

# Clustering / Unsupervised Learning

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- The aim is to construct a natural classification that can be used to predict features of the data.
- The examples are partitioned 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  $X_1, \dots, X_n$   
 $X_j(e)$  is the value of feature  $X_j$  for example  $e$ .
- there is a class for each integer  $i \in \{1, \dots, k\}$ .

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The *k*-means algorithm outputs

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

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

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

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

# Minimizing the error

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

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

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- Given  $\hat{X}_j$  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  $X_j$ ,

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

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

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

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  $\hat{X}_j(c)$

$$pn(j, c) =$$

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

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

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

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

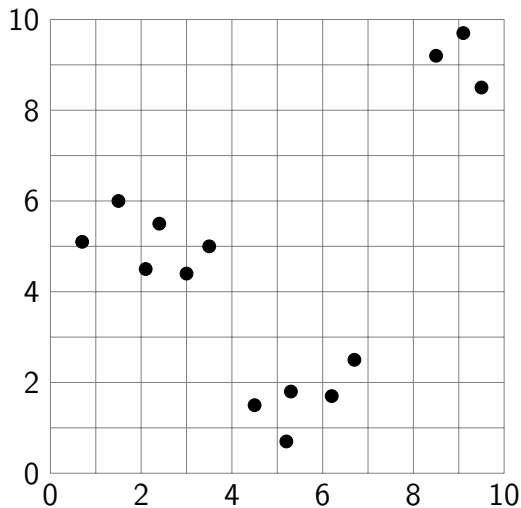


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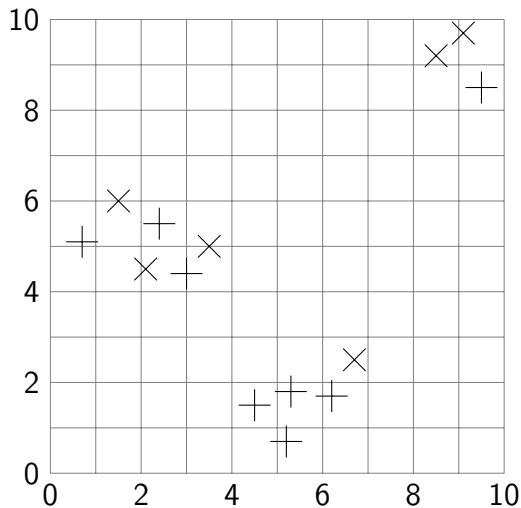
1: procedure k-means( $Xs, Es, k$ )
2:   Initialize  $fs$  and  $cc$  randomly (based on data)
3:   def  $pn(j, c) = fs[j, c]/cc[c]$ 
4:   def  $class(e) = \arg \min_c \sum_{j=1}^n (pn(j, c) - X_j(e))^2$ 
5:   repeat
6:      $fsn$  and  $ccn$  initialized to be all zero
7:     for each example  $e \in Es$  do
8:        $c := class(e)$ 
9:        $ccn[c] += 1$ 
10:      for each feature  $X_j \in Xs$  do
11:         $fsn[j, c] += X_j(e)$ 
12:       $stable := (fsn=fs)$  and  $(ccn=cc)$ 
13:       $fs := fsn$ 
14:       $cc := ccn$ 
15:   until  $stable$ 
16:   return  $class, pn$ 

```

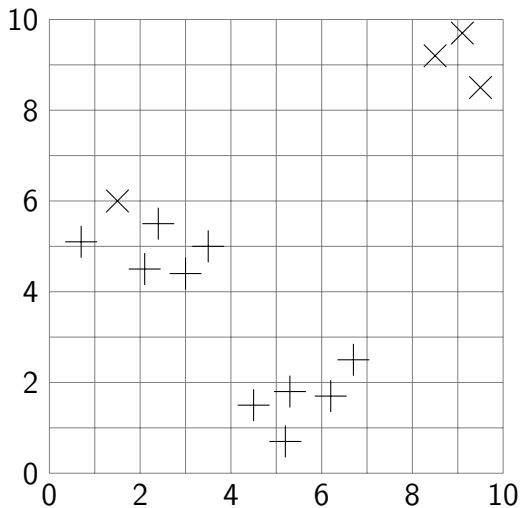
# Example Data



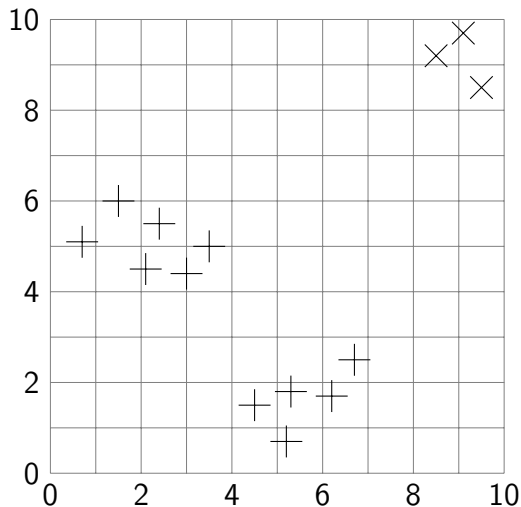
# Random Assignment to Classes



# Assign Each Example to Closest Mean



# Reassign Each Example to Closest Mean



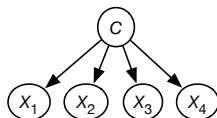
# Properties of $k$ -means

- 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 until  $k$  is the number of different examples.

# EM Algorithm

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

Model



Data

$X_1$	$X_2$	$X_3$	$X_4$
$t$	$f$	$t$	$t$
$f$	$t$	$t$	$f$
$f$	$f$	$t$	$t$
		...	

⇒ Probabilities

$$P(C)$$

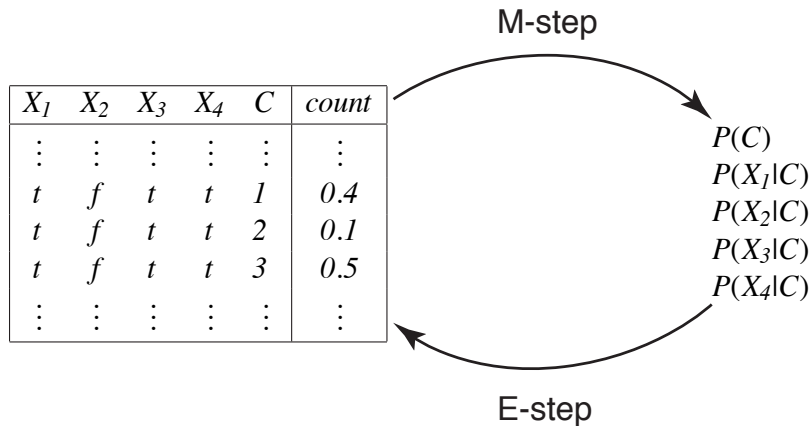
$$P(X_1|C)$$

$$P(X_2|C)$$

$$P(X_3|C)$$

$$P(X_4|C)$$

# EM Algorithm





# 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 a posteriori 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  $dom(C) = \{1, 2, 3\}$ .

$$P(C = 1 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.407$$

$$P(C = 2 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.121$$

$$P(C = 3 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.472:$$

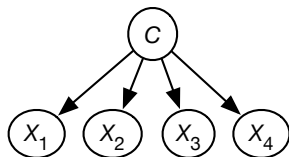
$X_1$	$X_2$	$X_3$	$X_4$	$Count$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$t$	$f$	$t$	$t$	100
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

→

$A[X_1, \dots, X_4, C]$					
$X_1$	$X_2$	$X_3$	$X_4$	$C$	$Count$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$t$	$f$	$t$	$t$	1	40.7
$t$	$f$	$t$	$t$	2	12.1
$t$	$f$	$t$	$t$	3	47.2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

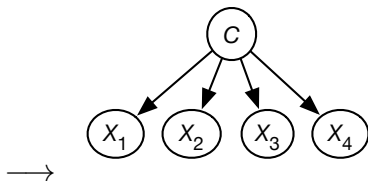
# M step

$X_1$	$X_2$	$X_3$	$X_4$	$C$	<i>Count</i>
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$t$	$f$	$t$	$t$	1	40.7
$t$	$f$	$t$	$t$	2	12.1
$t$	$f$	$t$	$t$	3	47.2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$



# M step

$X_1$	$X_2$	$X_3$	$X_4$	$C$	<i>Count</i>
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$t$	$f$	$t$	$t$	1	40.7
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$t$	$f$	$t$	$t$	3	47.2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$



$$P(C=v_i)$$

$$P(X_k = v_j | C=v_i)$$

# 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  $class(t) = c$ .

```

1: procedure  $EM(Xs, Es, k)$ 
2:    $cc[c] := 0; fc[i, v, c] := 0$ 
3:   repeat
4:      $cc\_new[c] := 0; fc\_new[i, v, c] := 0$ 
5:     for each example  $\langle v_1, \dots, v_n \rangle \in Es$  do
6:       for each  $c \in [1, k]$  do
7:          $dc := P(C = c \mid X_1 = v_1, \dots, X_n = v_n)$ 
8:          $cc\_new[c] := cc\_new[c] + dc$ 
9:         for each  $i \in [1, n]$  do
10:           $fc\_new[i, v_i, c] := fc\_new[i, v_i, c] + dc$ 
11:         $stable := (cc \approx cc\_new) \text{ and } (fc \approx fc\_new)$ 
12:         $cc := cc\_new$ 
13:         $fc := fc\_new$ 
14:   until  $stable$ 
15:   return  $cc, fc$ 

```