Clustering / Unsupervised Learning

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- 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 $i \in \{1, \ldots, k\}$.

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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.

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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

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- 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)

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until

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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 $\widehat{X}_j(c)$

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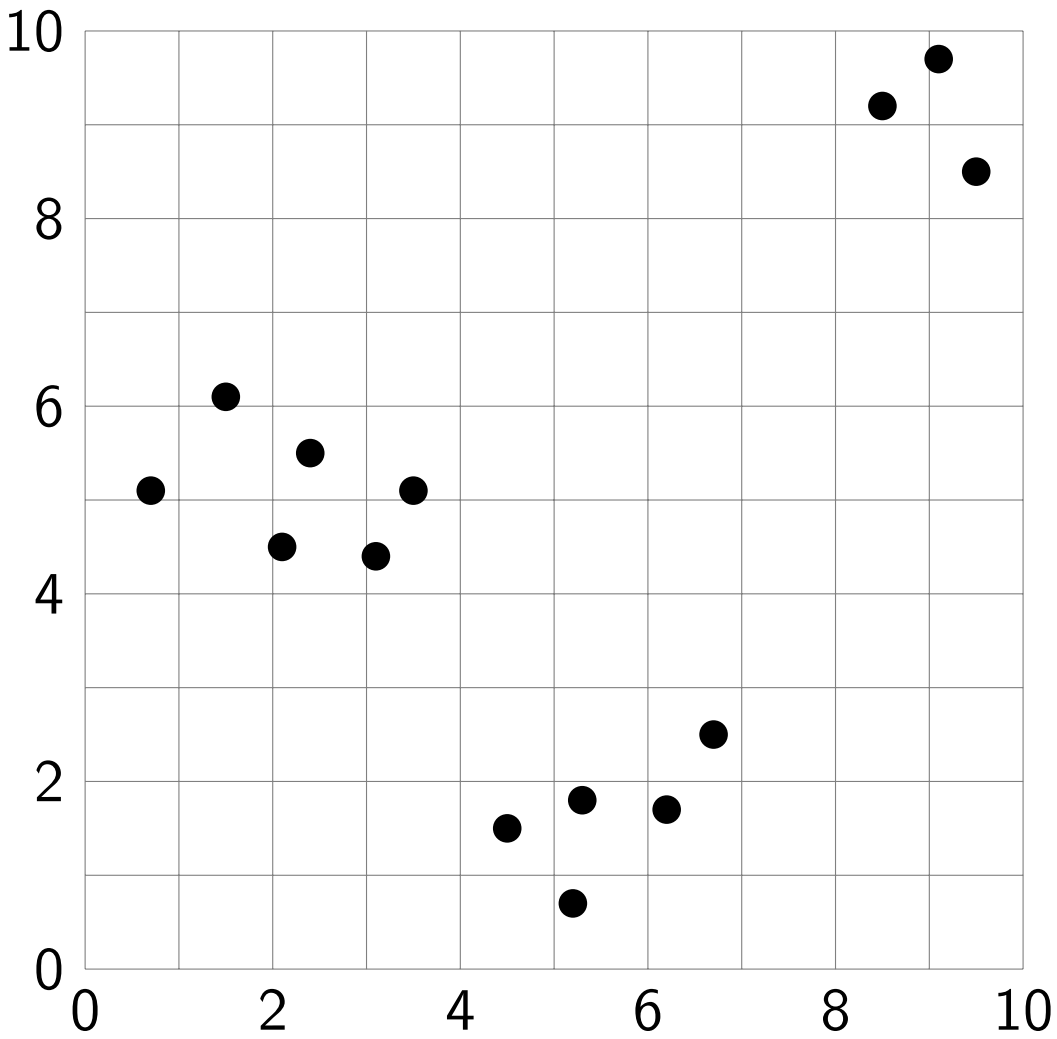
$$class(e) = \arg\min_c \sum_{j=1}^{n} (pn(j, c) - X_j(e))^2$$

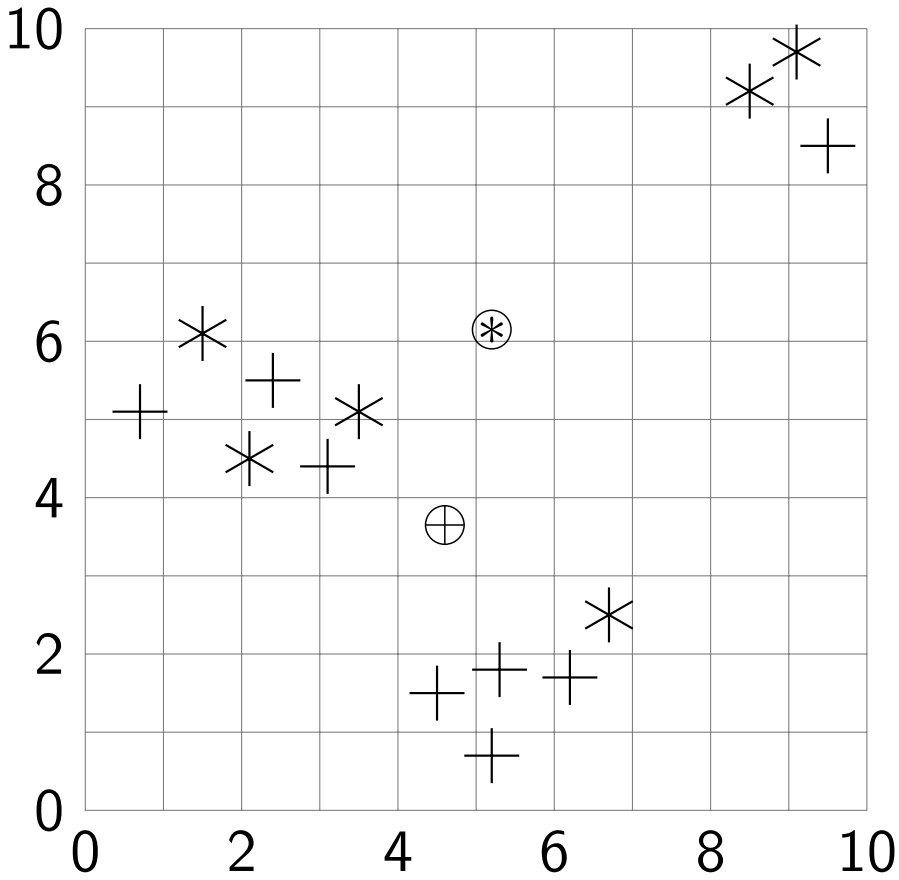
These can be updated in one pass through the training data.

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

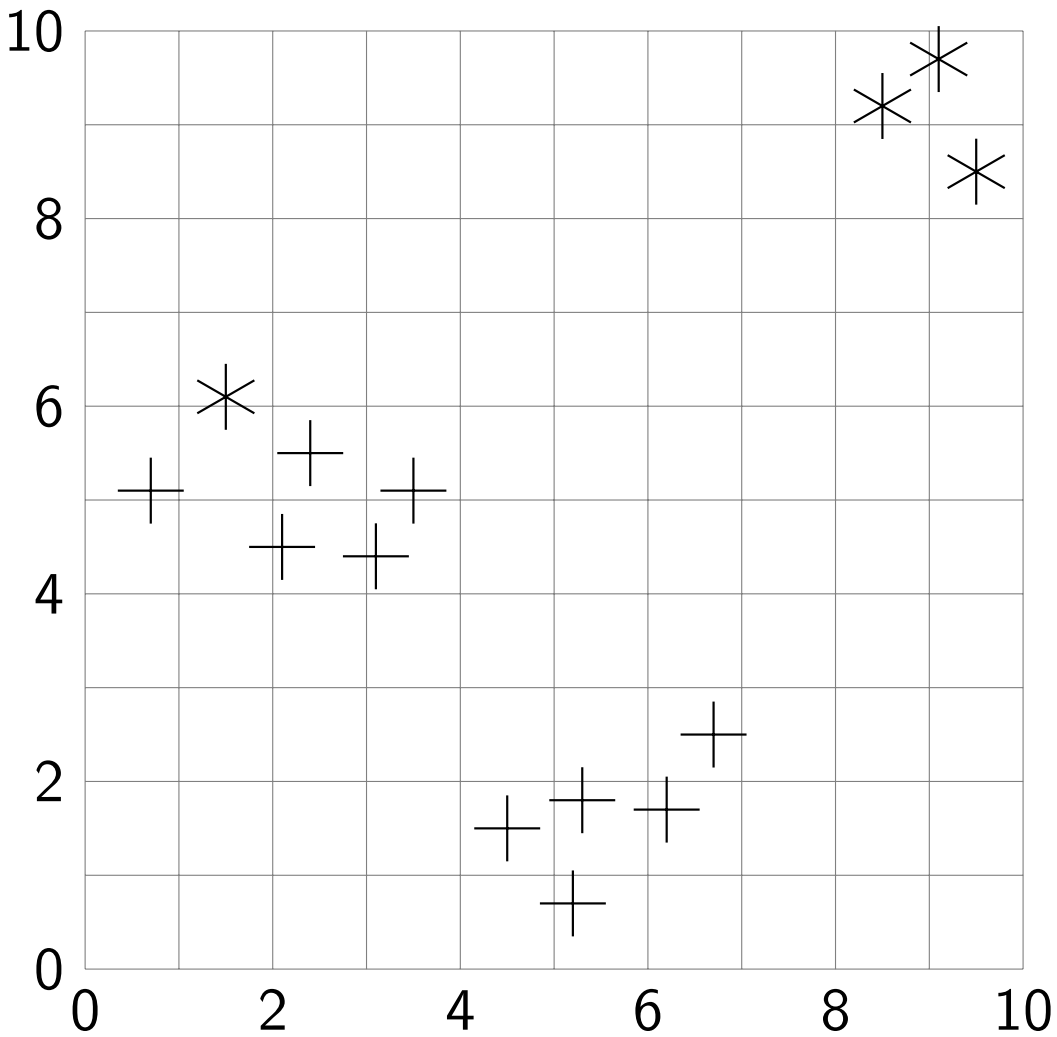


Random Assignment to Classes

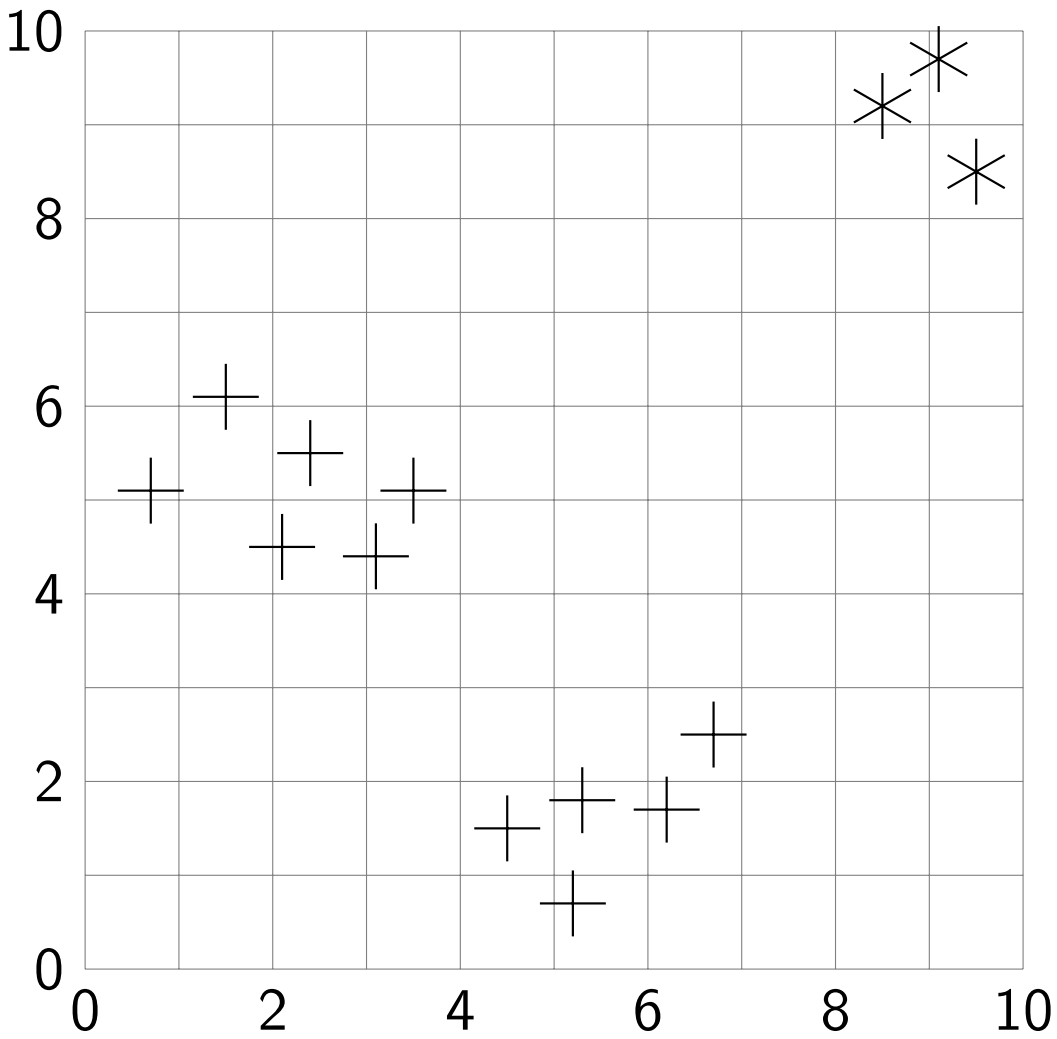


$\oplus$ is mean of $+$ and $\circledast$ is mean of $*$

Assign Each Example to Closest Mean



Ressign Each Example to Closest Mean



Properties of k-means

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  How?

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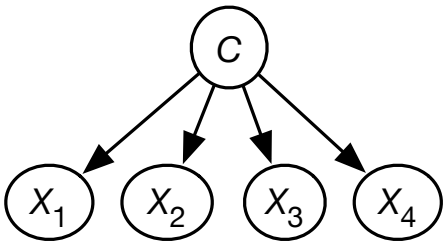
- It is sensitive to the relative scale of the dimensions.
- Increasing k *can* always decrease error (but does not always) until k is the number of different examples.
  How? Given an assignment with k classes, for $k+1$ classes start with the same assignment, but with the point most distant from its class center in its own new cluster.

EM Algorithm

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

Model



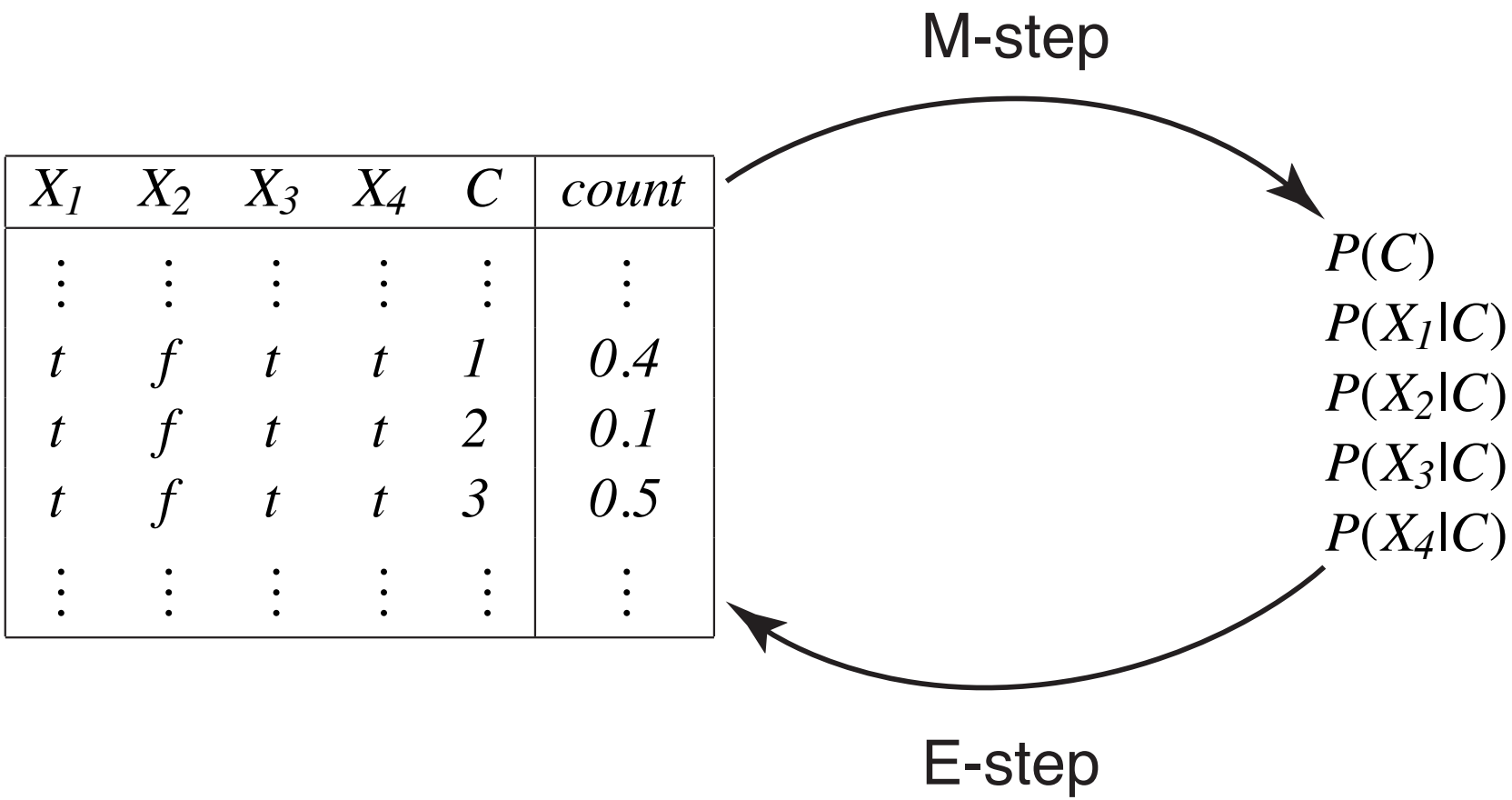
Data

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

⇨ 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 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
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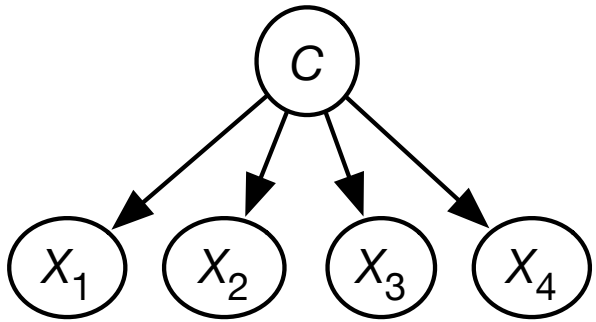
⋮	⋮	⋮	⋮	⋮	⋮

$\longrightarrow$



M step

X_1	X_2	X_3	X_4	C	*Count*
⋮	⋮	⋮	⋮	⋮	⋮
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t	f	t	t	2	12.1
t	f	t	t	3	47.2
⋮	⋮	⋮	⋮	⋮	⋮

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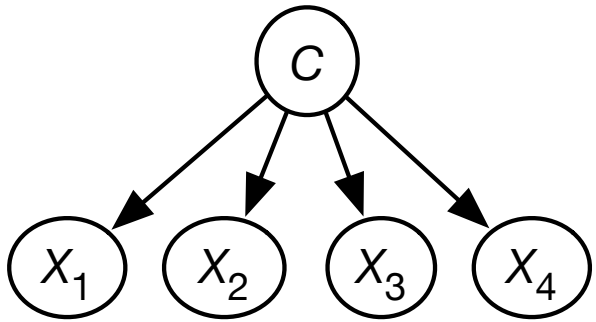

$P(C{=}c)$

$P(X_i = v | C{=}c)$

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 $class(t) = c$.

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- The probabilites can be computed by:

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

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

```
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 ⟨v_1, ..., v_n⟩ ∈ Es do
6:              for each c ∈ [1, k] do
7:                  dc := P(C = c | X_1 = v_1, ..., X_n = v_n)
8:                  cc_new[c] := cc_new[c] + dc
9:                  for each i ∈ [1, n] do
10:                     fc_new[i, v_i, c] := fc_new[i, v_i, c] + dc
11:         stable := (cc ≈ cc_new) and (fc ≈ fc_new)
12:         cc := cc_new
13:         fc := fc_new
14:     until stable
15:     return cc,fc
```