Clustering / Unsupervised Learning

- The target features are not given in the training examples
- The aim is to construct a natural classification that can be used to predict features of the data.
- The examples are partitioned in into clusters or classes. Each class predicts feature values for the examples in the class.
  - In hard clustering each example is placed definitively in a class.
  - In soft clustering each example has a probability distribution over its class.
- Each clustering has a prediction error on the examples. The best clustering is the one that minimizes the error.

k-means algorithm

The k-means algorithm is used for hard clustering.
Inputs:

- training examples
- the number of classes, k

Outputs:

- a prediction of a value for each feature for each class
- an assignment of examples to classes

k-means algorithm formalized

- E is the set of all examples
- the input features are $X_1, \ldots, X_n$
  $X_j(e)$ is the value of feature X_j for example e.
- there is a class for each integer $i \in \{1, \ldots, k\}$.

The k-means algorithm outputs

- function $class : E \to \{1, \ldots, k\}$.
  $class(e) = i$ means e is in class i.
- prediction $\widehat{X}_j(i)$ for each feature X_j and class i.

The sum-of-squares error for $class$ and $\widehat{X}_j(i)$ is

$$\sum_{e \in E} \sum_{j=1}^{n} \left(\widehat{X}_j(class(e)) - X_j(e) \right)^2 .$$

Aim: find $class$ and prediction function that minimize sum-of-squares error.

Minimizing the error

The sum-of-squares error for *class* and $\widehat{X}_j(i)$ is

$$\sum_{e \in E} \sum_{j=1}^{n} \left(\widehat{X}_j(class(e)) - X_j(e) \right)^2 .$$

- Given *class*, the $\widehat{X}_j$ that minimizes the sum-of-squares error is the mean value of X_j for that class.
- Given $\widehat{X}_j$ for each j, each example can be assigned to the class that minimizes the error for that example.

k-means algorithm

Initially, randomly assign the examples to the classes.
Repeat the following two steps:

- For each class i and feature X_j, let

$$\widehat{X}_j(i) \leftarrow \frac{\sum_{e:class(e)=i} X_j(e)}{|\{e : class(e) = i\}|}$$

  (the prediction of class i on feature X_j)

- For each example e, assign e to the class i that minimizes

$$\sum_{j=1}^{n} \left(\widehat{X}_j(i) - X_j(e)\right)^2 .$$

until the second step does not change the assignment of any example.

k-means algorithm

Sufficient statistics:

- $cc[c]$ is the number of examples in class c,
- $fs[j, c]$ is the sum of the values for $X_j(e)$ for examples in class c.

then define $pn(j, c)$, current estimate of $\widehat{X}_j(c)$

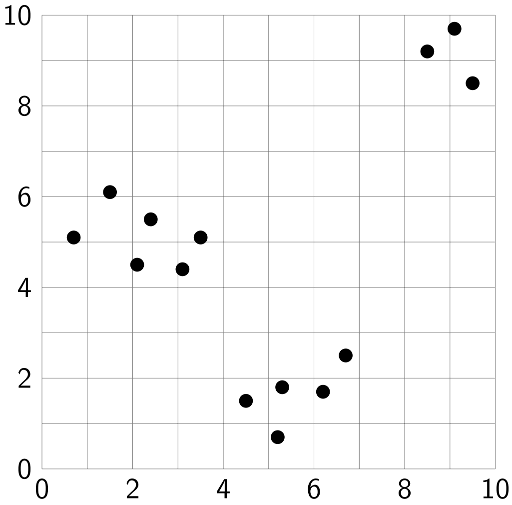
$$pn(j, c) = fs[j, c]/cc[c]$$

$$class(e) = \arg\min_c \sum_{j=1}^{n} (pn(j, c) - X_j(e))^2$$

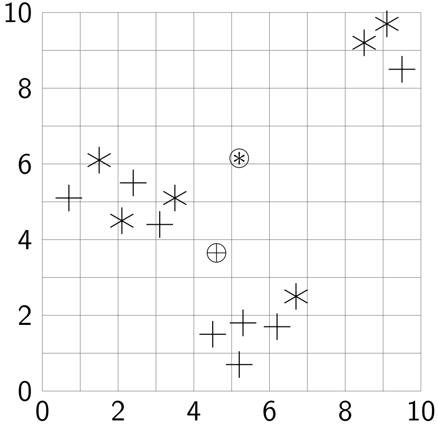
These can be updated in one pass through the training data.

procedure *k-means*(Xs, Es, k)
    Initialize *fs* and *cc* randomly (based on data)
    def $pn(j,c) = fs[j,c]/cc[c]$
    def $class(e) = \arg\min_c \sum_{j=1}^{n} \left(pn(j,c) - X_j(e)\right)^2$
    repeat
        fsn and *ccn* initialized to be all zero
        for each example $e \in Es$ **do**
            $c := class(e)$
            $ccn[c] += 1$
            for each feature $X_j \in Xs$ **do**
                $fsn[j,c] += X_j(e)$
        $stable := (fsn = fs)$ and $(ccn = cc)$
        $fs := fsn$
        $cc := ccn$
    until *stable*
    return *class*, *pn*

Example Data

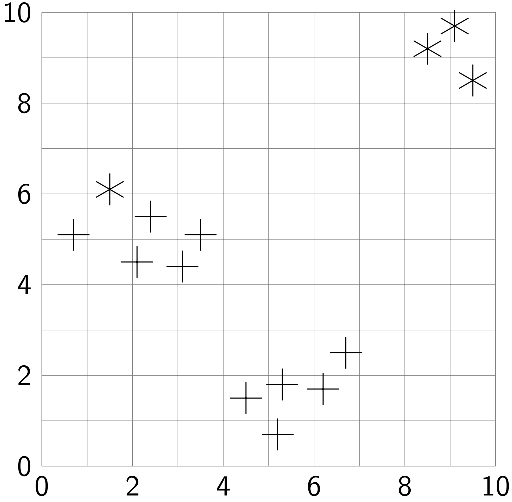


Random Assignment to Classes

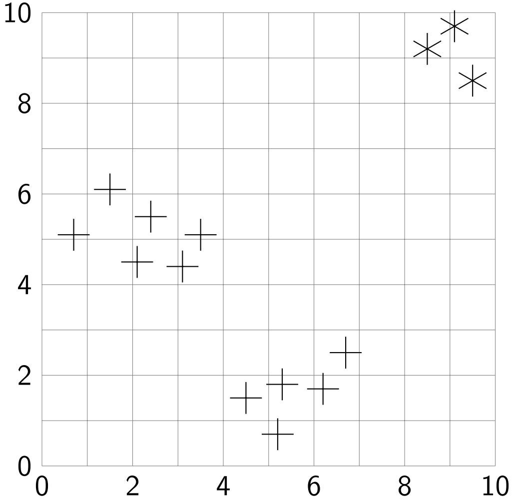


$\oplus$ is mean of $+$ and $\circledast$ is mean of $*$

Assign Each Example to Closest Mean



Ressign Each Example to Closest Mean



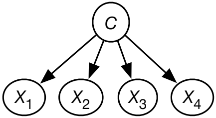
Properties of k-means

- An assignment of examples to classes is stable if running both the M step and the E step does not change the assignment.
- This algorithm will eventually converge to a stable local minimum.
- Any permutation of the labels of a stable assignment is also a stable assignment.
- It is not guaranteed to converge to a global minimum.
- It is sensitive to the relative scale of the dimensions.
- Increasing k *can* always decrease error (but does not always) until k is the number of different examples.
  How? Given an assignment with k classes, for $k+1$ classes start with the same assignment, but with the point most distant from its class center in its own new cluster.

EM Algorithm

- Used for soft clustering — examples are probabilistically in classes.
- k-valued random variable C

Model



Data

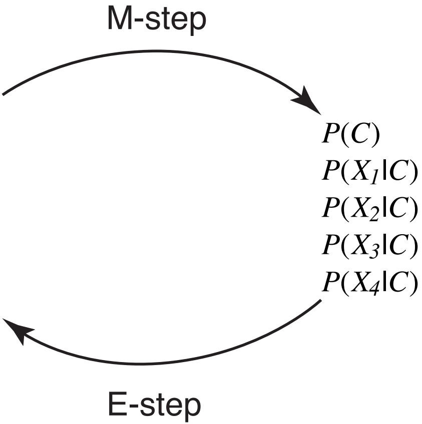
X_1	X_2	X_3	X_4
t	f	t	t
f	t	t	f
f	f	t	t
	$\cdots$		

➪ Probabilities

$P(C)$
$P(X_1|C)$
$P(X_2|C)$
$P(X_3|C)$
$P(X_4|C)$

EM Algorithm

X_1	X_2	X_3	X_4	C	*count*
⋮	⋮	⋮	⋮	⋮	⋮
t	*f*	*t*	*t*	*1*	*0.4*
t	*f*	*t*	*t*	*2*	*0.1*
t	*f*	*t*	*t*	*3*	*0.5*
⋮	⋮	⋮	⋮	⋮	⋮



EM Algorithm Overview

- Repeat the following two steps:
  - E-step give the expected number of data points for the unobserved variables based on the given probability distribution.
  - M-step infer the (maximum likelihood or maximum aposteriori probability) probabilities from the data.
- Start either with made-up data or made-up probabilities.
- EM will converge to a local maxima.

Augmented Data — E step

Suppose $k = 3$, and $dom(C) = \{1, 2, 3\}$.
$P(C = 1 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.407$
$P(C = 2 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.121$
$P(C = 3 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.472$:

X_1	X_2	X_3	X_4	$Count$
⋮	⋮	⋮	⋮	⋮
t	f	t	t	100
⋮	⋮	⋮	⋮	⋮

$\longrightarrow$

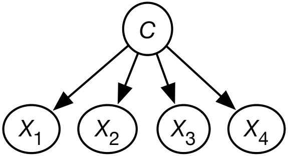
$A[X_1, \ldots, X_4, C]$

X_1	X_2	X_3	X_4	C	$Count$
⋮	⋮	⋮	⋮	⋮	⋮
t	f	t	t	1	40.7
t	f	t	t	2	12.1
t	f	t	t	3	47.2
⋮	⋮	⋮	⋮	⋮	⋮

M step

X_1	X_2	X_3	X_4	C	$Count$
⋮	⋮	⋮	⋮	⋮	⋮
t	f	t	t	1	40.7
t	f	t	t	2	12.1
t	f	t	t	3	47.2
⋮	⋮	⋮	⋮	⋮	⋮

$\longrightarrow$



$P(C{=}c)$

$P(X_i = v \mid C{=}c)$

EM sufficient statistics

- cc, a k-valued array, $cc[c]$ is the sum of the counts for $class{=}c$.
- fc, a 3-dimensional array such that $fc[i, v, c]$, is the sum of the counts of the augmented examples t with $X_i(t) = val$ and $class(t) = c$.
- The probabilites can be computed by:

$$P(C{=}c) = \frac{cc[c]}{|Es|}$$

$$P(X_i = v | C{=}c) = \frac{fc[i, v, c]}{cc[c]}$$

procedure $EM(Xs, Es, k)$
  $cc[c] := 0;\ fc[i, v, c] := 0$
  repeat
    $cc\_new[c] := 0;\ fc\_new[i, v, c] := 0$
    for each example $\langle v_1, \ldots, v_n \rangle \in Es$ **do**
      for each $c \in [1, k]$ **do**
        $dc := P(C = c \mid X_1 = v_1, \ldots, X_n = v_n)$
        $cc\_new[c] := cc\_new[c] + dc$
        for each $i \in [1, n]$ **do**
          $fc\_new[i, v_i, c] := fc\_new[i, v_i, c] + dc$
    $stable := (cc \approx cc\_new)$ and $(fc \approx fc\_new)$
    $cc := cc\_new$
    $fc := fc\_new$
  until $stable$
  return cc,fc