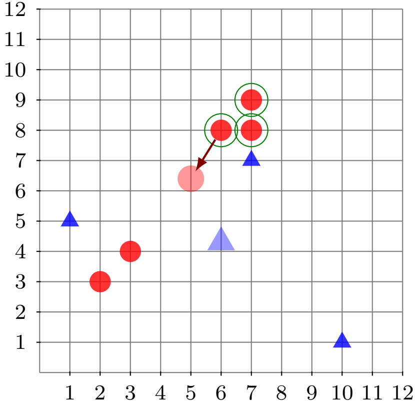
Alternative Run – Different Order



assign second point

k-means Clustering – MacQueen Algorithm

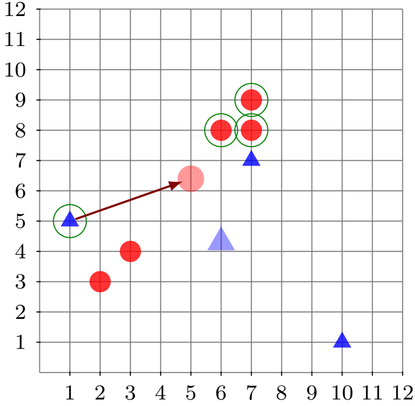
Alternative Run – Different Order



assign third point

k-means Clustering – MacQueen Algorithm

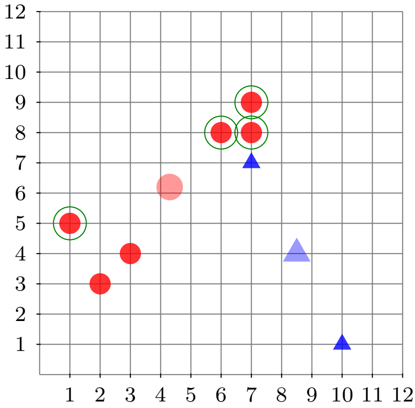
Alternative Run – Different Order



assign fourth point

k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



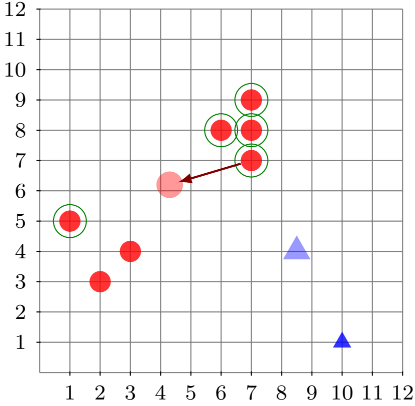
recompute centroids:

$\mu \approx (4.0, 8.5)$

$\mu \approx (4.3, 6.2)$

k-means Clustering – MacQueen Algorithm

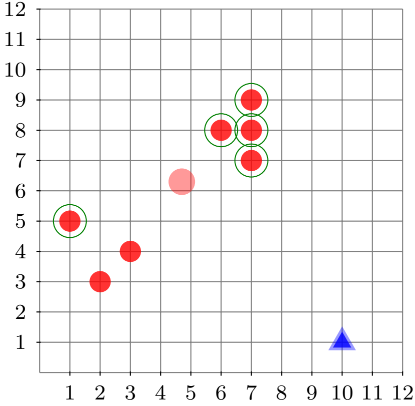
Alternative Run – Different Order



assign fifth point

k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



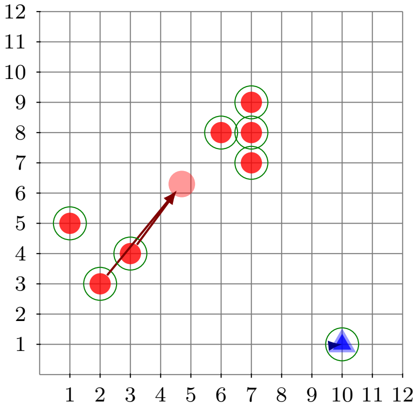
recompute centroids:

$\mu \approx (10.0, 1.0)$

$\mu \approx (4.7, 6.3)$

k-means Clustering – MacQueen Algorithm

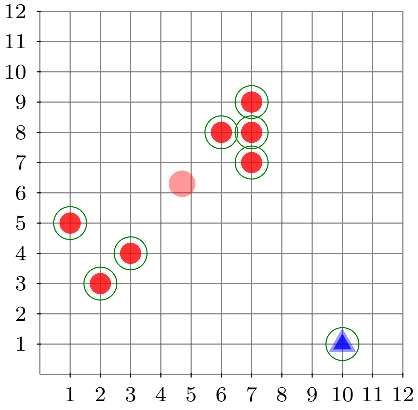
Alternative Run – Different Order



reasign more points

k-means Clustering – MacQueen Algorithm

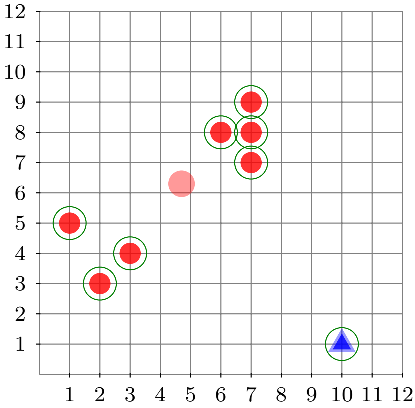
Alternative Run – Different Order



reasign more points
possibly more iterations

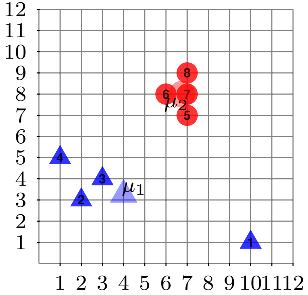
k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



reasign more points
possibly more iterations
convergence

k-means Clustering – Quality



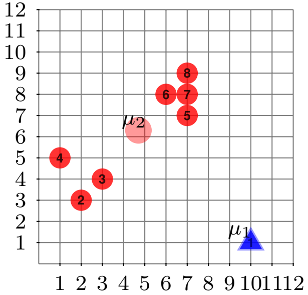
First solution: $TD^2 = 61\frac{1}{2}$

$SSQ(\mu_1, p_1) = |4 - 10|^2 + |3.25 - 1|^2 = 36 + 5\frac{1}{16} = 41\frac{1}{16}$
$SSQ(\mu_1, p_2) = |4 - 2|^2 + |3.25 - 3|^2 = 4 + \frac{1}{16} = 4\frac{1}{16}$
$SSQ(\mu_1, p_3) = |4 - 3|^2 + |3.25 - 4|^2 = 1 + \frac{9}{16} = 1\frac{9}{16}$
$SSQ(\mu_1, p_4) = |4 - 1|^2 + |3.25 - 5|^2 = 9 + 3\frac{1}{16} = 12\frac{1}{16}$
$TD^2(C_1) = 58\frac{3}{4}$

$SSQ(\mu_2, p_5) = |6.75 - 7|^2 + |8 - 7|^2 = \frac{1}{16} + 1 = 1\frac{1}{16}$
$SSQ(\mu_2, p_6) = |6.75 - 6|^2 + |8 - 8|^2 = \frac{9}{16} + 0 = \frac{9}{16}$
$SSQ(\mu_2, p_7) = |6.75 - 7|^2 + |8 - 8|^2 = \frac{1}{16} + 0 = \frac{1}{16}$
$SSQ(\mu_2, p_8) = |6.75 - 7|^2 + |8 - 9|^2 = \frac{1}{16} + 1 = 1\frac{1}{16}$
$TD^2(C_2) = 2\frac{3}{4}$

Note: $SSQ(\mu, p) = ||\mu - p||_2^2$.

k-means Clustering – Quality



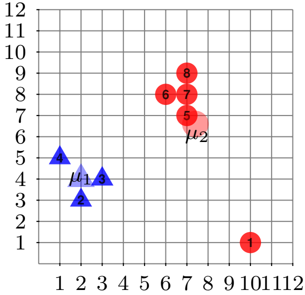
$SSQ(\mu_1, p_1) = |10 - 10|^2 + |1 - 1|^2 = 0$
$TD^2(C_1) = 0$

$SSQ(\mu_2, p_2) \approx |4.7 - 2|^2 + |6.3 - 3|^2 \approx 18.2$
$SSQ(\mu_2, p_3) \approx |4.7 - 3|^2 + |6.3 - 4|^2 \approx 8.2$
$SSQ(\mu_2, p_4) \approx |4.7 - 1|^2 + |6.3 - 5|^2 \approx 15.4$
$SSQ(\mu_2, p_5) \approx |4.7 - 7|^2 + |6.3 - 7|^2 \approx 5.7$
$SSQ(\mu_2, p_6) \approx |4.7 - 6|^2 + |6.3 - 8|^2 \approx 4.6$
$SSQ(\mu_2, p_7) \approx |4.7 - 7|^2 + |6.3 - 8|^2 \approx 8.2$
$SSQ(\mu_2, p_7) \approx |4.7 - 7|^2 + |6.3 - 9|^2 \approx 12.6$
$TD^2(C_2) \approx 72.86$

First solution: $TD^2 = 61\frac{1}{2}$
Second solution: $TD^2 \approx 72.68$

Note: $SSQ(\mu, p) = ||\mu - p||_2^2$.

k-means Clustering – Quality



$SSQ(\mu_1, p_2) = |2-2|^2 + |4-3|^2 = 0 + 1 = 1$
$SSQ(\mu_1, p_3) = |2-3|^2 + |4-4|^2 = 1 + 0 = 1$
$SSQ(\mu_1, p_4) = |2-1|^2 + |4-5|^2 = 1 + 1 = 2$
$TD^2(C_1) = 4$

$SSQ(\mu_2, p_1) = |7.4-10|^2 + |6.6-1|^2 = 6\frac{19}{25} + 31\frac{9}{25} = 38\frac{3}{25}$
$SSQ(\mu_2, p_5) = |7.4-7|^2 + |6.6-7|^2 = \frac{4}{25} + \frac{4}{25} = \frac{8}{25}$
$SSQ(\mu_2, p_6) = |7.4-6|^2 + |6.6-8|^2 = 1\frac{24}{25} + 1\frac{24}{25} = 3\frac{23}{25}$
$SSQ(\mu_2, p_7) = |7.4-7|^2 + |6.6-8|^2 = \frac{4}{25} + 1\frac{24}{25} = 2\frac{3}{25}$
$SSQ(\mu_2, p_8) = |7.4-7|^2 + |6.6-9|^2 = \frac{4}{25} + 5\frac{19}{25} = 5\frac{23}{25}$
$TD^2(C_2) = 50\frac{2}{5}$

First solution: $TD^2 = 61\frac{1}{2}$
Second solution: $TD^2 \approx 72.68$
Optimal solution: $TD^2 = 54\frac{2}{5}$

Note: $SSQ(\mu, p) = ||\mu - p||_2^2$.

Discussion

pros

- efficient: $\mathcal{O}(k \cdot n)$ per iteration, number of iterations is usually in the order of 10.
- easy to implement, thus very popular

cons

- k-means converges towards a **local** minimum
- k-means (MacQueen-variant) is order-dependent
- deteriorates with noise and outliers (all points are used to compute centroids)
- clusters need to be convex and of (more or less) equal extension
- number k of clusters is hard to determine
- strong dependency on initial partition (in result quality as well as runtime)