

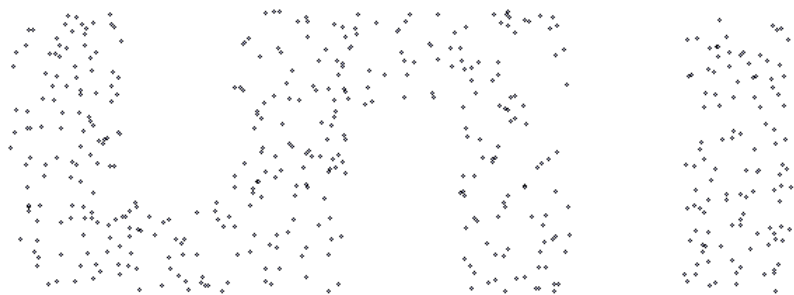
# *Artificial Intelligence*

## *Unsupervised Learning*

Marco Piastra

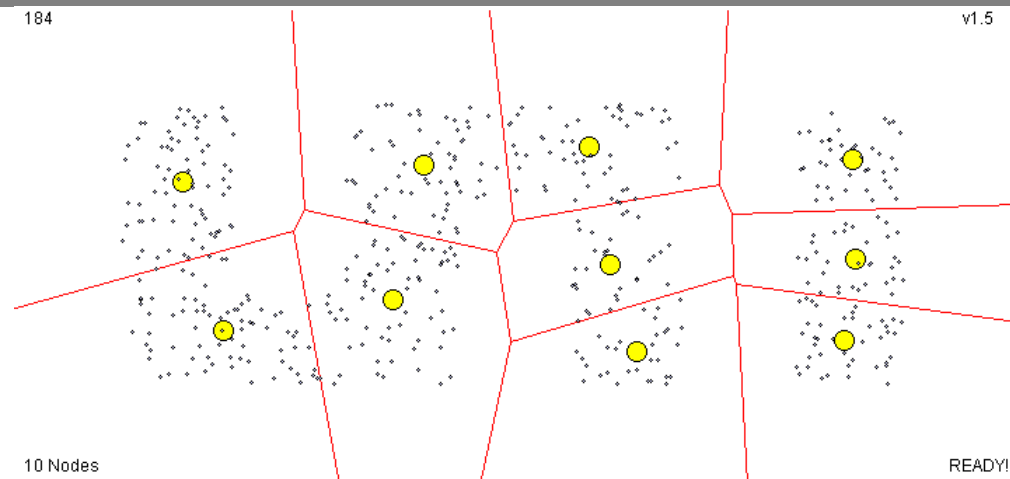
# Vector quantization

184



v1.5

184



v1.5

10 Nodes

READY!

10 Nodes

READY!

Original data

Quantization (compression via prototypes)

The basic idea is to replace each real-valued vector  $\mathbf{x} \in \mathbb{R}^d$  with a discrete symbol  $\mathbf{w}_j \in \mathbb{R}^d$  which belongs to a codebook of  $k$  prototypes  $\theta := \{\mathbf{w}_1, \dots, \mathbf{w}_k\}$

Each data vector is encoded by using the index of the most similar prototype, where similarity is measured in terms, for instance, of Euclidean distance:

$$w(\mathbf{x}) := \operatorname{argmin}_{\mathbf{w}_j} \|\mathbf{x} - \mathbf{w}_j\|$$

For instance, part of mpeg4 and QuickTime (Apple) video compression algorithms work in this way and so does the Ogg Vorbis audio compression algorithm

# *k-means* (Generalized Lloyd's Algorithm – Vector quantization)

Given a set  $D := \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  of observations (i.e. vectors in  $\mathbb{R}^d$ ) and a set  $\theta := \{\mathbf{w}_1, \dots, \mathbf{w}_k\}$  of  $k$  prototypes (i.e. vectors in  $\mathbb{R}^d$ )

Clustering problem: find an assignment function  $w : \mathbb{R}^d \rightarrow W$  such that the objective (loss) function:

$$J(D, \theta) := \frac{1}{2} \sum_{i=1}^N \|\mathbf{x}_i - w(\mathbf{x}_i)\|^2$$

is minimized.

# *k-means* (Generalized Lloyd's Algorithm – Vector quantization)

## **k-means algorithm:**

- 1) Position the  $k$  prototypes at random
- 2) Assign each observation to its closest prototype

$$w(\mathbf{x}_i) := \operatorname{argmin}_{\mathbf{w}_j} \|\mathbf{x}_i - \mathbf{w}_j\|$$

- 3) Position each prototype at the *centroid* of the observations assigned to it

$$\mathbf{w}_j = \frac{1}{|D(\mathbf{w}_j)|} \sum_{D(\mathbf{w}_j)} \mathbf{x}_i \quad \text{where } D(\mathbf{w}_j) := \{\mathbf{x}_i \in D \mid w(\mathbf{x}_i) = \mathbf{w}_j\}$$

- 4) Unless no prototype was moved in step 3), go back to step 2)

This algorithm converges to a local minimum of  $J(D, \theta)$

# *k-means* (Generalized Lloyd's Algorithm – Vector quantization)

Why does the algorithm work: *alternate optimization* (also 'coordinate descent')

**Step 2):** Assign observations while keeping the  $k$  prototype fixed

$$w(\mathbf{x}_i) := \operatorname{argmin}_{\mathbf{w}_j} \|\mathbf{x}_i - \mathbf{w}_j\|$$

which minimizes each of the terms in  $J(D, \theta) := \frac{1}{2} \sum_{i=1}^N \|\mathbf{x}_i - w(\mathbf{x}_i)\|^2$

**Step 3):** Reposition the  $k$  prototypes while keeping the assignments fixed

$$J(D, \theta) := \frac{1}{2} \sum_{i=1}^N \|\mathbf{x}_i - w(\mathbf{x}_i)\|^2 = \frac{1}{2} \sum_j \sum_{D(\mathbf{w}_j)} (\mathbf{x}_i - \mathbf{w}_j)^2$$

$$\begin{aligned} \frac{\partial}{\partial \mathbf{w}_j} J(D, \theta) &= \frac{\partial}{\partial \mathbf{w}_j} \frac{1}{2} \sum_{D(\mathbf{w}_j)} (\mathbf{x}_i - \mathbf{w}_j)^2 = \frac{\partial}{\partial \mathbf{w}_j} \frac{1}{2} \sum_{D(\mathbf{w}_j)} (\mathbf{x}_i - \mathbf{w}_j)^T (\mathbf{x}_i - \mathbf{w}_j) \\ &= \frac{\partial}{\partial \mathbf{w}_j} \frac{1}{2} \sum_{D(\mathbf{w}_j)} (\mathbf{x}_i^2 + \mathbf{w}_j^2 - 2 \mathbf{x}_i^T \mathbf{w}_j) = \sum_{D(\mathbf{w}_j)} (\mathbf{w}_j - \mathbf{x}_i) \end{aligned}$$

then, by imposing  $\frac{\partial}{\partial \mathbf{w}_j} J(D, \theta) = 0$  we obtain

$$\mathbf{w}_j = \frac{1}{|D(\mathbf{w}_j)|} \sum_{D(\mathbf{w}_j)} \mathbf{x}_i$$

# *k-means* (Generalized Lloyd's Algorithm – Vector quantization)

## Discussion of the *k-means* algorithm

- a) At each step of the algorithm  $J(D, \theta)$  cannot increase: only decrease or stay equal
- b) The algorithm is a variant of a *gradient descent*, in which at each step the *gradient descent* is performed on one subset of variables only
- c) It must reach a *fixed point*, where both gradients vanish
- d) But the only guarantee is that the algorithm reaches a local minimum  
(unless it gets stuck in a saddle point)

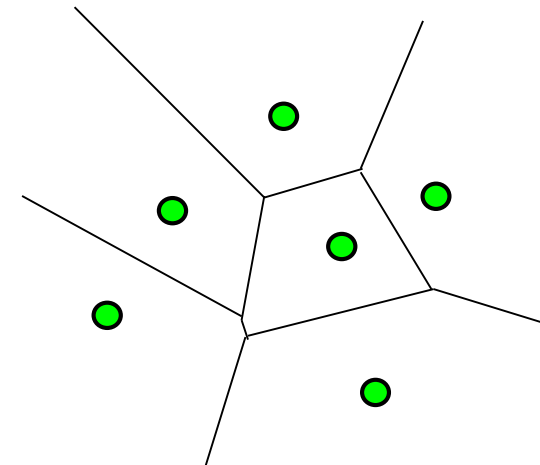
# *k-means* (Generalized Lloyd's Algorithm – Vector quantization)

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## **Voronoi cell:**

$$V(\mathbf{w}_j) := \{\mathbf{x} \in \mathbb{R}^d \mid \|\mathbf{x} - \mathbf{w}_j\| \leq \|\mathbf{x} - \mathbf{w}_l\|, \forall l \neq j\}$$

**Voronoi tessellation:** the complex of all Voronoi cells of  $\theta$



## **Algorithm** (rewritten):

- 1) Position the  $k$  prototypes at random
- 2) Assign each observation to its Voronoi cell

$$w(\mathbf{x}_i) := \mathbf{w}_j \mid \mathbf{x}_i \in V(\mathbf{w}_j)$$

- 3) Position each prototype at the *centroid* of the observations in its Voronoi cell

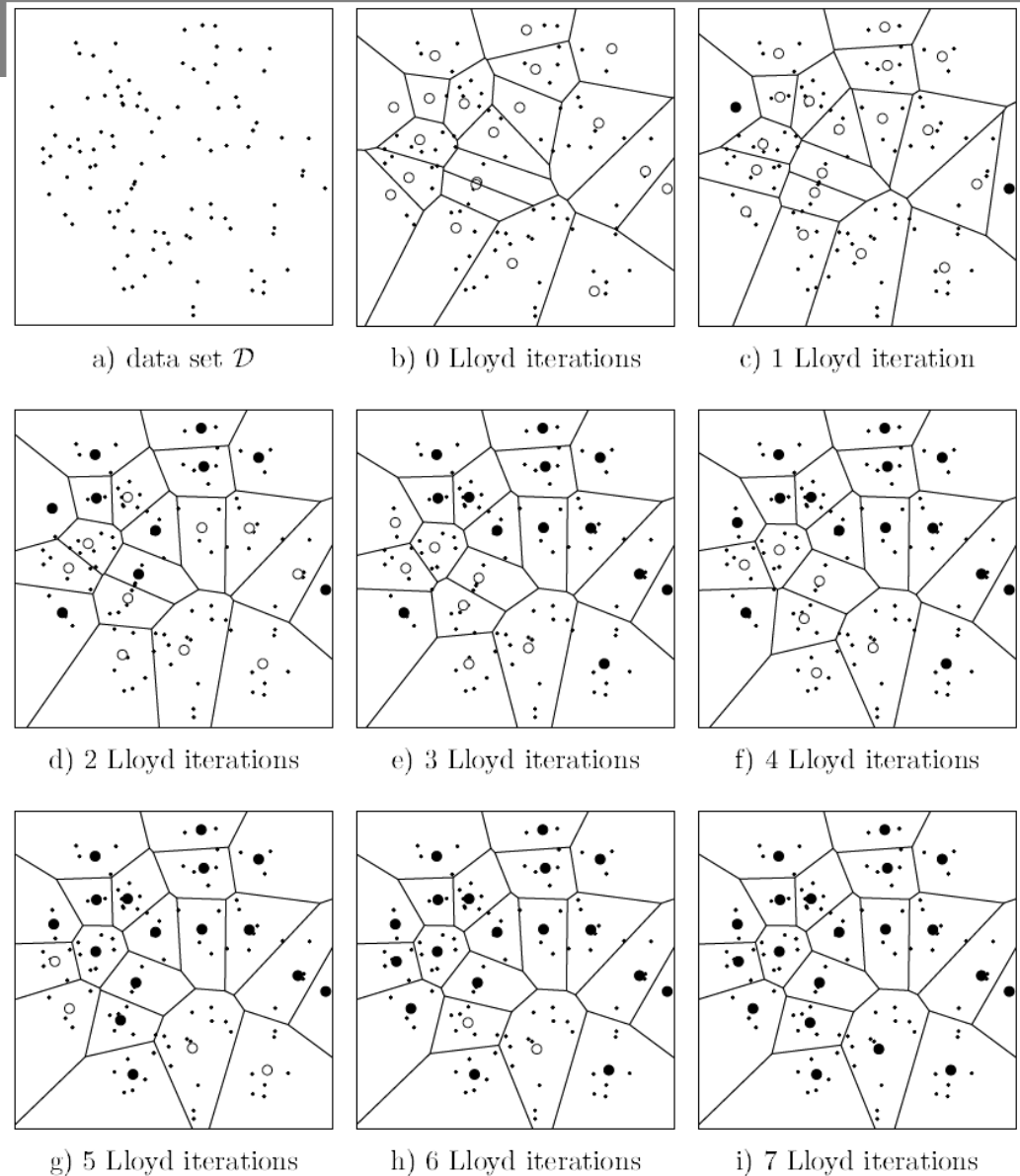
$$\mathbf{w}_j = \frac{1}{|\{\mathbf{x}_i \in V(\mathbf{w}_j)\}|} \sum_{\{\mathbf{x}_i \in V(\mathbf{w}_j)\}} \mathbf{x}_i$$

- 4) Unless no prototype was moved in step 3), go back to step 2)

# *k-means*

*An example run of the algorithm*

*The landmarks (empty circles) become black when they cease to move*





# Expected value of a random variable

(also *expectation*)

## Basic definition

$$\mathbb{E}_X[X] := \sum_{x \in \mathcal{X}} x P(X = x)$$

*More concise notation*

$$\mathbb{E}[X] := \sum_{x \in \mathcal{X}} x P(x)$$

## A linear operator

$$\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$$

$$\mathbb{E}[cX] = c\mathbb{E}[X]$$

*Continuous case*

$$\mathbb{E}[X] := \int_{x \in \mathcal{X}} x p(x) dx$$

## Conditional expectation

$$\mathbb{E}_X[X|Y = y] = \mathbb{E}[X|Y = y] := \sum_{x \in \mathcal{X}} x P(X = x|Y = y)$$

## Iterated expectation (*see Wikipedia*)

$$\mathbb{E}_X[X] = \mathbb{E}_Y[\mathbb{E}_X[X|Y]]$$

# Joint Expected Value

The **expected value** of a function  $f$  of a set of random variables  $\{X_i\}$  is

$$\mathbb{E}[f(\{X_i\})] := \sum_{\{X_i\}} f(\{X_i\}) P(\{X_i\})$$

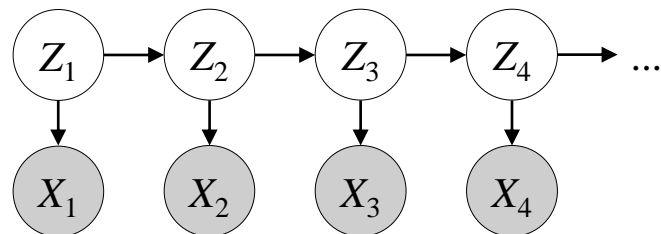
*the sum is over all possible combinations of values of the random variables*

(Unless specified otherwise, the  $\mathbb{E}$  operator acts over *all* the random variables enclosed)

*The extension to the continuous case is obvious*

# Incomplete observations

## Example: 'Hidden Markov' model



Terminology:

*hidden = latent = always unobserved*

*missing = unobserved (in a data set)*

Typically,  $Z_i$  nodes are *hidden*,  
i.e. *non-observables*

$$P(\{X_i\}, \{Z_j\}) = P(Z_1) P(X_1 | Z_1) \prod_{i=2}^n P(Z_i | Z_{i-1}) P(X_i | Z_i) \quad \text{Joint distribution}$$

## ■ Problem

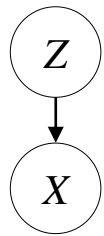
*MLE* of parameters  $\theta$  starting from *partial* observations of the  $\{X_i\}$  variables only

In other terms, this is the *MLE* of the *likelihood function*

$$L(\theta | D) = P(D | \theta) = \sum_{\{Z_j\}} P(D, \{Z_j\} | \theta)$$

*Note that the model (= the probability function) and the (partial) observations are known, the parameters and the values of some variables are hidden*

# Expectation Maximization: a preliminary example



**a** Maximum likelihood

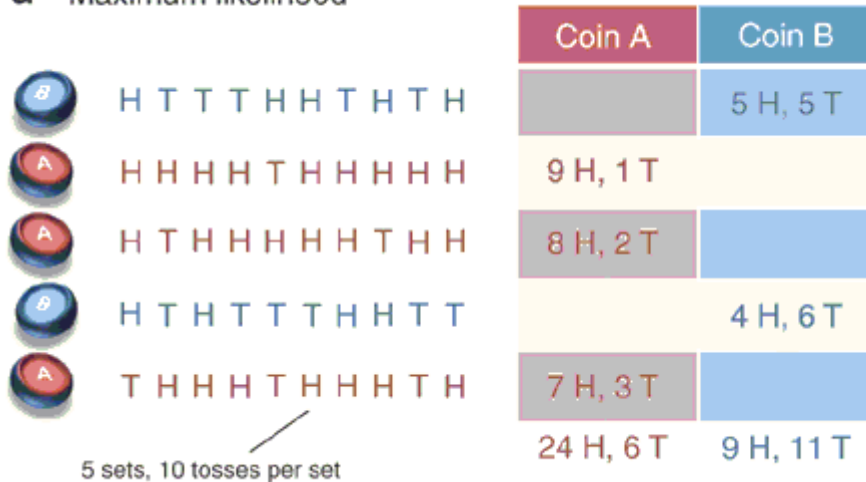


Figure from <http://www.nature.com/nbt/journal/v26/n8/full/nbt1406.html>

$$\hat{\theta}_A = \frac{24}{24 + 6} = 0.80$$

$$\hat{\theta}_B = \frac{9}{9 + 11} = 0.45$$

- An experiment with two coins

At each step, one coin is selected at random (*with equal probability*) and then tossed ten times

Random variables:  $X$  number of heads,  $Z$  selected coin (i.e A or B)

Parameters to be learnt:  $\theta = \{ \theta_A, \theta_B \}$  probabilities of landing on head of A and B, resp.

When the results are fully observable, by MLE:

$$\theta_A^* = \frac{N_{X=1, Z=A}}{N_{Z=A}} \qquad \theta_B^* = \frac{N_{X=1, Z=B}}{N_{Z=B}}$$

# Expectation Maximization: a preliminary example

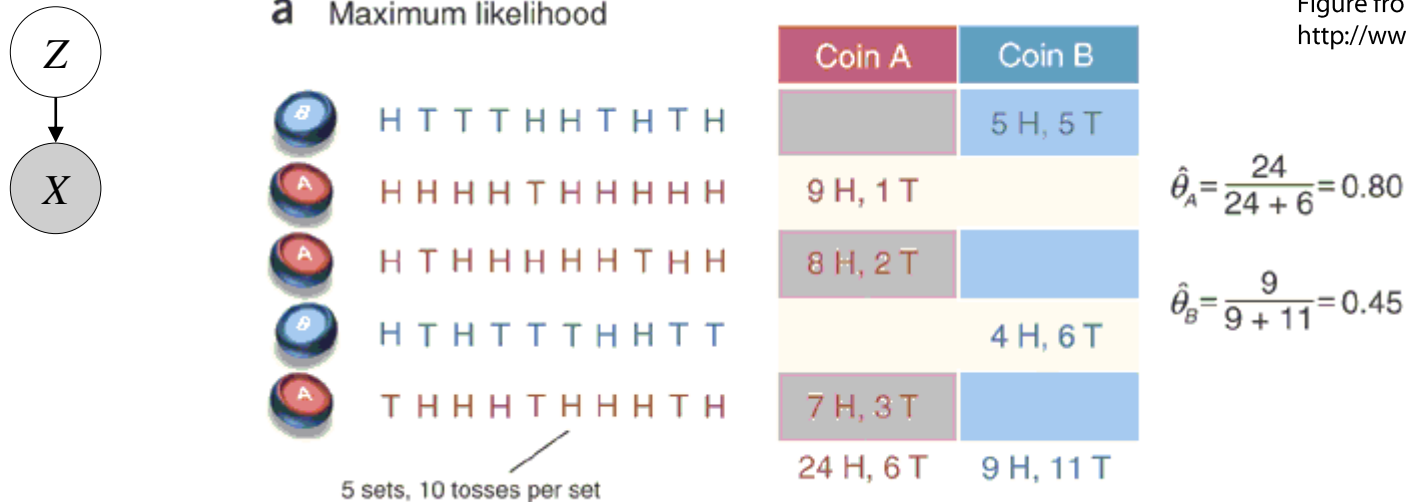


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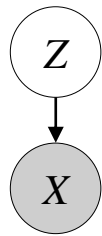
Random variables:  $X$  number of heads,  $Z$  selected coin (i.e A or B)

Parameters to be learnt:  $\theta = \{ \theta_A, \theta_B \}$  probabilities of landing on head of A and B, resp.

- What if  $Z$  is *hidden* (= *latent*, = *unobserved*)?

*The results of each sequence of coin tosses are known, but not the coin selected*

# Expectation Maximization: a preliminary example



**a** Maximum likelihood

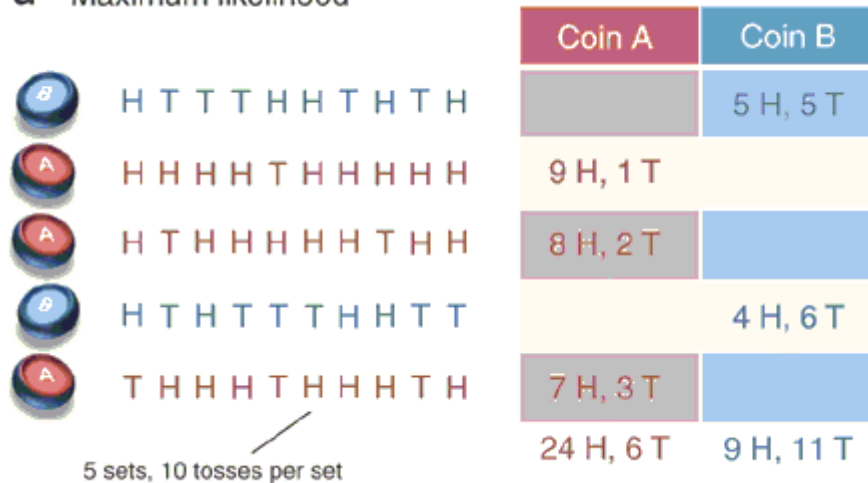


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- What if  $Z$  is *hidden* (= *latent*, = *unobserved*)?

*Likelihood*

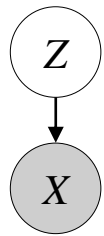
$$P(D | \theta) = P(\{x^{(i)}\} | \theta) = \sum_{\{Z^{(i)}\}} P(\{\langle x^{(i)}, Z^{(i)} \rangle\} | \theta)$$

*MLE*

$$\theta^* := \operatorname{argmax}_{\theta} \sum_{\{Z^{(i)}\}} P(\{\langle x^{(i)}, Z^{(i)} \rangle\} | \theta)$$

\* This optimization is intractable, in general

# Expectation Maximization: a preliminary example



**a** Maximum likelihood

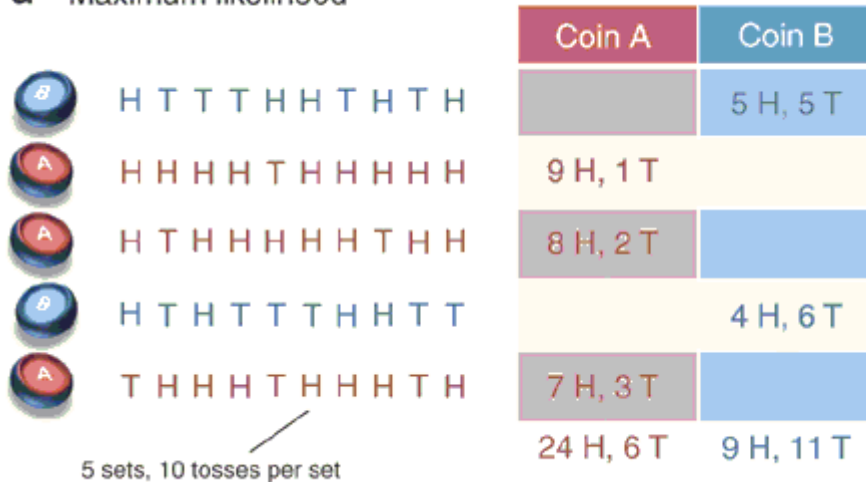


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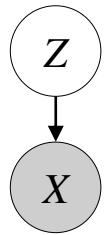
*Intuitive idea: use expected values for unobserved variables*

- Define an initial (random) guess  $\hat{\theta}^{(0)}$
- Create an intermediate function  $Q(\{\langle x^{(i)}, Z^{(i)} \rangle\} | \hat{\theta}^{(t)})$  based on  $\mathbb{E}_{Z^{(i)}} [X^{(i)} | \hat{\theta}^{(t)}]$
- Maximize

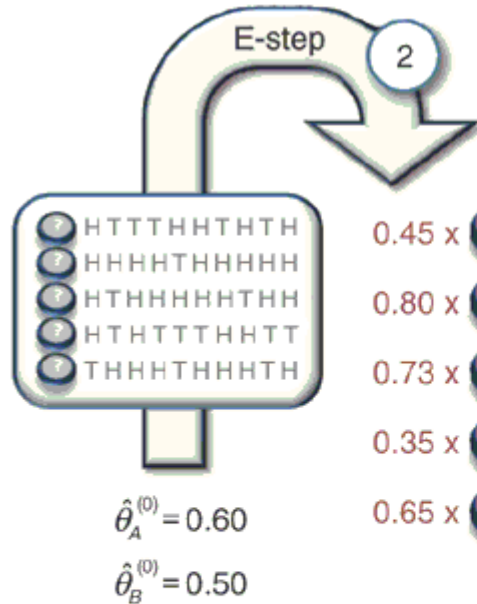
$$\hat{\theta}^{(t+1)} = \operatorname{argmax}_{\theta} \sum_i Q(\{\langle x^{(i)}, Z^{(i)} \rangle\} | \hat{\theta}^{(t)})$$

- Unless some convergence criterion has been met, go to step 2.

# Expectation Maximization: a preliminary example



	5 H, 5 T
9 H, 1 T	
8 H, 2 T	
	4 H, 6 T
7 H, 3 T	
24 H, 6 T	9 H, 11 T



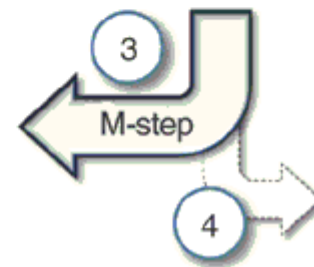
Coin A	Coin B
≈ 2.2 H, 2.2 T	≈ 2.8 H, 2.8 T
≈ 7.2 H, 0.8 T	≈ 1.8 H, 0.2 T
≈ 5.9 H, 1.5 T	≈ 2.1 H, 0.5 T
≈ 1.4 H, 2.1 T	≈ 2.6 H, 3.9 T
≈ 4.5 H, 1.9 T	≈ 2.5 H, 1.1 T
≈ 21.3 H, 8.6 T	≈ 11.7 H, 8.4 T

Initial random estimate of  $\hat{\theta}_A, \hat{\theta}_B$



$$\hat{\theta}_A^{(1)} \approx \frac{21.3}{21.3 + 8.6} \approx 0.71$$

$$\hat{\theta}_B^{(1)} \approx \frac{11.7}{11.7 + 8.4} \approx 0.58$$



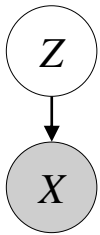
$$\hat{\theta}_A^{(10)} \approx 0.80$$

$$\hat{\theta}_B^{(10)} \approx 0.52$$

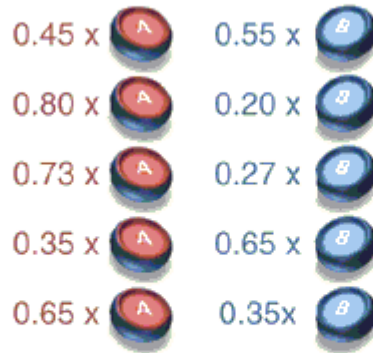
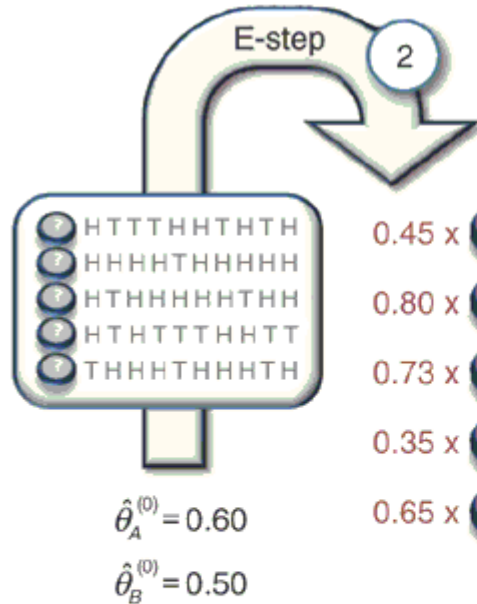
Converged?



# Expectation Maximization: a preliminary example



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9 H, 1 T	
8 H, 2 T	
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7 H, 3 T	
24 H, 6 T	9 H, 11 T

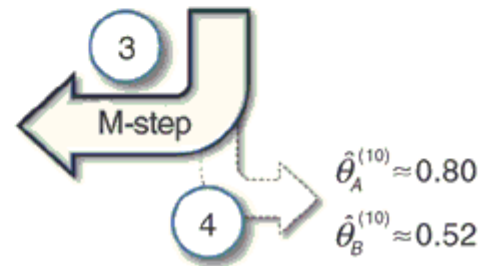


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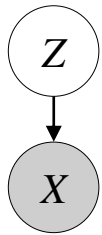
$$\hat{\theta}_B^{(1)} \approx \frac{11.7}{11.7 + 8.4} \approx 0.58$$



MLE given expected observations

Converged?

# Expectation Maximization: a preliminary example



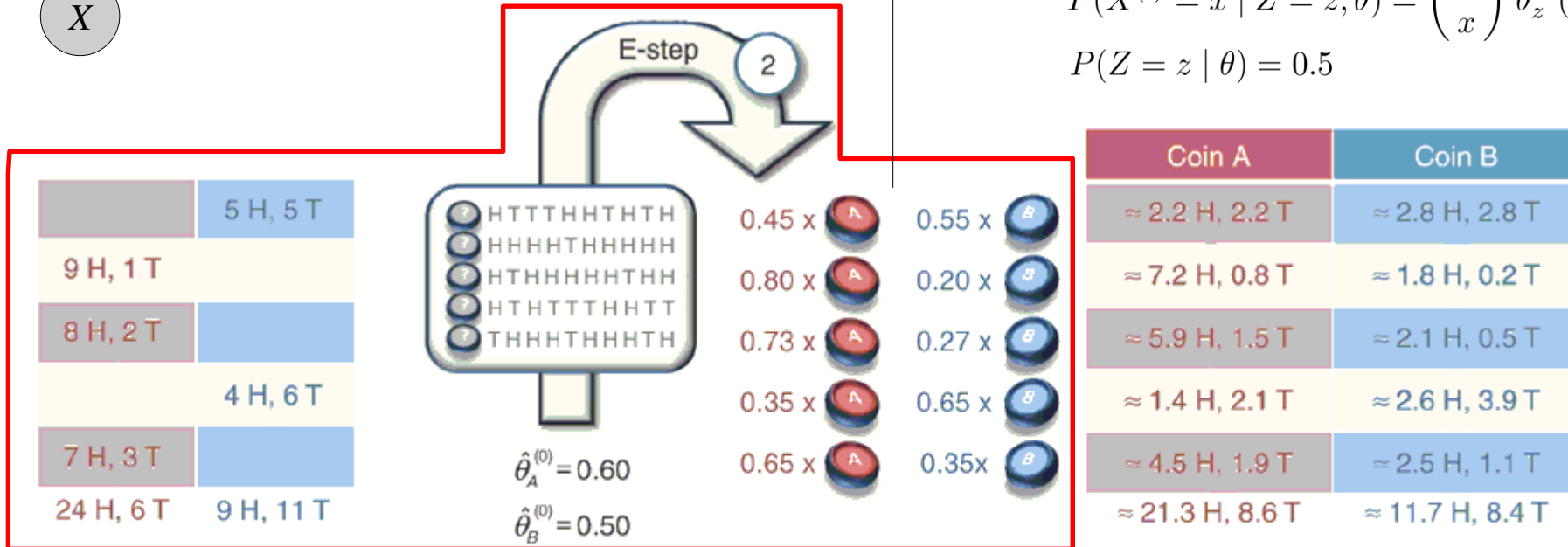
Compute the probability distribution of hidden observations

$$P(Z = z | X^{(i)} = x, \theta) = \frac{P(X^{(i)} = x | Z = z, \theta)P(Z = z | \theta)}{\sum_z P(X^{(i)} = x | Z = z, \theta)P(Z = z | \theta)}$$

where

$$P(X^{(i)} = x | Z = z, \theta) = \binom{10}{x} \theta_z^x (1 - \theta_z)^{10-x}$$

$$P(Z = z | \theta) = 0.5$$

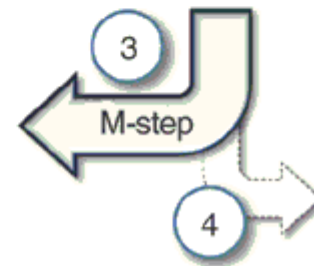


Initial random estimate of  $\hat{\theta}_A, \hat{\theta}_B$



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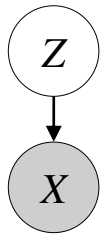


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Converged?

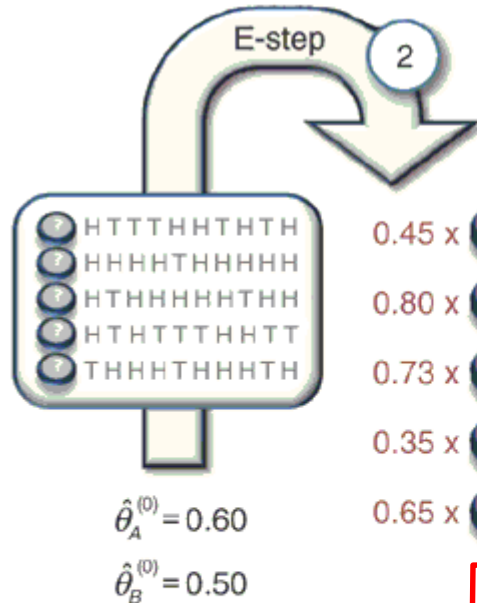
# Expectation Maximization: a preliminary example



Use 'expected observations' instead of actual observations to update ML estimations

$$\mathbb{E}_Z[x \mid X = x, \theta] = \sum_z x P(Z = z \mid X = x, \theta) = x$$

	5 H, 5 T
9 H, 1 T	
8 H, 2 T	
	4 H, 6 T
7 H, 3 T	
24 H, 6 T	9 H, 11 T



Coin A	Coin B
$\approx 2.2$ H, $2.2$ T	$\approx 2.8$ H, $2.8$ T
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$\approx 5.9$ H, $1.5$ T	$\approx 2.1$ H, $0.5$ T
$\approx 1.4$ H, $2.1$ T	$\approx 2.6$ H, $3.9$ T
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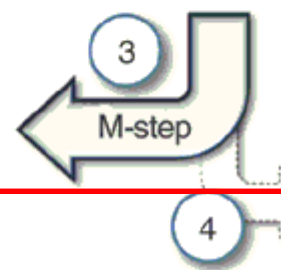
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MLE using 'expected observations'



$$\hat{\theta}_A^{(10)} \approx 0.80$$

$$\hat{\theta}_B^{(10)} \approx 0.52$$

Converged?

# An aside: Jensen's inequality

A relationship between probability and geometry

When  $f$  is convex function

$$f(E[\{X_i\}]) \leq E[f(\{X_i\})]$$

$f$  is **convex** when for any two points  $p_i$  and  $p_j$  the segment  $(p_i - p_j)$  is not below  $f$

That is, when

$$\lambda f(x_i) + (1-\lambda)f(x_j) \geq f(\lambda x_i + (1-\lambda)x_j) \quad \forall \lambda \in [0,1]$$

Furthermore,  $f$  is **strictly convex** when

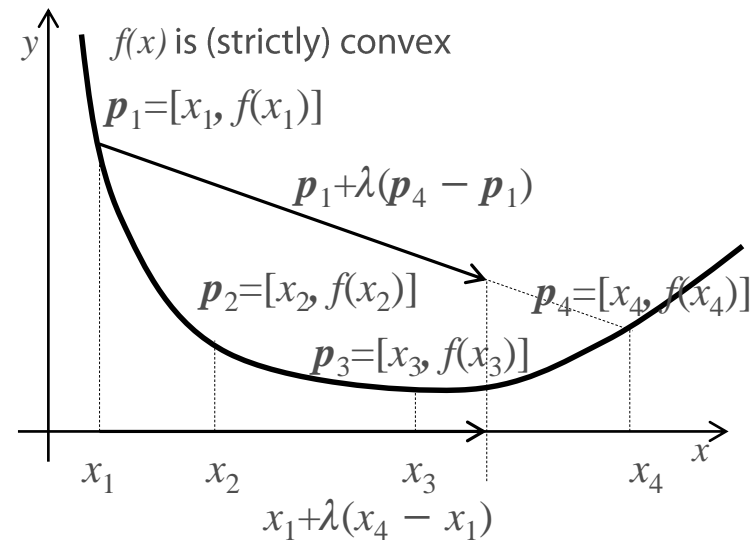
$$\lambda f(x_i) + (1-\lambda)f(x_j) > f(\lambda x_i + (1-\lambda)x_j) \quad \forall \lambda \in (0,1)$$

Corollary:

when  $f$  is *strictly convex*, if and only if all the variables in  $\{X_i\}$  are constant it is true that

$$f(E[\{X_i\}]) = E[f(\{X_i\})]$$

Dual results also hold for concave functions



# An aside: Jensen's inequality

A relationship between probability and geometry

When  $f$  is convex function

$$f(E[\{X_i\}]) \leq E[f(\{X_i\})]$$

To see this, consider

$$p = \lambda_1 p_1 + \lambda_2 p_2 + \lambda_3 p_3 + \lambda_4 p_4$$

i.e. a **linear combination** of  $p_i$  points

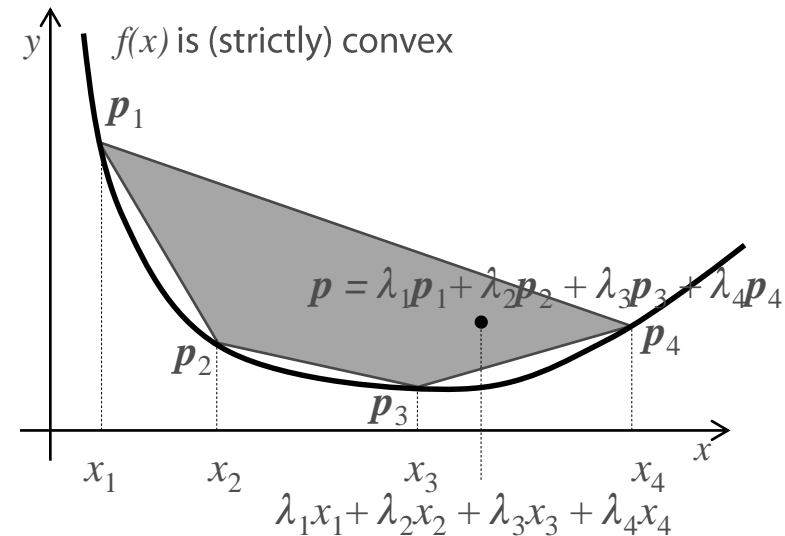
This is an **affine** combination if  $\sum \lambda_i = 1$   
and it is a **convex** combination if also  $\lambda_i \geq 0, \forall i$

When the  $\lambda_i$  define a probability, then  $p$  is a **convex combination** of  $p_i$  points

Any convex combination of  $p_i$  points lies inside their **convex hull** (see figure)  
and therefore above  $f$  :

$$\sum_i \lambda_i f(x_i) \geq f(\sum_i \lambda_i x_i)$$

*Corollary: the only way to make the convex hull be on  $f$  is to shrink it to a single point (i.e. the Jensen's corollary)*



# Incomplete observations

*Likelihood function with hidden random variables*

$$L(\theta | D) = P(D | \theta) = \prod_m P(D_m | \theta)$$

$$\lambda(\theta | D) = \sum_m \log P(D_m | \theta) = \sum_m \log \sum_{\{Z_i\}} P(D_m, \{Z_i\} | \theta)$$

*Arbitrary probability distributions*

$$= \sum_m \log \sum_{\{Z_i\}} Q_m(\{Z_i\}) \frac{P(D_m, \{Z_i\} | \theta)}{Q_m(\{Z_i\})}$$

*Jensen's inequality: log is concave*

$$= \sum_m \log E_{Q_m(\{Z_i\})} \left[ \frac{P(D_m, \{Z_i\} | \theta)}{Q_m(\{Z_i\})} \right] \geq \sum_m E_{Q_m(\{Z_i\})} \left[ \log \frac{P(D_m, \{Z_i\} | \theta)}{Q_m(\{Z_i\})} \right]$$
$$= \sum_m \sum_{\{Z_i\}} Q_m(\{Z_i\}) \log \frac{P(D_m, \{Z_i\} | \theta)}{Q_m(\{Z_i\})}$$

# Expectation–Maximization (EM) Algorithm

Alternate optimization (coordinate ascent)

Log-likelihood function:

$$\lambda(\theta | D) \geq \sum_m \sum_{\{Z_i\}} Q_m(\{Z_i\}) \log \frac{P(D_m, \{Z_i\} | \theta)}{Q_m(\{Z_i\})}$$

This inequality becomes equality when this term is constant (see Jensen's corollary)

Keep  $\theta$  constant, define  $Q_m(\{Z_i\})$  so that the right side of the inequality is maximized

$$Q_m(\{Z_i\}) := \frac{P(D_m, \{Z_i\} | \theta)}{\sum_{\{Z_i\}} P(D_m, \{Z_i\} | \theta)} = \frac{P(D_m, \{Z_i\} | \theta)}{P(D_m | \theta)} = P(\{Z_i\} | D_m, \theta) =: p_{\{Z_i\}}^{(m)}$$

These numbers can be computed from the graphical model (i.e. as an inference step)

Then maximize the log-likelihood while keeping  $Q_m(\{Z_i\})$  constant

$$\begin{aligned} \theta^* &= \arg \max_{\theta} \sum_m \sum_{\{Z_i\}} p_{\{Z_i\}}^{(m)} \log \frac{P(D_m, \{Z_i\} | \theta)}{p_{\{Z_i\}}^{(m)}} \\ &= \arg \max_{\theta} \sum_m \left( \sum_{\{Z_i\}} p_{\{Z_i\}}^{(m)} \log P(D_m, \{Z_i\} | \theta) - \sum_{\{Z_i\}} p_{\{Z_i\}}^{(m)} \log p_{\{Z_i\}}^{(m)} \right) \\ &= \arg \max_{\theta} \sum_m \sum_{\{Z_i\}} p_{\{Z_i\}}^{(m)} \log P(D_m, \{Z_i\} | \theta) \end{aligned}$$

*This is also called the entropy of  $Q_m(\{Z_i\})$  (i.e. a constant measure of the distribution)*

# Expectation– Maximization (EM) Algorithm

*Alternate optimization (coordinate ascent)*

Log-likelihood function and its estimator:

$$\lambda(\theta | D) \geq \sum_m \sum_{\{Z_i\}} Q_m(\{Z_i\}) \log \frac{P(D_m, \{Z_i\} | \theta)}{Q_m(\{Z_i\})}$$

**Algorithm:**

- 1) Assign the  $\theta$  at random
- 2) (*E-step*) Compute the probabilities

$$p_{\{Z_i\}}^{(m)} = Q_m(\{Z_i\}) = P(\{Z_i\} | D_m, \theta)$$

- 3) (*M-step*) Compute a new estimate of  $\theta$

$$\theta^* = \arg \max_{\theta} \sum_m \sum_{\{Z_i\}} p_{\{Z_i\}}^{(m)} \log P(D_m, \{Z_i\} | \theta)$$

- 4) Go back to step 2) until some convergence criterion is met

*The algorithm converges to a local maximum of the log-likelihood*

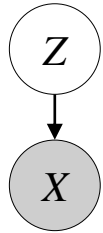
*The effectiveness of algorithm depends on the form of the distribution (see step3):*

$$P(D_m, \{Z_i\} | \theta)$$

*In particular, when this distribution is exponential... (e.g. Gaussian – see next slide)*



# EM Algorithm: mixture of Gaussians



## Model:

The hidden variable  $Z$  has  $k$  possible values, the observable variable  $X$  is a point in  $\mathbb{R}^d$

$$P(Z = k) := \phi_k$$

← Multivariate normal distribution

$$P(X = x | Z = k) = N(x; \mu_k, \Sigma_k) := (2\pi)^{-d/2} (\det \Sigma_k)^{-1/2} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)\right)$$

i.e. the condition probabilities are normal distributions

The observations are a set  $D = \{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}$  of points in  $\mathbb{R}^d$

## Algorithm:

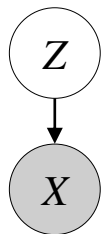
- 1) For each value  $k$ , assign  $\phi_k$ ,  $\mu_k$  and  $\Sigma_k$  at random
- 2) (E-step) For all the  $x_i$  in  $D$  compute the probabilities  
 $p_k^{(m)} = P(Z = k | x^{(m)}, \phi_k, \mu_k, \Sigma_k) = \phi_k \cdot N(x^{(m)}; \mu_k, \Sigma_k)$
- 3) (M-step) Compute the new estimates for the parameters

$$\phi_k = \frac{1}{n} \sum_m p_k^{(m)}$$

$$\mu_k = \frac{\sum_m p_k^{(m)} x^{(m)}}{\sum_m p_k^{(m)}} \quad \Sigma_k = \frac{\sum_m p_k^{(m)} (x - \mu_k)(x - \mu_k)^T}{\sum_m p_k^{(m)}}$$

- 4) Go back to step 2) until some convergence criterion is met

# EM Algorithm: mixture of Gaussians



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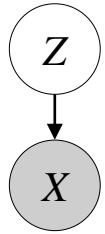
i.e. the condition probabilities are normal distributions

The observations are a set  $D = \{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}$  of points in  $\mathbb{R}^d$

## Proof (of the M-step):

$$\begin{aligned} \sum_m \sum_k p_k^{(m)} \log P(X^{(m)}, Z = k | \phi_k, \mu_k, \Sigma_k) &= \sum_m \sum_k p_k^{(m)} \log P(X^{(m)} | Z = k, \mu_k, \Sigma_k) P(Z = k | \phi_k) \\ &= \sum_m \sum_k p_k^{(m)} \left( \log(2\pi^{-d/2} (\det \Sigma_k)^{-1/2}) + \left( -\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) \right) + \log \phi_k \right) \end{aligned}$$

# EM Algorithm: mixture of Gaussians



## Model:

The hidden variable  $Z$  has  $k$  possible values, the variable  $X$  is a point in  $\mathbb{R}^d$

$$P(Z = k) := \phi_k$$

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## Proof (of the M-step):

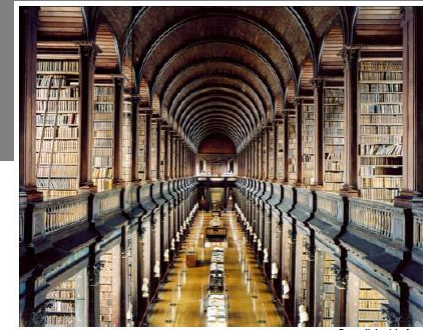
$$\begin{aligned} & \frac{\partial}{\partial \mu_j} \sum_m \sum_k p_k^{(m)} \left( \log\left((2\pi)^{-d/2} (\det \Sigma_k)^{-1/2}\right) + \left(-\frac{1}{2}(x^{(m)} - \mu_k)^T \Sigma_k^{-1}(x^{(m)} - \mu_k)\right) + \log \phi_k \right) \\ &= \frac{\partial}{\partial \mu_j} \sum_m \sum_k p_k^{(m)} \left( -\frac{1}{2}(x^{(m)} - \mu_k)^T \Sigma_k^{-1}(x^{(m)} - \mu_k) \right) \\ &= \frac{\partial}{\partial \mu_j} \sum_m \sum_k p_k^{(m)} \left( -\frac{1}{2}(x^{(m)T} \Sigma_k^{-1} x^{(m)} + \mu_k^T \Sigma_k^{-1} \mu_k - 2x^{(m)T} \Sigma_k^{-1} \mu_k) \right) = \sum_m p_j^{(m)} (x^T \Sigma_j^{-1} - \mu_j^T \Sigma_j^{-1}) \end{aligned}$$

By imposing:  $\sum_m p_j^{(m)} (x^T \Sigma_j^{-1} - \mu_j^T \Sigma_j^{-1}) = 0$

$$\mu_j = \frac{\sum_m p_j^{(m)} x^{(m)}}{\sum_m p_j^{(m)}}$$

See the link in the web page for the derivations of other parameters ...

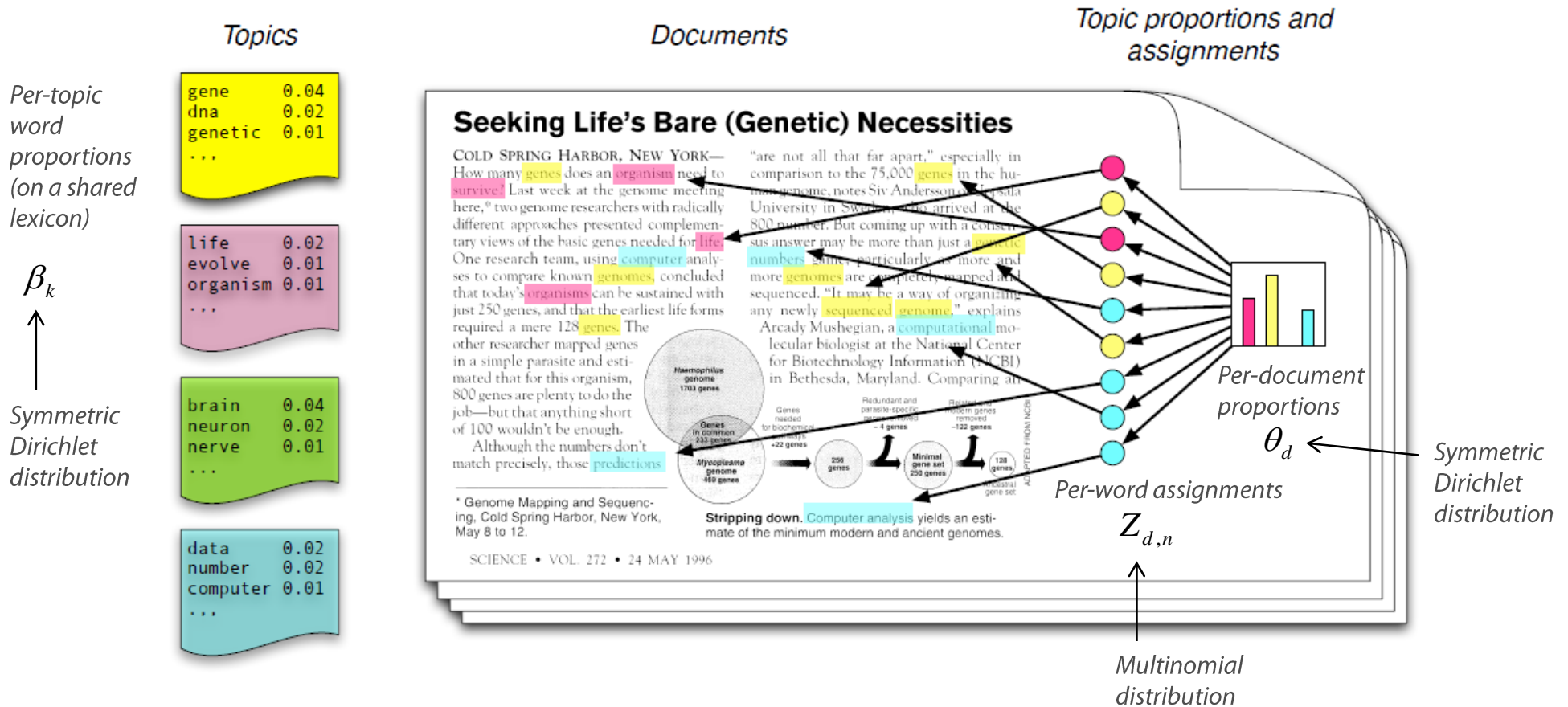
# Topic modeling



Candida Hofer

## Topic modeling

Classifying a (large) corpus of digital documents relying on word counting only



# Multinomial distribution

- Bernoulli

*Head or Tail?*

$$P(X = 1) = \theta, \quad P(X = 0) = 1 - \theta$$

- Binomial

*n heads out of N coin tosses*

$$P(X = n) = \binom{N}{n} \theta^n (1 - \theta)^{(N-n)}$$

- Categorical

*The result of throwing a dice with k faces*

$$P(X = 1) = \theta_1, \quad P(X = k) = \theta_k, \quad \sum_{i=1}^k \theta_i = 1$$

- Multinomial

Obtaining an outcome combination  $x_1, \dots, x_k$  in  $N$  throws of a  $k$ -faced dice, with  $\sum_{i=1}^k x_i = N$

$$P(X_1 = x_1, \dots, X_k = x_k) = \frac{N!}{x_1! \dots x_k!} \prod_{i=1}^k \theta_i^{x_i}$$

# Dirichlet distribution

## ■ Beta distribution

What do you think about a coin after obtaining  $(\alpha_1 - 1)$  heads and  $(\alpha_2 - 1)$  tails?

$$\text{Beta}(x_1, x_2; \alpha_1, \alpha_2) := \frac{x_1^{\alpha_1-1} \cdot x_2^{\alpha_2-1}}{\text{B}(\alpha_1, \alpha_2)}, \quad x_1 + x_2 = 1$$

This is just a re-writing of the 'standard' formula:

$$\text{Beta}(x; \alpha, \beta) := \frac{x^{\alpha-1} (1-x)^{\beta-1}}{\text{B}(\alpha, \beta)}$$

## ■ Dirichlet distribution

What do you think about a  $k$ -faced dice after obtaining  $(\alpha_1 - 1)$ ,  $(\alpha_2 - 1)$  ...  $(\alpha_k - 1)$  outcomes?

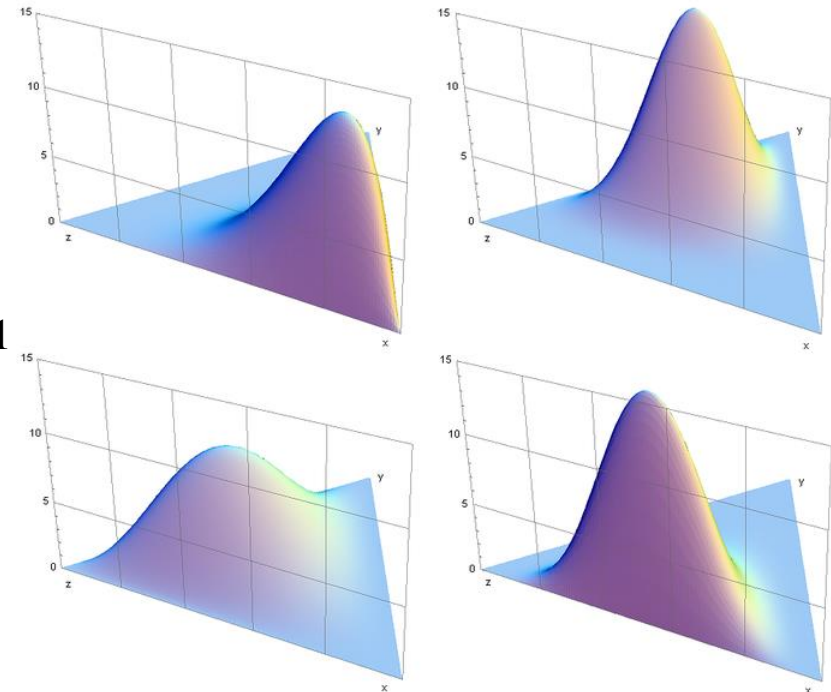
$$\text{D}(x_1, \dots, x_k; \alpha_1, \dots, \alpha_k) := \frac{\prod_{i=1}^k x_i^{\alpha_i-1}}{\text{B}(\alpha_1, \dots, \alpha_k)}, \quad \sum_{i=1}^k x_i = 1$$

where

$$\text{B}(\alpha_1, \dots, \alpha_k) := \frac{\prod_{i=1}^k \Gamma(\alpha_i)}{\Gamma\left(\sum_{i=1}^k \alpha_i\right)}$$

is the *multivariate Beta function*.

The Dirichlet distribution is the **conjugate prior** of the Multinomial distribution



examples of Dirichlet distributions, for  $k = 3$   
(from Wikipedia)

# Dirichlet distribution

- Symmetric Beta distribution

*i.e. when  $\alpha = \beta$*

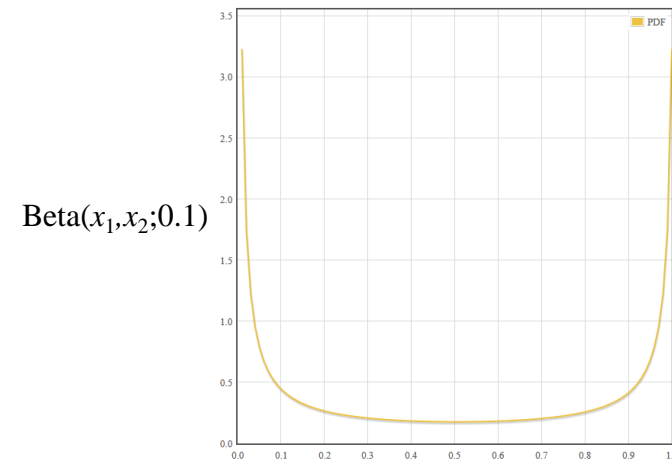
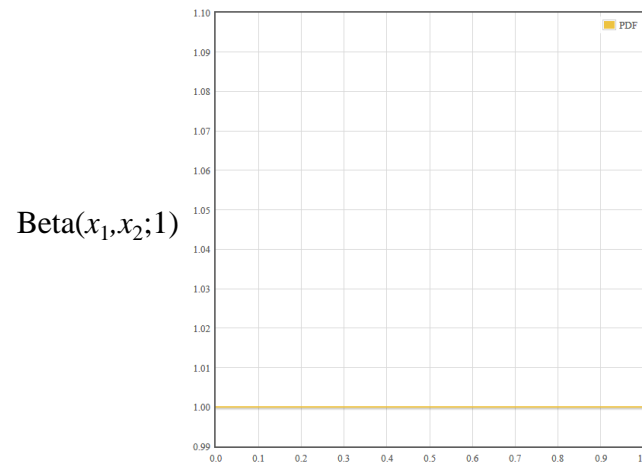
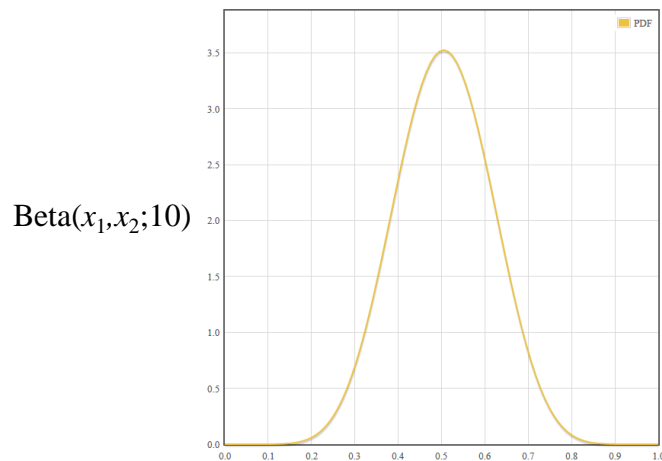
$$\text{Beta}(x_1, x_2; \alpha) := \frac{x_1^{\alpha-1} \cdot x_2^{\alpha-1}}{B(\alpha, \alpha)}, \quad x_1 + x_2 = 1$$

- Symmetric Dirichlet distribution

*i.e. when  $\alpha_1 = \alpha_2 = \dots = \alpha_k$*

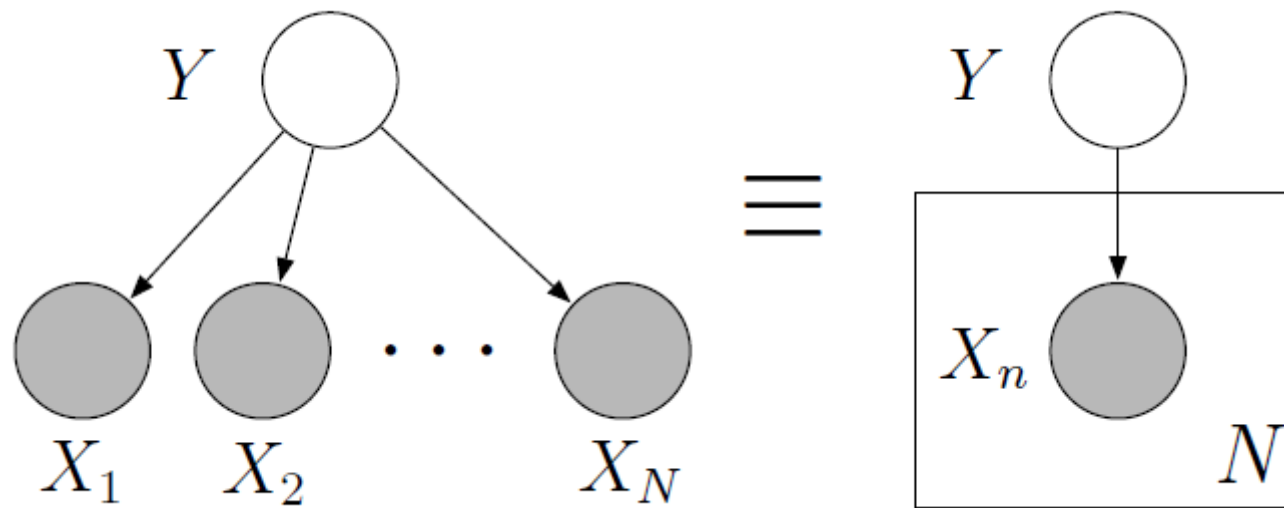
$$D(x_1, \dots, x_k; \alpha) := \frac{\prod_{i=1}^k x_i^{\alpha-1}}{B(\alpha, \dots, \alpha)}, \quad \sum_{i=1}^k x_i = 1$$

*Note: in both distributions, the parameters can be  $< 1$   
(this is true of the non-symmetric versions as well)*



# An aside: plate notation

A shorthand notation for graphical models



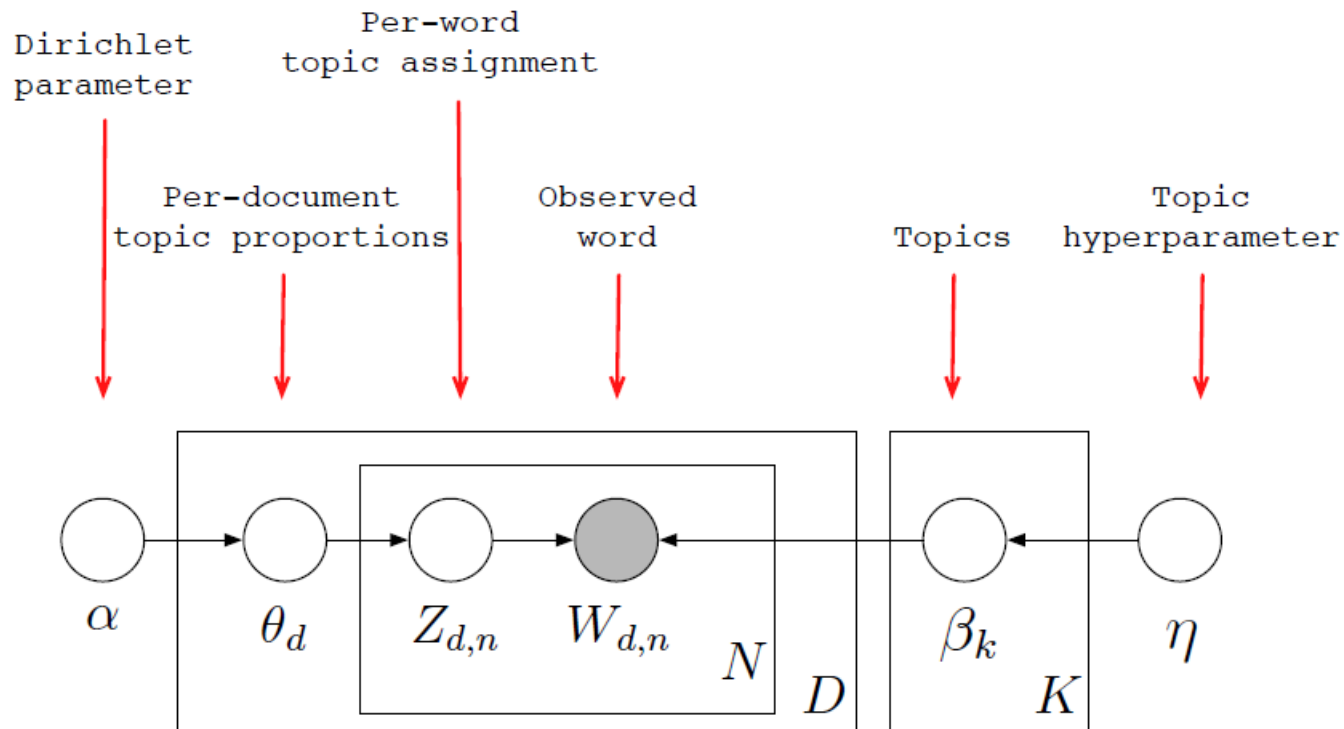


# An example: Probabilistic Topic Models (Blei & Lafferty, 2009)

Classifying a corpus of documents with  $k$  (unknown) topics  
when the only observable variables is the multiple occurrence of words

A *mixture model*:

*each document belongs to multiple topics, with different probabilities*

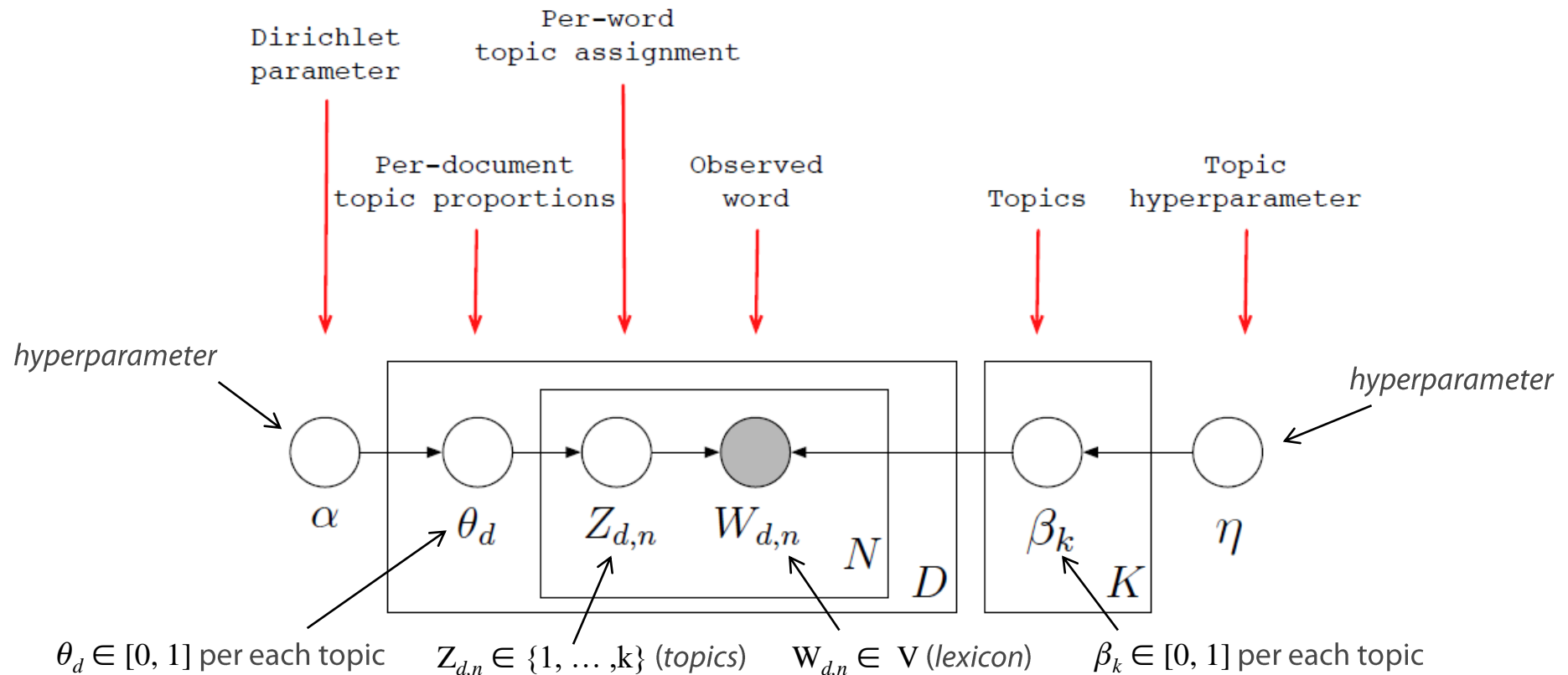


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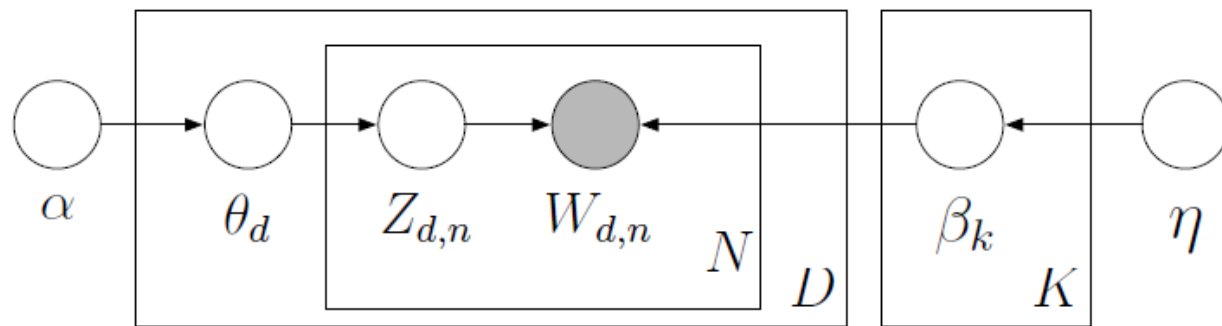


# An example: Probabilistic Topic Models (Blei & Lafferty, 2009)

Classifying a corpus of documents as *mixtures* of  $K$  (unknown) topics when the only observable variables is the multiple occurrence of words

*A three-level, mixture model:*

*each document belongs to multiple topics, with different probabilities*



$$\prod_{i=1}^K p(\beta_i | \eta) \prod_{d=1}^D p(\theta_d | \alpha) \left( \prod_{n=1}^N p(z_{d,n} | \theta_d) p(w_{d,n} | \beta_{1:K}, z_{d,n}) \right)$$

↑
↑
↑
↑

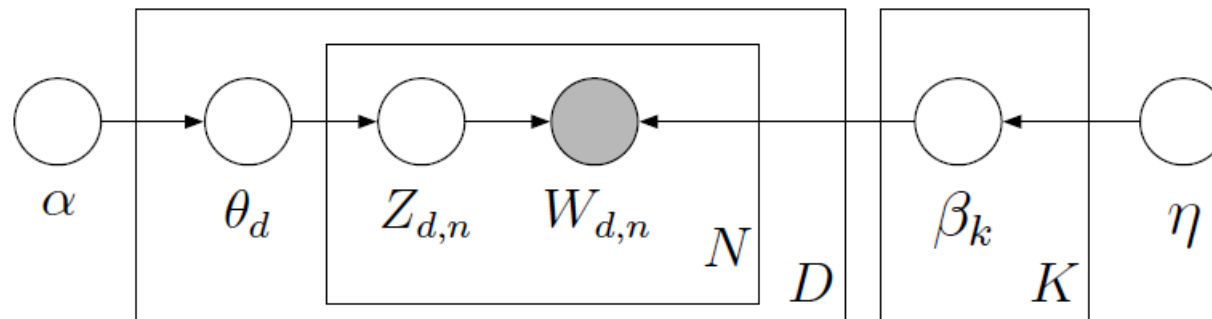
*Symmetric Dirichlet distributions*
*Multinomial distributions*

# Latent Dirichlet Allocation (LDA)

Classifying a corpus of documents as *mixtures* of  $K$  (unknown) topics when the only observable variables is the multiple occurrence of words

*A three-level, mixture model:*

*each document belongs to multiple topics, with different probabilities*



A generative procedure:

- 1 Draw each topic  $\beta_i \sim \text{Dir}(\eta)$ , for  $i \in \{1, \dots, K\}$ .
- 2 For each document:
  - 1 Draw topic proportions  $\theta_d \sim \text{Dir}(\alpha)$ .
  - 2 For each word:
    - 1 Draw  $Z_{d,n} \sim \text{Mult}(\theta_d)$ .
    - 2 Draw  $W_{d,n} \sim \text{Mult}(\beta_{Z_{d,n}})$ .

# LDA: which results?

Identifying topics:  
relative frequencies  
of words that define a class

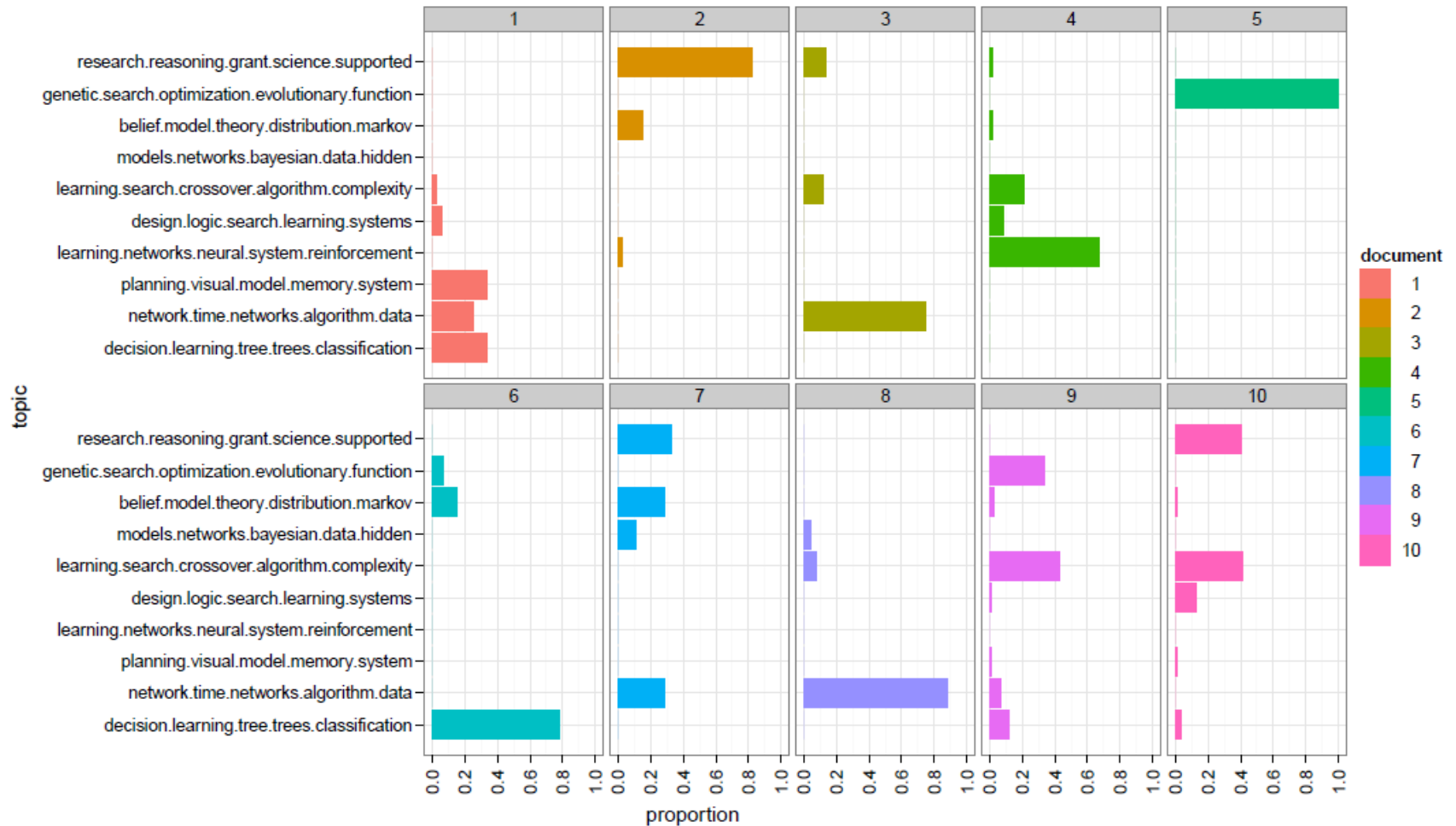
*Each box represents a topic  
The size of words in a box  
represents its relative proportion*



# LDA: which results?

Classifying documents: *relative topic assignment proportions*

*Each topic is represented by a list of most relevant words*



# LDA in practice

*There exist multiple methods*

## *Mean-Field Variational Inference (Blei et al. 2003)*

*(not discussed here – see links to the literature)*

*(It is a sort of generalization of the EM algorithm)*

*Many software implementations around: e.g. Apache Mahout*

## *Real-world examples*

*The OCR'ed collection of Science from 1990-2000 [2009]*

- *17K documents*
- *11M words*
- *20K unique terms (stop words and rare words removed)*

*Model: 100 Topics*

*The New York Times online recommender system [2015]*

*See <http://open.blogs.nytimes.com/2015/08/11/building-the-next-new-york-times-recommendation-engine/>*