# Machine Intelligence 10. Unsupervised Learning: Clustering Learning on your own!

#### Álvaro Torralba



Fall 2022

Thanks to Thomas D. Nielsen and Jörg Hoffmann for slide sources

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 Clustering
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 Evaluation
 Preprocessing
 EM
 Autoencoders
 Semi-supervised
 Conclusion

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## Agenda

- Introduction
- Clustering
- $\bigcirc$  k-Mean
- Evaluation of Clustering Model
- 5 Preprocessing Optimizations: Excluding Outliers and Normalization
- 6 Soft clustering: The EM Algorithm
- Autoencoders
- Semi-supervised Learning
- Conclusions

# So far... Supervised Learning

Supervised Learning: Learn from labelled data



#### **Example: Iris Dataset**

Measurement of petal width/length and sepal width/length for 150 flowers of 3 different species of Iris.

first reported in:

Fisher,R.A. "The use of multiple measurements in taxonomic problems" Annual Eugenics, 7 (1936).

	Attri	Class variable		
SL	SW	PL	PW	Species
5.1	3.5	1.4	0.2	Setosa
4.9	3.0	1.4	0.2	Setosa
6.3	2.9	6.0	2.1	Virginica
6.3	2.5	4.9	1.5	Versicolor

 $\rightarrow\!\text{Given}$  the value of the input attributes, predict the value of the target variable

#### Unsupervised Learning

- Obtaining labelled data is expensive (typically done manually) or even impossible
- Sometimes we have a lot of data but we do not know what kind of question to ask

Suppose that we have a dataset without any target variable:

Attributes					
	SL	SW	PL	PW	
	5.1	3.5	1.4	0.2	
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Can we learn something, even if we do not know the answers (or the questions for that matter)?

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Can we learn something, even if we do not know the answers (or the questions for that matter)?

Yes! We can try to learn patterns or structural properties of the data

 $\rightarrow$  In the case of the Iris, instead of predicting the species as defined by humans, our learning algorithm can "invent" or "discover" its own species classification!

- Clustering. A problem for unsupervised learning
  - ightarrow What does clustering mean and what is it useful for?

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- Clustering. A problem for unsupervised learning
  - → What does clustering mean and what is it useful for?
- k-means: A clustering method
  - → How can we find clusters in the dataset?

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  - $\rightarrow$  Is it possible to do it better?

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  - → Using probabilities once again

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  - → What the hell is that?

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  - → What the hell is that?
- Semi-supervised learning: Combining supervised and unsupervised learning
  - ightarrow Taking advantage of the information we already have

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# Clustering Definition

**Definition (Clustering).** A clustering of the data examples  $E = \mathbf{e}_1, \dots, \mathbf{e}_N$  consists of a set  $C = \{c_1, \dots, c_k\}$  of *cluster labels*, and a *cluster assignment ca* :  $E \to C$ .

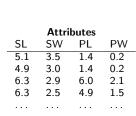
In the unlabelled Iris-Dataset, can get find a pattern in the data?

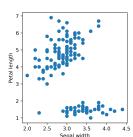
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Unlabeled Iris

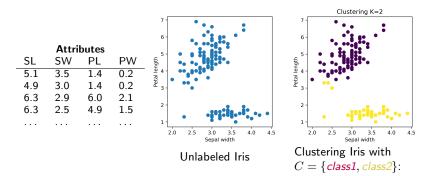
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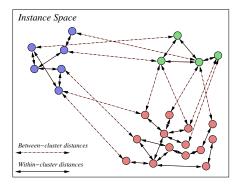
In the unlabelled Iris-Dataset, can get find a pattern in the data?



Yes, we can divide our data into two distinct clusters!

Note: Here we are only plotting 2 of the 4 dimensions (so there may be further patterns hidden in the data)

#### What is a Good Clustering?



A candidate clustering (indicated by colors) of data cases in instance space. Arrows indicate between- and within-cluster distances (selected).

In this lecture, we will focus on finding clusterings such that:

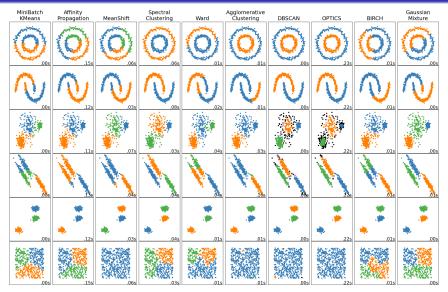
- large between-cluster variation (sum of between-cluster distances)
- small within-cluster variation (sum of within-cluster distances)

(where distance function can be e.g. the Euclidean distance).

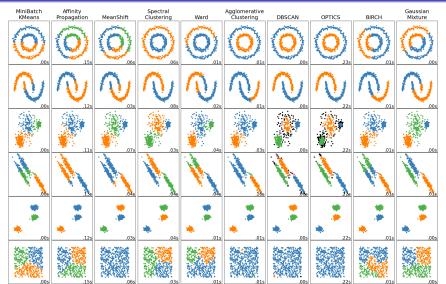
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#### What is a Good Clustering?



## What is a Good Clustering?



Note: There are many clustering algorithms and distance metrics are not the only option to extract useful patterns

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#### Clustering: Applications

- Based on customer data, find groups of customers with similar profiles.
- Based on image data, find groups of images with similar motif.
- Based on article data, find groups of articles with the same topics.
- . . .

Also, unsupervised learning can be used as a preparation to perform supervised learning (see end of this chapter)

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#### The k-means algorithm

We consider the scenario, where

- the number k of clusters is known.
- we have a distance measure  $d(\mathbf{x}_i, \mathbf{x}_j)$  between pairs of data points (feature vectors).
- we can calculate a centroid for a collection of data points  $S = \{\mathbf{x}_1, \dots \mathbf{x}_n\}$ .

Initialize: randomly pick k data points as initial cluster centers  $\mathbf{c}=c_1,\ldots,c_k$  from S repeat

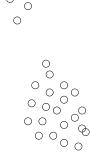
Form k clusters by assigning each point in S to its closest centroid.

Recompute the centroid for each cluster.

until Centroids do not change

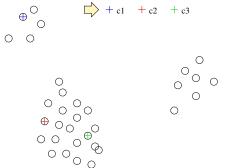
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$$k = 3$$
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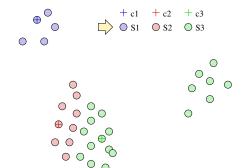




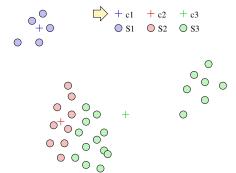
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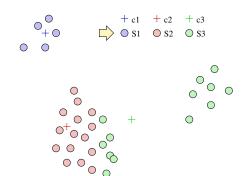
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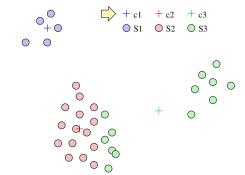
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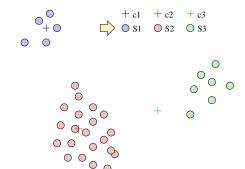
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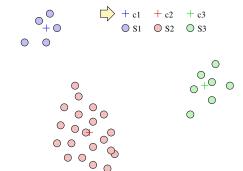
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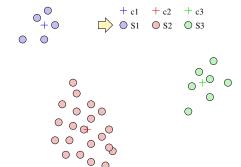
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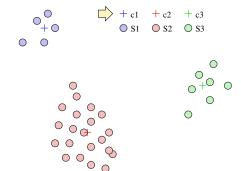
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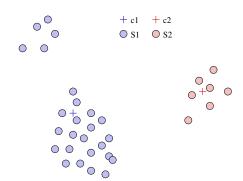


$$k = 3$$
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#### Different k

Result for clustering the same data with k=2:



Result can depend on choice of initial cluster centers!

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#### The k-means algorithm: Properties

#### Convergence

The k-means algorithm is guaranteed to converge

- Each step reduces the sum of squared errors
- There is only a finite number of cluster assignments

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#### The k-means algorithm: Properties

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The k-means algorithm is guaranteed to converge

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#### **Optimality Analysis**

k-means is not guaranteed to reach the global optimum:

- Performance depends on the random initialization
- Improve by running with multiple random restarts

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#### The k-means algorithm: Background

#### k-means as an optimization problem

Assume that we use the Euclidean distance d as proximity measure and that the quality of the clustering is measured by the sum of squared errors:

$$SSE = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} d(\mathbf{c}_i, \mathbf{x})^2,$$

#### where:

- c<sub>i</sub> is the i'th centroid
- $C_i \subseteq S$  is the points closets to  $\mathbf{c}_i$  according to d.

#### In principle ...

We can minimize the SSE by looking at all possible partitionings  $\sim$  not feasible!

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## The k-means algorithm: Background

### k-means as an optimization problem

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### In principle ...

We can minimize the SSE by looking at all possible partitionings → not feasible!

#### Instead, k-means

The centroid that minimizes the SSE is the *mean* of the data-points in that cluster:

$$\mathbf{c}_i = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \mathbf{x}$$

Álvaro Torralba

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### Cluster evaluation

A clustering algorithm applied to a dataset will return a clustering - even if there is no meaningful structure in the data!

Question: Do the clusters actually correspond to meaningful groups of data instances? Question: Are all the clusters relevant, or are there some real and some meaningless

clusters?

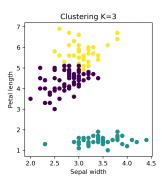
Two types of evaluation:

- Supervised
- Unsupervised

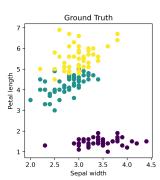
# Supervised Evaluation of Clustering Approaches

Uses external information, e.g. a true class label as the "gold standard" for actual groups in the data

#### **Example: Clustering Iris with 3-means**



Clustering found by k-means



Iris true classes

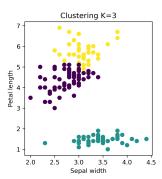
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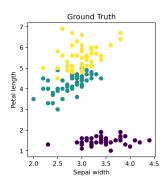
# Supervised Evaluation of Clustering Approaches

Uses external information, e.g. a true class label as the "gold standard" for actual groups in the data

#### **Example: Clustering Iris with 3-means**



Clustering found by k-means



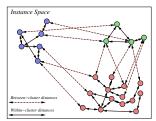
Iris true classes

- Not representative for actual clustering applications
- Can be useful to evaluate clustering algorithms
- Caveat: no guarantee that the class labels actually describe the most natural or relevant

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# Unsupervised Evaluation of Clustering Approaches

- Uses only the data as given to the clustering algorithm, and the resulting clustering
- The realistic scenario: If you have labelled data, why not doing supervised learning instead?
- Example: distance between clusters:



 $\rightarrow$  Other metrics are out of the scope of this course

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### Agenda

- Introduction
- Clustering
- $\bigcirc$  k-Mear
- Evaluation of Clustering Model
- Preprocessing Optimizations: Excluding Outliers and Normalization
- 6 Soft clustering: The EM Algorithm
- Autoencoders
- Semi-supervised Learning
- Conclusions

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### Some Practical Issues

Some Practical Issues:

- Outliers
- Different Measuring Scales

We can address them by some "massaging" of the data

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### **Outliers**

#### Issue: Outliers

The result of partitional clustering can be skewed by outliers

Example with k=2:









### **Outliers**

#### Issue: Outliers

The result of partitional clustering can be skewed by outliers

Example with k=2:









 $\sim$  useful preprocessing: outlier detection and elimination.

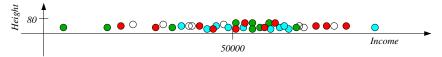
# Different Measuring Scales

#### Issue: Different Measuring Scales

If attributes are measured in different scales, the Euclidean distance is heavily biased and completely ignores those in smaller scales!

Example: Dataset with two attributes

 $A_1 = height in inches and <math>A_2 = annual income in \$$ :

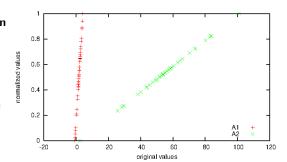


- Height is irrelevant because distances are dominated by the difference in income
- Problem is that we are comparing attributes in different units/magnitudes
- $\bullet \mbox{ } \sim \mbox{ } \text{may need to } \textit{rescale}$  or normalize continuous attributes. We see two ways to do so:
  - Min-Max Normalization
  - Z-score Normalization

### Min-Max Normalization

#### Min-Max Normalization

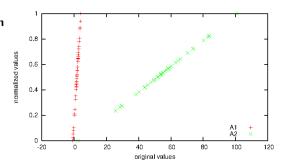
replace 
$$A_i$$
 with 
$$\frac{A_i - \min(A_i)}{\max(A_i) - \min(A_i)}$$
 ( $\min(A_i), \max(A_i)$  are  $\min/\max$  values of  $A_i$  appearing in the data)



### Min-Max Normalization

#### Min-Max Normalization

replace  $A_i$  with  $\frac{A_i - \min(A_i)}{\max(A_i) - \min(A_i)}$  ( $\min(A_i), \max(A_i)$  are  $\min/\max$  values of  $A_i$  appearing in the data)



#### **Properties**

- Ensures that all attributes have only values between 0 and 1
- Very sensitive with respect to outliers

### **Z-Score Standardization**

### Z-score Standardization

replace 
$$A_i$$
 with  $A_i - mean(A_i)$ 

 $\overline{standarddeviation(A_i)}$ 

where

$$mean(A_i) = \frac{1}{n} \sum_{j=1}^{n} a_{j,i}$$

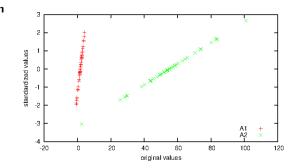
$$standarddeviation(A_i) = \sqrt{\frac{1}{n} \sum_{j=1}^{n} (a_{j,i} - mean(A_i))^2}$$

Clustering Evaluation Preprocessing 000000

## **Z-Score Standardization**

### **Z-score Standardization**

replace 
$$A_i$$
 with 
$$\frac{A_i - mean(A_i)}{standard deviation(A_i)}$$



where

$$mean(A_i) = \frac{1}{n} \sum_{j=1}^{n} a_{j,i}$$

$$standarddeviation(A_i) = \sqrt{\frac{1}{n} \sum_{j=1}^{n} (a_{j,i} - mean(A_i))^2}$$

#### **Properties**

- Intuitively, it measures how many standard deviations is each example far from the mean
- Less sensitive to outliers
- Not all attributes have the same range (but they are still relatively close)

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- Introduction
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# Soft Clustering

The k-means algorithm generates a hard clustering: each example is assigned to a single cluster.

#### Original dataset

$F_1$	$F_2$	$F_3$
t	t	t
t	f	t
t	f	f
f	f	t

# Soft Clustering

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$F_1$	$F_2$	$F_3$
t	t	t
t	f	t
t	f	f
f	f	t

Har	d clus	tering	(K=2)
$F_1$	$F_2$	$F_3$	C
t	t	t	class1
t	f	t	class2
t	f	f	class1
f	f	$\mid t \mid$	class1

## Soft Clustering

The k-means algorithm generates a hard clustering: each example is assigned to a single cluster.

Original dataset

$F_1$	$\mid F_2$	$F_3$	Har	d clus	tering	(K=2)			Soft	cluste	ring (K=2	2)
$\frac{1}{t}$	t.	t.	$F_1$	$F_2$	$F_3$	C	1	$F_1$	$F_2$	$F_3$	class1	class2
t	f	t	 t	t	t	class1		t	t	t	0.9	0.1
t	$\int_{f}^{J}$	f	t	f	t	class2		t	f	t	0.2	0.8
f	$\int_{f}^{J}$	t.	t	f	f	class1		t	f	f	0.7	0.3
J	J	1	f	f	t	class1		f	f	t	1	0

**Soft Clustering:** Each example is assigned to a cluster with a certain probability We need:

4 A way of representing the mapping from examples to probabilities. Any ideas?

## Soft Clustering

The k-means algorithm generates a *hard* clustering: each example is assigned to a single cluster.

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$F_1$	$F_2$	$F_3$
t	t	t
t	f	t
t	f	f
f	f	t

$F_1$	$F_2$	$F_3$	C
t	t	t	class1
t	f	t	class2
t	f	f	class1
f	f	t	class1

Hard clustering (K=2)

	Soft	ciuste	ring (K=2	()
$F_1$	$F_2$	$F_3$	class1	class2
t	t	t	0.9	0.1
t	f	t	0.2	0.8
t	f	f	0.7	0.3
f	f	t	1	0

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**Soft Clustering:** Each example is assigned to a cluster with a certain probability We need:

A way of representing the mapping from examples to probabilities. Any ideas?
 → This is just a probabilistic model! We will use the simplest (Naive Bayes)
 (Note that in this section, we assume for simplicity that our features are discrete)

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### Soft Clustering

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Original dataset

$F_1$	$F_2$	$F_3$
t	t	t
t	f	t
t	f	f
f	f	t

$F_1$	$F_2$	$F_3$	C
t	t	t	class1
t	f	t	class2
t	f	f	class1
f	f	t	class1

Hard clustering (K=2)

	3011	Ciuste	ning (N-2	.)
$F_1$	$F_2$	$F_3$	class1	class2
t	t	t	0.9	0.1
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t	f	f	0.7	0.3
f	f	t	1	0

Caft alustoring (K-2)

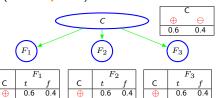
**Soft Clustering:** Each example is assigned to a cluster with a certain probability We need:

- A way of representing the mapping from examples to probabilities. Any ideas?
   → This is just a probabilistic model! We will use the simplest (Naive Bayes)
   (Note that in this section, we assume for simplicity that our features are discrete)
- ② An algorithm to decide how to cluster the data (an alternative to k-means that works with probabilities) → Expectation-Maximization

## Soft Clustering Using Naive Bayes

We use a Naive Bayes Network to represent the soft clustering

We can compute  $P(C|F_1, F_2, F_3)$  to retrieve the probability of belonging to each class! (c.f. Chapter 6)



0.4 0.6

$F_1$	$F_2$	$F_3$	$P(C F_1, F_2, F_3)$
t	t	t	?
t	f	t	?
t	f	f	?
f	f	t	?

#### Question!

0.4 0.6

Considering the network above, compute the probability that each example belongs to  $\oplus$ . Which of them have probability > 0.5?

0.4 0.6

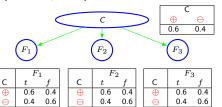
(A): ttt (B): tft

(C): tff (D): fft

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t $t$ $t$ $(0.84, 0.16)$	
$t \mid f \mid t \parallel$ ?	
$t \mid f \mid f \mid$ ?	
$f \mid f \mid t \mid$ ?	

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(A): ttt

(B): *tft* 

(C): tff

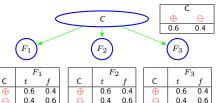
**(D)**: *fft* 

$$P(C|F_1 = t, F_2 = t, F_3 = t) = \langle 0.6 \cdot 0.6 \cdot 0.6 \cdot 0.6, 0.4 \cdot 0.4 \cdot 0.4 \cdot 0.4 \rangle = \alpha \langle 0.1296, 0.0256 \rangle = \langle 0.84, 0.16 \rangle$$

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t	t	t	(0.84, 0.16)
t	f	t	(0.69, 0.31)
t	f	f	?
f	f	t	?
-	-	'	'

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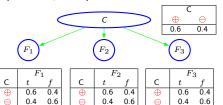
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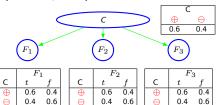
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Álvaro Torralba

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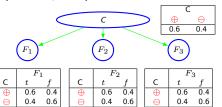
Álvaro Torralba

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→The question of how to find a good clustering becomes how to fill the probability tables!

(D): fft

# How to Fill In Probability Tables: Expectation Maximization

We need to estimate P(C),  $P(C|F_1)$ ,  $P(C|F_2)$ ,  $P(C|F_3)$  How to do that?

# How to Fill In Probability Tables: Expectation Maximization

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- ullet When learning the probability distributions of the model, the variable C is hidden
- → we cannot directly estimate the probabilities using frequency counts
- In supervised learning we used the frequency counts. However, here, we do not have any values for C!

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#### Instead we employ the Expectation-maximization algorithm

- The expectation maximization or EM algorithm can be used to learn probabilistic models with hidden variables
- Combined with a naive Bayes classifier, it does soft clustering, similar to the -means algorithm, but where examples are probabilistically in classes

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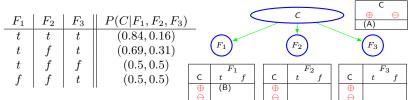
The main idea: Similar to k-means (set centroids, recompute class, repeat until convergence)

- Use hypothetical completions of the data using the current probability estimates
- Infer the maximum likelihood probabilities for the model based on completed data set

### The Expectation Maximization (EM) Algorithm

- ullet Create a model with the right number of clusters (K)
- Initialize probabilities of the model (P(C),  $P(F_1|C)$ ,  $P(F_2|C)$ , and  $P(F_3|C)$ ) at random
- Until convergence:
  - Expectation: for each example in the training set, compute estimated class probabilities based on the current table probabilities
  - Maximization: Re-compute the current table probabilities based on the estimated class probabilities

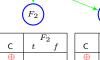
Re-compute the current table probabilities based on the estimated class probabilities



Re-compute the current table probabilities based on the estimated class probabilities

$F_1$	$F_2$	$F_3$	$P(C F_1,F_2,$
t	t	t	(0.84, 0.16)
t	f	t	(0.69, 0.31)
t	f	f	(0.5, 0.5)
f	f	t	(0.5, 0.5)





	$F_3$	
C	t	f
$\oplus$		
$\Theta$		

(A)

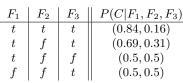
#### Question!

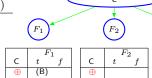
Compute the following:

(A): 
$$P(C = \oplus)$$

**(B)**: 
$$P(F_1 = t \mid C = \oplus)$$

Re-compute the current table probabilities based on the estimated class probabilities





#### Question!

Compute the following:

(A): 
$$P(C = \oplus)$$

**(B)**: 
$$P(F_1 = t \mid C = \oplus)$$

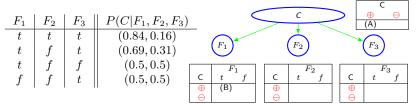
(A)

C

 $\oplus$ 

$$P(C = \oplus) =$$

Re-compute the current table probabilities based on the estimated class probabilities



#### Question!

### Compute the following:

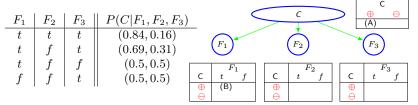
(A): 
$$P(C = \oplus)$$

**(B)**: 
$$P(F_1 = t \mid C = \oplus)$$

$$P(C = \oplus) = \frac{0.84 + 0.69 + 0.5 + 0.5}{4} = 0.63$$

# Maximization Step

Re-compute the current table probabilities based on the estimated class probabilities



#### Question!

#### Compute the following:

(A): 
$$P(C = \oplus)$$

**(B)**: 
$$P(F_1 = t \mid C = \oplus)$$

$$P(C = \oplus) = \frac{0.84 + 0.69 + 0.5 + 0.5}{4} = 0.63$$

$$P(F_1 = t \mid C = \oplus) =$$

# Maximization Step

Re-compute the current table probabilities based on the estimated class probabilities

$F_1$	$F_2$	$F_3$	$ P(C F_1, F_2, F_3) $		C	⊕ ⊕ (A)
$t \ t$	f	$egin{pmatrix} t \ t \end{bmatrix}$	$(0.84, 0.16) \\ (0.69, 0.31)$	$F_1$	$F_2$	$F_3$
f	$\begin{array}{c c} f \\ f \end{array}$	$\begin{array}{ c c c }\hline f \\ t \end{array}$	(0.5, 0.5)  (0.5, 0.5)	$ \begin{array}{c c}  & F_1 \\ C & t & f \\ \hline \oplus & (B) \\ \hline \end{array} $	$\begin{array}{c c} C & t & F_2 \\ \oplus & & & \\ \Theta & & & \end{array}$	$ \begin{array}{ c c c } \hline C & t & f \\ \hline \oplus & & & \\ \hline \Theta & & & & \\ \hline \end{array} $

#### Question!

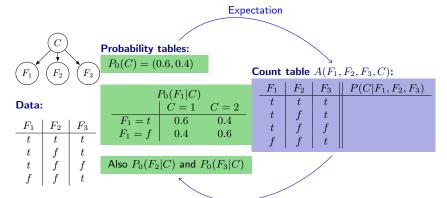
#### Compute the following:

(A): 
$$P(C = \oplus)$$

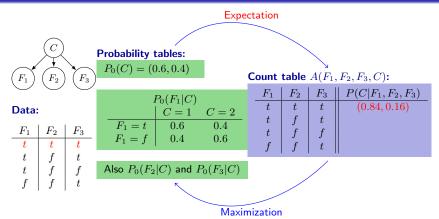
**(B)**: 
$$P(F_1 = t \mid C = \oplus)$$

$$P(C = \oplus) = \frac{0.84 + 0.69 + 0.5 + 0.5}{4} = 0.63$$

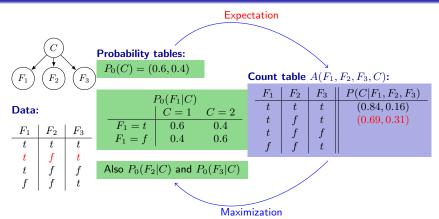
$$P(F_1 = t \mid C = \oplus) = \frac{P(F_1 = t, C = \oplus)}{P(C = \oplus)} = \frac{\frac{0.84 + 0.69 + 0.5}{4}}{\frac{0.84 + 0.69 + 0.5 + 0.5}{4}} = \frac{0.84 + 0.69 + 0.5}{0.84 + 0.69 + 0.5 + 0.5} = 0.8$$



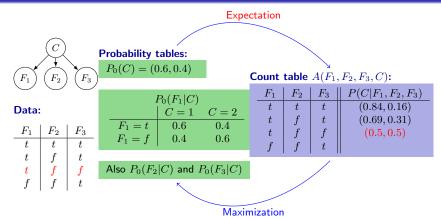
Maximization



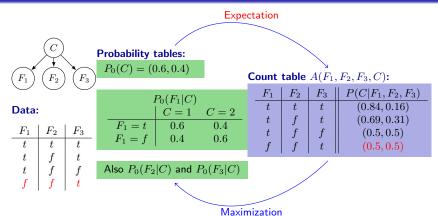
### Expectation



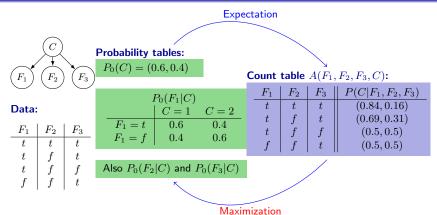
#### **Expectation**



### **Expectation**



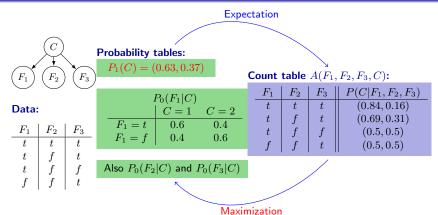
#### **Expectation**



#### **Maximization**

$$P_1(C) = \frac{1}{4} \sum_{F_1, F_2, F_3} A(F_1, F_2, F_3, C) = \frac{1}{4} (0.84 + 0.69 + 0.5 + 0.5, 0.16 + 0.31 + 0.5 + 0.5)$$

$$= (0.63, 0.37)$$

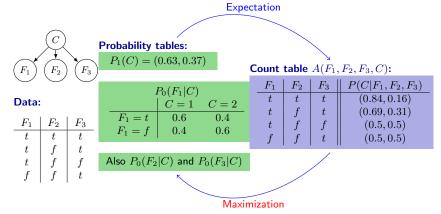


#### **Maximization**

$$\frac{P_1(C)}{I} = \frac{1}{4} \sum_{F_1, F_2, F_3} A(F_1, F_2, F_3, C) = \frac{1}{4} (0.84 + 0.69 + 0.5 + 0.5, 0.16 + 0.31 + 0.5 + 0.5)$$

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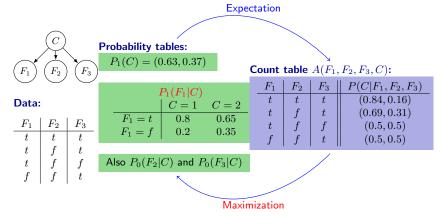
#### Maximization

$$P_{1}(F_{1}|C) = \frac{\sum_{F_{2},F_{3}} A(F_{1}, F_{2}, F_{3}, C)}{\sum_{F_{1},F_{2},F_{3}} A(F_{1}, F_{2}, F_{3}, C)} = \frac{\begin{pmatrix} 0.84 + 0.69 + 0.5 + 0 & 0.16 + 0.31 + 0.5 + 0 \\ 0.40 + 0.40 + 0.40 & 0.40 + 0.40 \end{pmatrix}}{(2.53, 1.47)}$$

$$= \begin{pmatrix} 0.8 & 0.65 \\ 0.2 & 0.35 \end{pmatrix}$$

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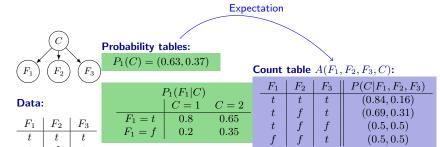




### Maximization

$$\frac{P_1(F_1|C)}{P_1(F_1|C)} = \frac{\sum_{F_2,F_3} A(F_1, F_2, F_3, C)}{\sum_{F_1,F_2,F_3} A(F_1, F_2, F_3, C)} = \frac{\begin{pmatrix} 0.84 + 0.69 + 0.5 + 0 & 0.16 + 0.31 + 0.5 + 0 \\ 0 + 0 + 0 + 0.5 & 0 + 0 + 0 + 0.5 \end{pmatrix}}{(2.53, 1.47)}$$

$$= \begin{pmatrix} 0.8 & 0.65 \\ 0.2 & 0.35 \end{pmatrix}$$

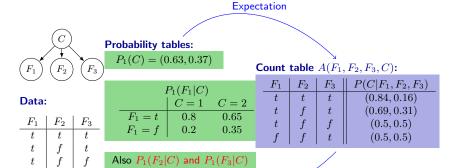


Also  $P_0(F_2|C)$  and  $P_0(F_3|C)$ 

Maximization

#### Maximization

$$P_1(F_2|C) = \dots = \begin{pmatrix} 0.33 & 0.11 \\ 0.67 & 0.89 \end{pmatrix}$$
  
 $P_1(F_3|C) = \dots = \begin{pmatrix} 0.80 & 066 \\ 0.20 & 0.34 \end{pmatrix}$ 

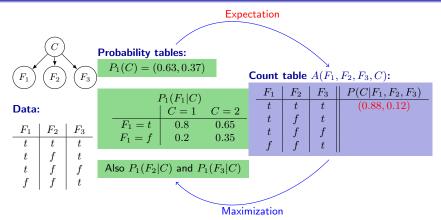


#### Maximization

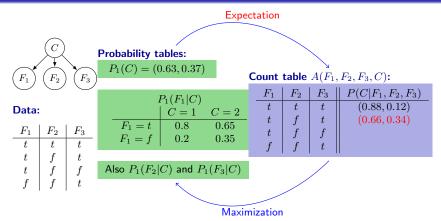
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Álvaro Torralba

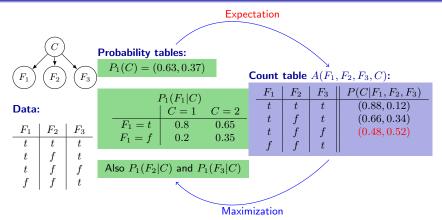
Maximization



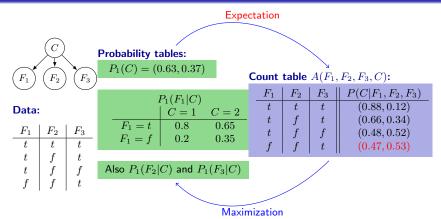
### **Expectation**



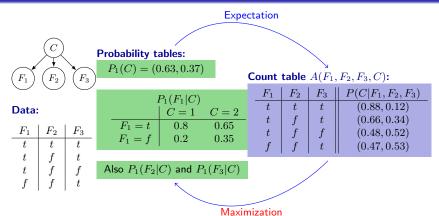
### **Expectation**



### **Expectation**

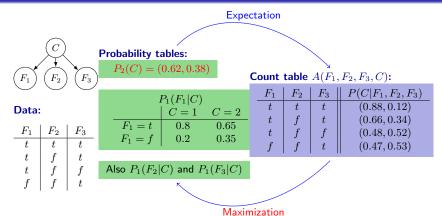


#### **Expectation**



#### Maximization

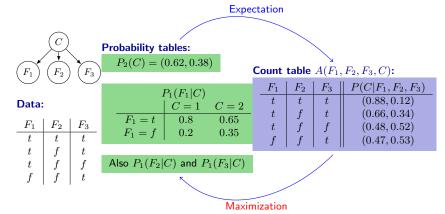
$$P_2(C) = \frac{1}{4} \sum_{F_1, F_2, F_3} A(F_1, F_2, F_3, C) = \frac{1}{4} (0.88 + 0.66 + 0.48 + 0.47, 0.12 + 0.34 + 0.52 + 0.62, 0.38)$$



#### Maximization

$$\frac{P_2(C)}{F_2(C)} = \frac{1}{4} \sum_{F_1, F_2, F_3} A(F_1, F_2, F_3, C) = \frac{1}{4} (0.88 + 0.66 + 0.48 + 0.47, 0.12 + 0.34 + 0.52 + 0.66, 0.38)$$





### Maximization

$$P_2(F_1|C) = \frac{\sum_{F_2,F_3} A(F_1, F_2, F_3, C)}{\sum_{F_1,F_2,F_3} A(F_1, F_2, F_3, C)} = \frac{\begin{pmatrix} 0.88 + 0.66 + 0.48 + 0 & 0.12 + 0.34 + 0.52 \\ 0 + 0 + 0 + 0.47 & 0 + 0 + 0 + 0.53 \end{pmatrix}}{(2.49, 1.51)}$$

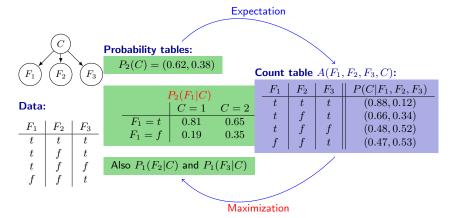
$$= \begin{pmatrix} 0.81 & 0.65 \end{pmatrix}$$

 $=\begin{pmatrix} 0.19 & 0.35 \end{pmatrix}$  Machine Intelligence

Chapter 10: Unsupervised Learning: Clustering

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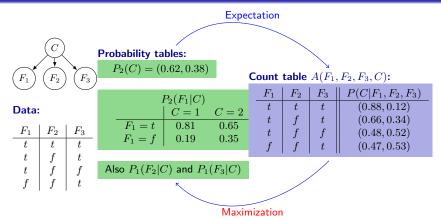
#### Maximization

$$P_{2}(F_{1}|C) = \frac{\sum_{F_{2},F_{3}} A(F_{1}, F_{2}, F_{3}, C)}{\sum_{F_{1},F_{2},F_{3}} A(F_{1}, F_{2}, F_{3}, C)} = \frac{\begin{pmatrix} 0.88 + 0.66 + 0.48 + 0 & 0.12 + 0.34 + 0.52 \\ 0 + 0 + 0 + 0.47 & 0 + 0 + 0 + 0.53 \end{pmatrix}}{(2.49, 1.51)}$$

$$= \begin{pmatrix} 0.81 & 0.65 \\ 0.10 & 0.27 \end{pmatrix}$$

- \( 0.19 \ 0.35 \)
Álvaro Torralba Machine Intelligence

Chapter 10: Unsupervised Learning: Clustering



#### Maximization

... and so we continue until a termination criterion is reached.

### The EM algorithm: Properties

- Convergence The sequence of probability estimates generated by the EM
  algorithm converges to a local maximum (in rare cases: a saddle point) of the
  marginal likelihood given the data.
- Non-optimality: May converge to a local maximum (non-necessarily the global maximum)
- To find better local maxima: run EM several times with different starting points.

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#### Notes

- Any permutation of the cluster labels of a local maximum will also be a local maximum
- Clustering an existing or new instance x amounts to calculating P(C|x).

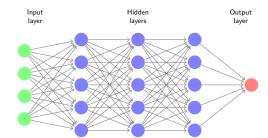
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### Agenda

- Introduction
- 2 Clustering
- $\bigcirc$  k-Mean
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# Neural Networks for Unsupervised Learning

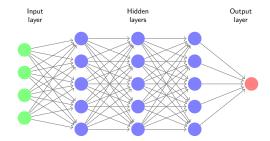
#### Can we use Neural Networks for Unsupervised Learning?



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### Neural Networks for Unsupervised Learning

#### Can we use Neural Networks for Unsupervised Learning?



### Problem:

The whole concept of training is to minimize the error with gradient descent. How do we compute the error if we do not have any target label?

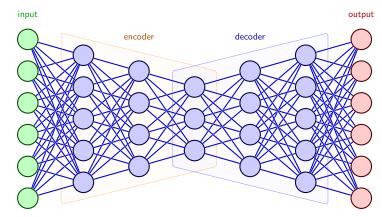
# Autoencoder

 $\bullet$   $\mbox{Output} = \mbox{Input} :$  Train the network to predict the input from the input

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### Autoencoder

- ullet Output = Input: Train the network to predict the input from the input
- Hidden layers have less neurons so the data needs to be compressed and then uncompressed
- After learning all weights, we can separate the encoder and the decoder

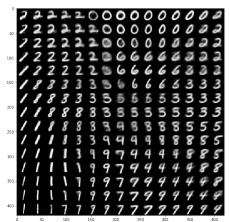


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# Embeddings

Aim: extract good representation from data without the need for any manual labels **Embeddings:** compressed representation of the original data



(example where images are reduced to two values (x, y), taken from https://github.com/lyeoni/keras-mnist-VAE/)

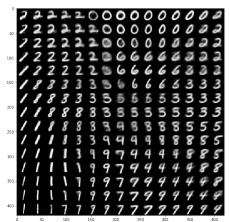
Why is this possible?

oduction Clustering k-Means Evaluation Preprocessing EM **Autoencoders** Semi-supervised Conclusion

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# Embeddings

Aim: extract good representation from data without the need for any manual labels **Embeddings:** compressed representation of the original data



(example where images are reduced to two values (x, y), taken from https://github.com/lyeoni/keras-mnist-VAE/)

Why is this possible? Most combinations of pixels are not possible in real images!

oduction Clustering k-Means Evaluation Preprocessing EM Autoencoders Semi-supervised Conclusion OO 00000 000000 00000 0000 $\bullet$  000 000

### Using Decoders

We can use decoders to obtain new examples that are not in our original dataset:

- Train Autoencoder on a large dataset (e.g. of face images)
- Identify which node in the latent representation correspond to smile (possibly forcing this by altering the training)
- Get a new image, and obtain its latent representation by using the encoder
- Modify the value of the value corresponding to "smile"
- Use the decoder to obtain a new image



(image taken from

https://gaussian37.github.io/deep-learning-chollet-8-4/)

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# Semi-supervised Learning

We have seen the two extremes:

- Supervised Learning: All our dataset is labelled
- Unsupervised Learning: We do not have any labels

### Semi-supervised Learning

We have seen the two extremes:

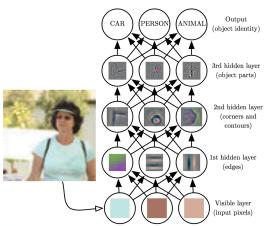
- Supervised Learning: All our dataset is labelled
- Unsupervised Learning: We do not have any labels

Semi-supervised Learning: We have only some examples labelled.

- Very realistic scenario: labelling data is expensive so we want to do it only for few examples
- Example: We have all images on the internet as our dataset. We label some of them (e.g. "like" and "dislike", or "dogs" and "cats"). In supervised learning, unlabelled images cannot be used. In semi-supervised learning we learn also from unlabelled data

# Autoencoders for Semi-supervised Learning

- Train Autoencoder on a large dataset (e.g. of face images)
- ② Get the (possibly few) labelled images
- Train a new "decoder"
- ightarrow The "compressed" representation obtained by the encoder makes much easier to learn the classifier



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### Summary

- Unsupervised Learning techniques learn from unlabelled examples.
- Clustering techniques divide the data into multiple clusters.
- K-means is a clustering technique, where each cluster is specified by its centroid.
   It alternates between setting the centroid and re-classifying the data.
- Soft clustering assigns each example a probability of belonging to each of the clusters.
- Expectation Maximization (EM) is a soft clustering algorithm, which can be used in combination with a Naive Bayes model.
- Autoencoders can be used to obtain a latent representation of the data.

### Reading

- Chapter 10.2 Unsupervised Learning from the book "Artificial Intelligence: Foundations of Computational Agents (2nd edition)
- Extra Reading: To go much further, you can read the Lecture Notes of the Stanford Course in Machine Learning. In this lecture we cover