ÉCOLE D'INGÉNIEURS EN INFORMATIQUE

Bayesian Machine Learning

November 2021 - François HU
https://curiousml.github.io/

Outline

1 **Bayesian statistics**

2 **Latent variable models**

3 **Variational Inference**
- Variational Inference for probabilistic models
- Introduction to NLP
- Application on textual data with LDA

4 **Markov Chain Monte Carlo**

5 **Extensions and oral presentations**

1 Variational Inference for probabilistic models

1. Variational Inference for probabilistic models

Reminder

Posterior distribution

Fixed by **model**

Fixed by **us**

Likelihood **Prior**

$$P(Z|X) = \frac{P(X,Z)}{P(X)} = \frac{P(X|Z) \times P(Z)}{P(X)}$$

Posterior

Evidence

Fixed by **data**

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Methods we have seen so far

- **Analytical inference.** Given $P(X|Z)$**,** we infer $P_X(Z) := P(Z|X)$ by
  - **Conjugate priors** : *easy* with a good matching prior
  - **Optimization** by EM algorithm : *tricky*,

    needs the computation of $\mathbb{E}_T\left[\log P(X,T|\theta)\right]$ with $Z = \{T, \theta\}$

1. Variational Inference for probabilistic models

Approximate inference

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In this lecture and (spoiler alert) in the next lecture

- **Approximate inference.** Approximate $P_X(Z) \approx \hat{P}_X(Z)$
  - **Deterministic approach** : Variational Inference
  - **Stochastic approach** : Markov Chain Monte Carlo

1. Variational Inference for probabilistic models

Variational Inference : Definition

Posterior distribution

Fixed by **model**

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$$\underbrace{P(Z|X)}_{\text{Posterior}} = \frac{P(X,Z)}{P(X)} = \frac{\overbrace{P(X|Z)}^{\text{Likelihood}} \times \overbrace{P(Z)}^{\text{Prior}}}{\underbrace{P(X)}_{\text{Evidence}}}$$

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(i) Select a family of distributions $\mathcal{Q}$

(ii) Find the « **best** » approximation $\hat{P}_X \in \mathcal{Q}$: « $P_X(Z) \approx \hat{P}_X(Z)$ »

1. Variational Inference for probabilistic models

Variational Inference : KL-divergence

Posterior distribution

Fixed by **model** — Likelihood

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Evidence — Fixed by **data**

Kullback-Leibler (KL) divergence

Consider P and Q two distributions

we want to compare the « differences » / divergence.

Ex. of measure : $D_{KL}(Q||P) = \int_{z \in Supp(Z)} Q(z) \cdot \log\left(\frac{Q(z)}{P(z)}\right) dz$

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Variational Inference : Mean Field Approximation

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Mean Field Approximation

(i) we choose $\mathcal{Q} = \left\{ Q = (Q_1, \ldots, Q_d) : Q(Z) = \prod_{i=1,\ldots,d} Q_i(Z_i) \right\}$

instead of $Q(Z_1, \ldots, Z_n) = \prod_{i=1,\ldots,n} Q(Z_i | pa(Z_i))$

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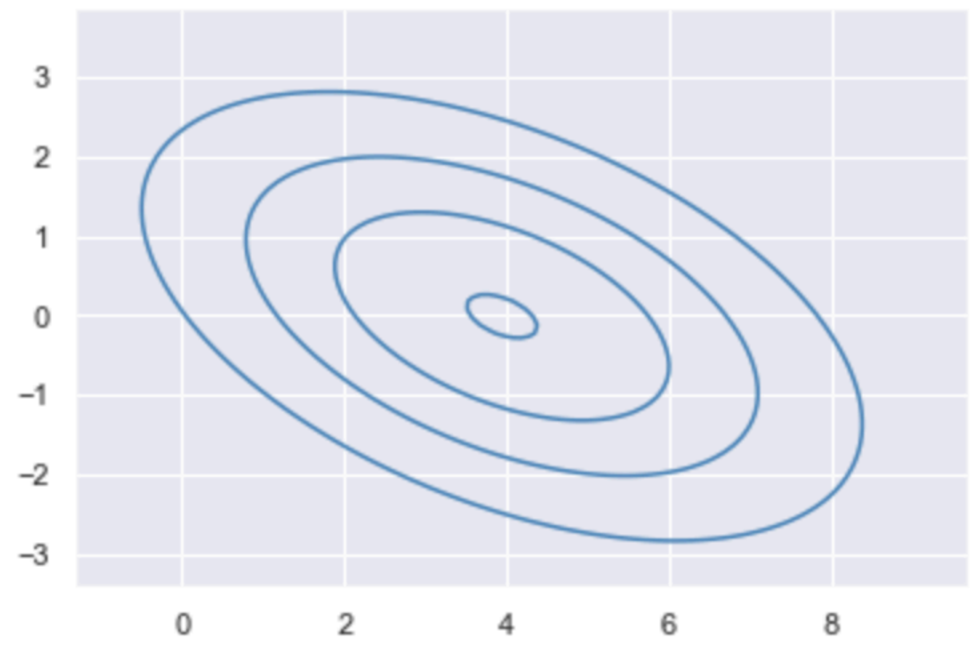
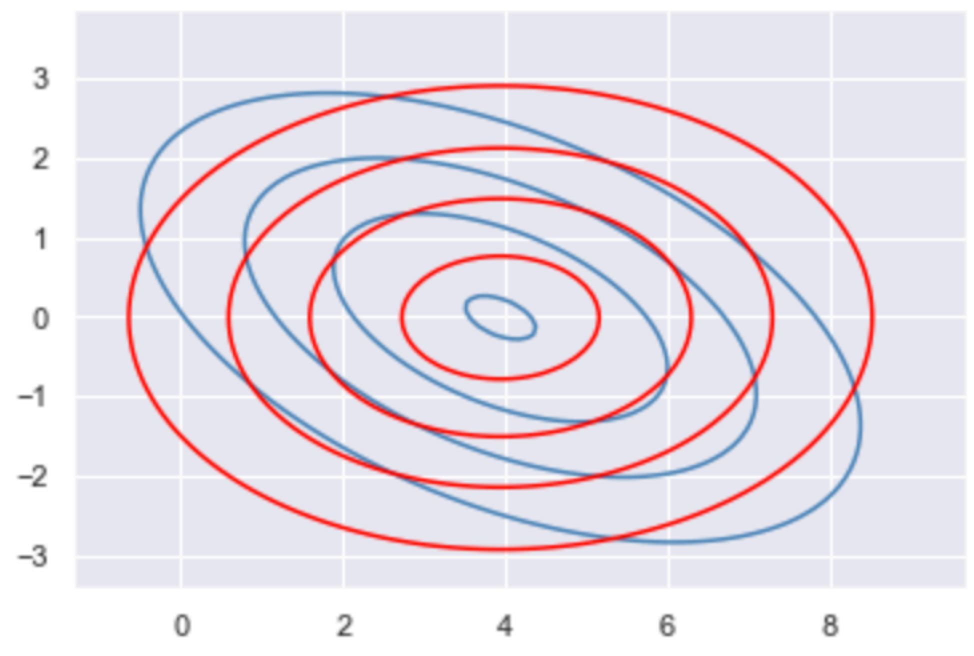
Example : Normal distribution

$P(z) = P(z_1, z_2) = \mathcal{N}_2(z | \mu, \Sigma)$



Mean Field

$P(z_1, z_2) \approx Q(z_1, z_2) = Q_1(z_1) \times Q_2(z_2)$ with $Q_i(z_i) = \mathcal{N}(z_i | \mu_i, \sigma_i^2)$



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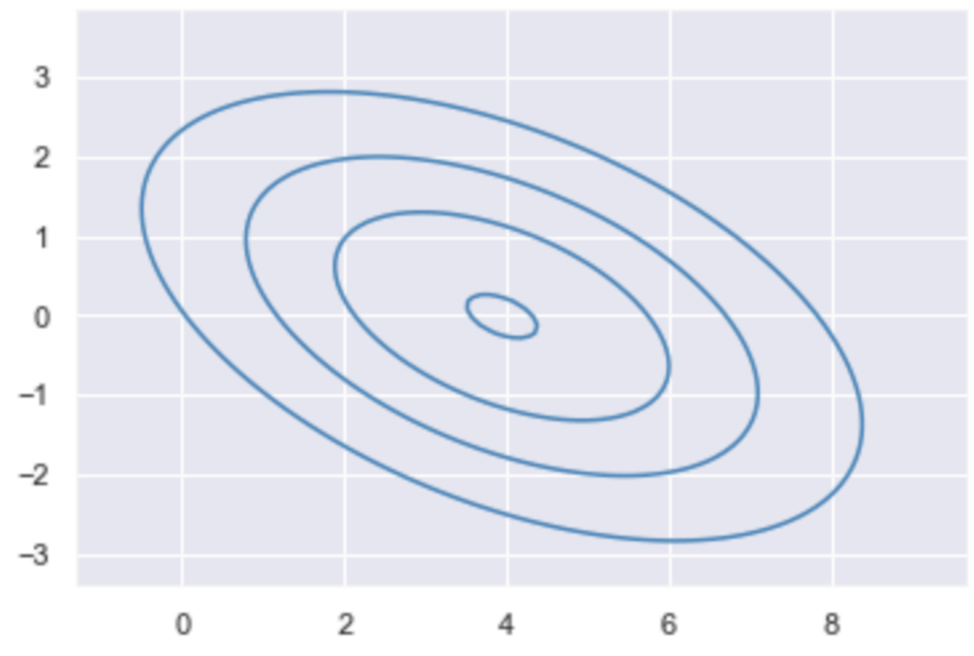

Mean Field $\longrightarrow$

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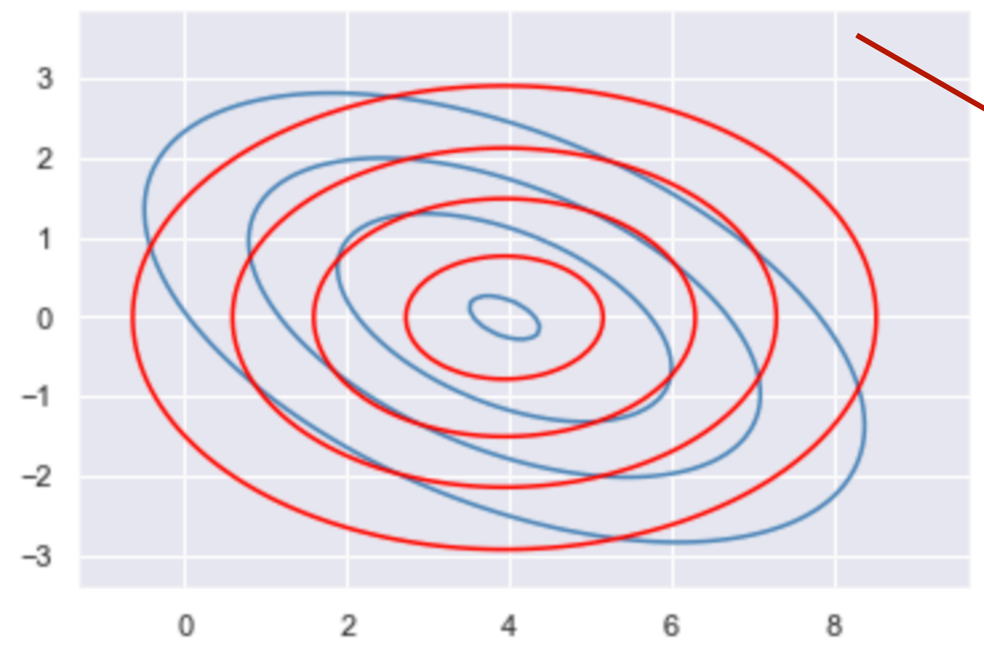

$\mathcal{N}_2\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}\right)$

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Optimization algorithm : coordinate descent

$$\hat{P} = \arg \min_{(Q_1, \dots, Q_d) \in \mathcal{Q}} D_{KL}(Q_1 \times Q_2 \times Q_3 \times \cdots \times Q_d \,||\, P)$$

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&\cdots\\
\hat{P}_d &= \arg\min_{Q_d} D_{KL}(\hat{P}_1 \times \hat{P}_2 \times \ldots \times Q_d \,||\, P)
\end{aligned}\right\}$$

Repeat until convergence with

$Q_1, \cdots, Q_d$
=
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Optimal solution in Mean Field

$$\log \hat{P}_i(Z_i) = \mathbb{E}_{Z_{-i}}\left[\log P(X,Z)\right] + \text{const}$$

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$$\mathbb{E}\left[\log P(X,Z)\right] - \mathbb{E}\left[\log P(Z)\right] \approx 0$$

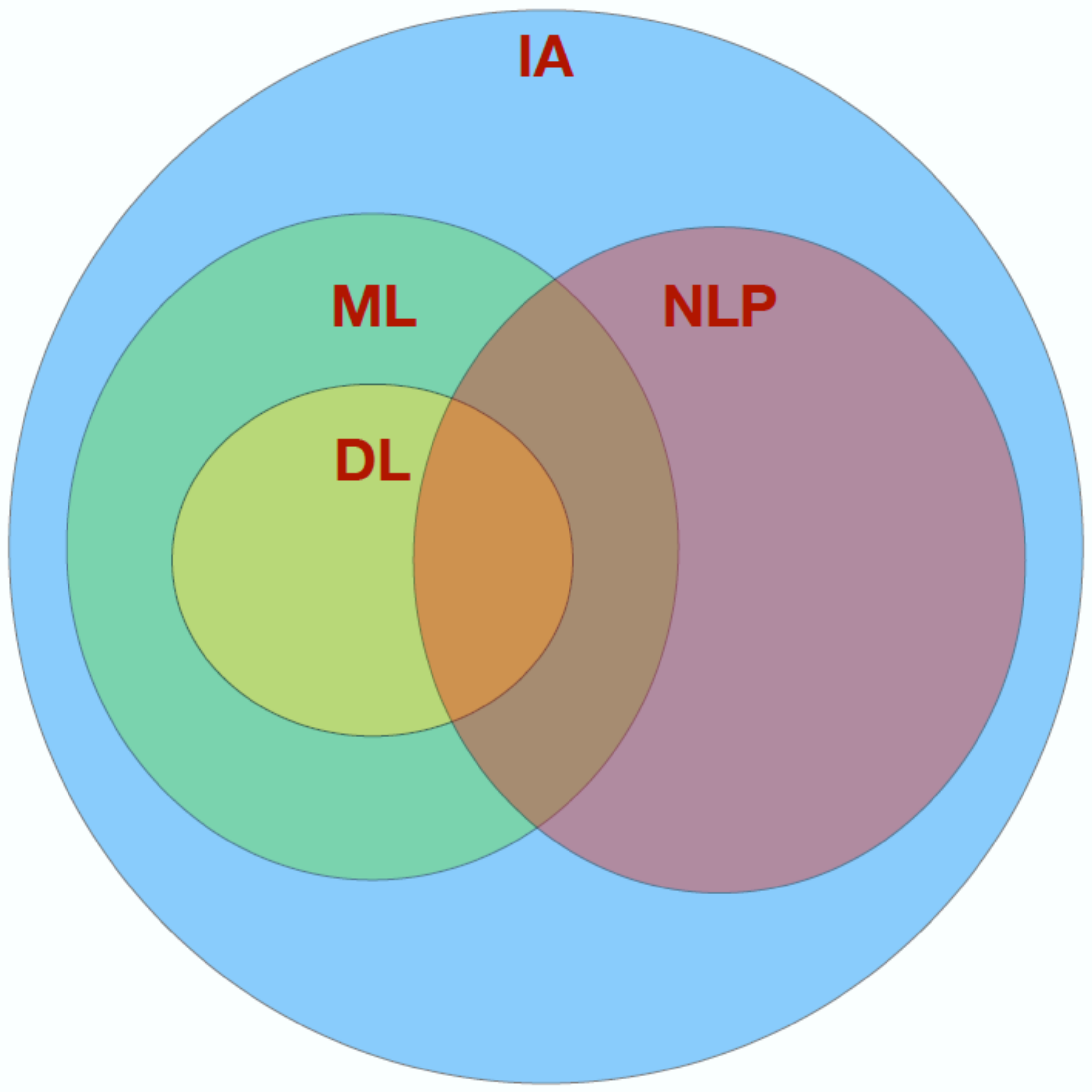
We will see in section 3 an example with the model LDA

2 Introduction to NLP

2. Introduction to NLP

Preprocessing : Tokenization

Natural Language Processing : The science of programming computers to understand human language



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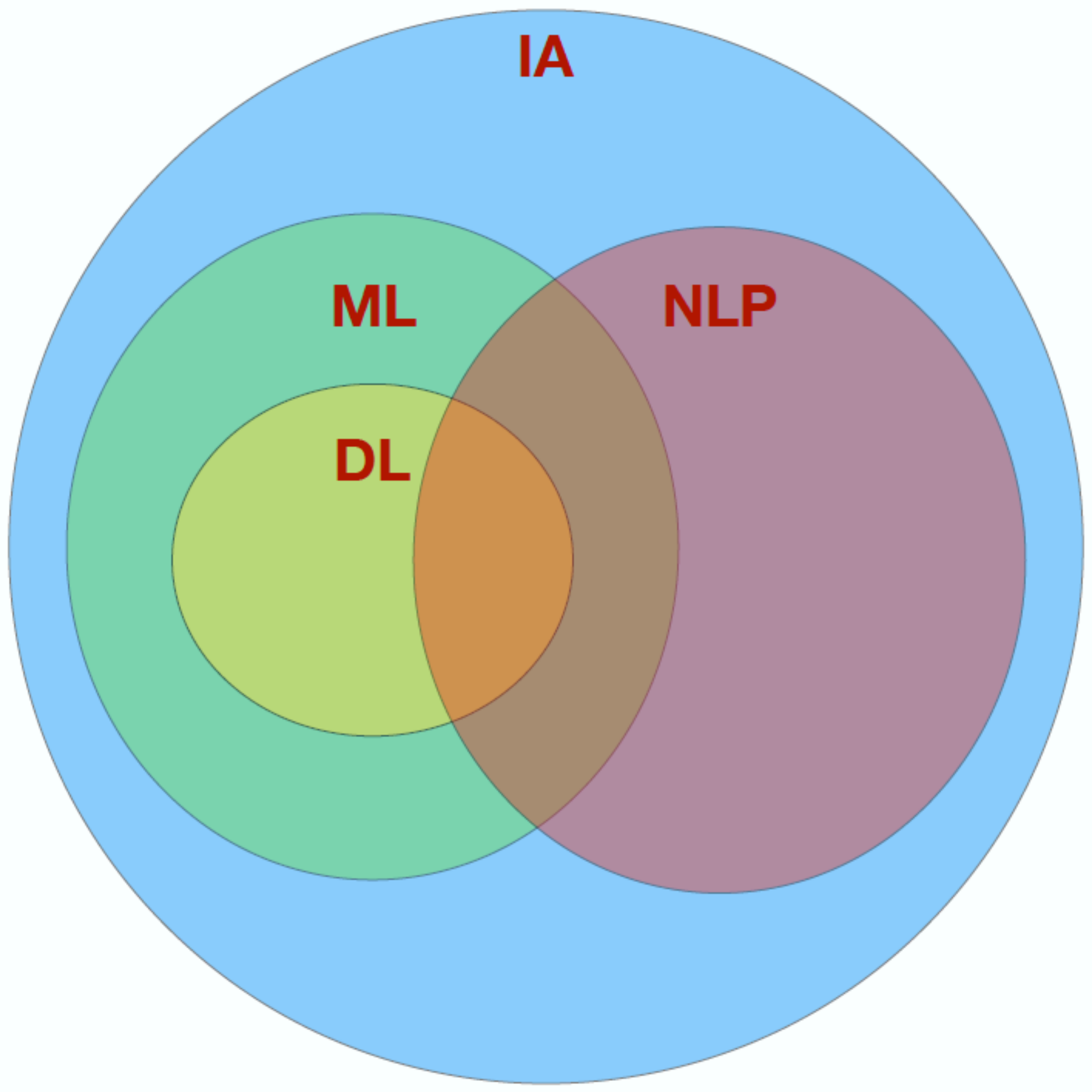

Some intuitions : we want to perform some learning tasks with textual data

- We know how to train a model with a tabular data. **How about textual data ?**
- Textual data can be highly sophisticated. **Can we simplify them ?**

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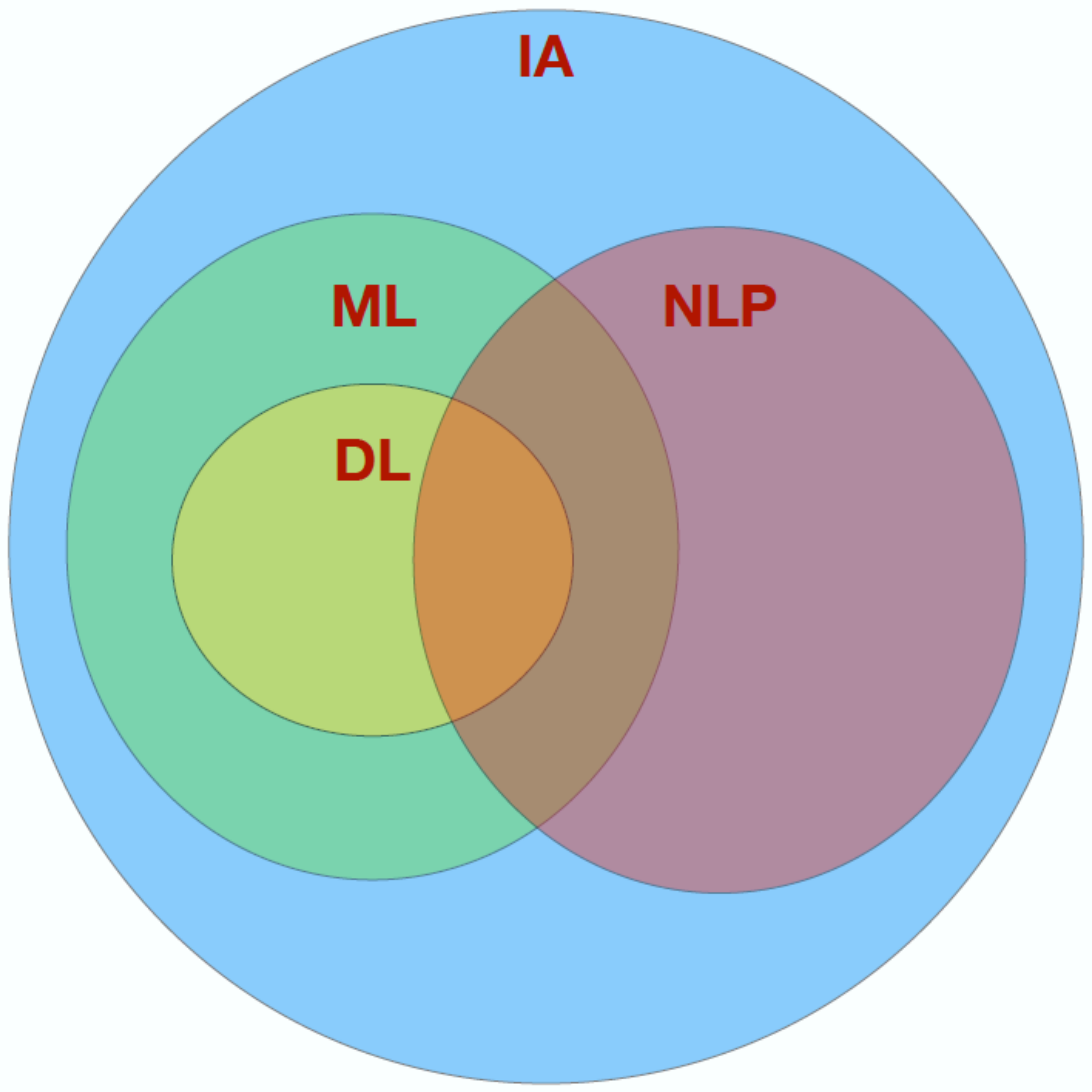

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- **Text** : sequence of words
- **Word** : sequence of logical characters
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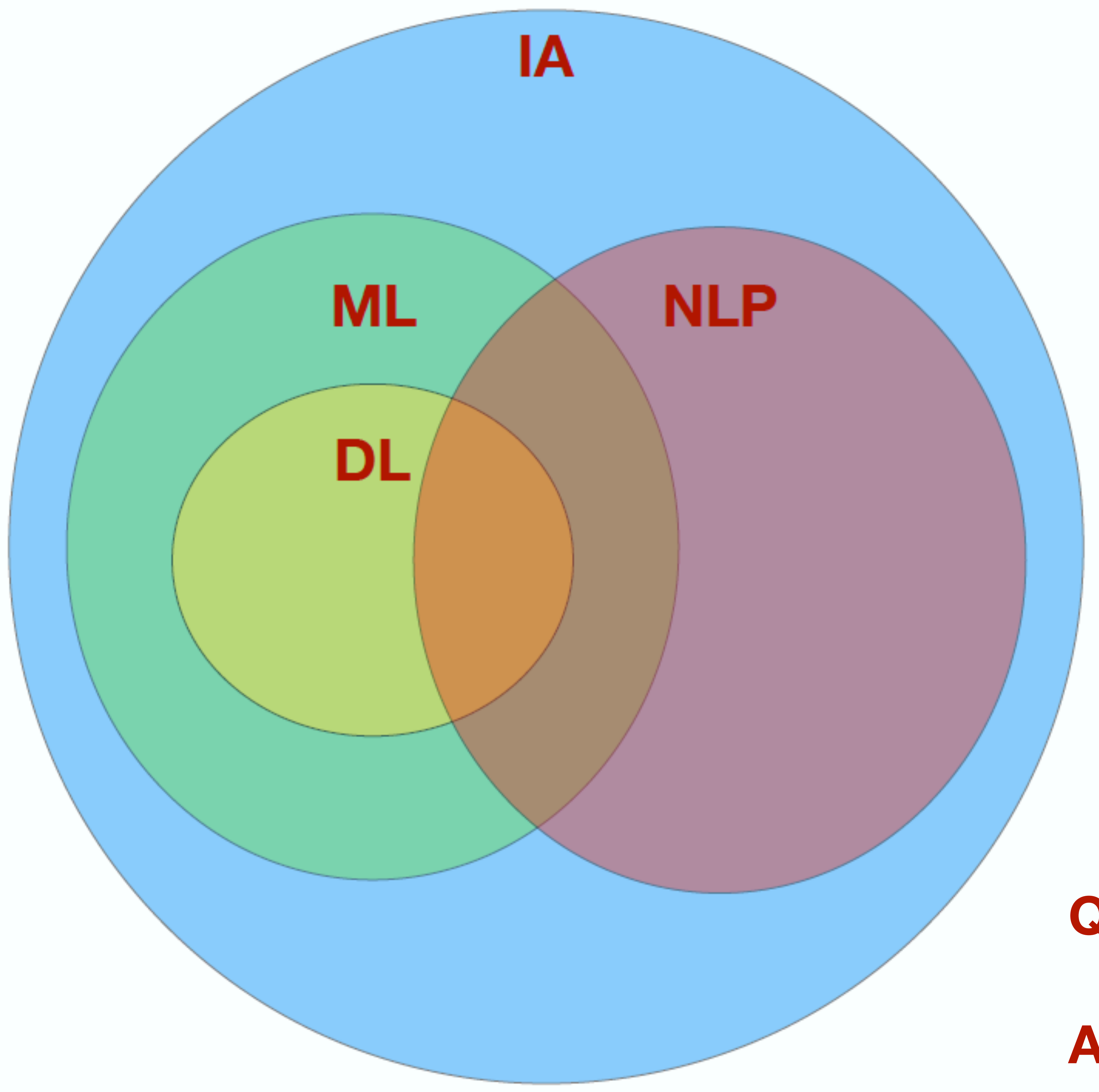

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Question : how to find the limits of a word?

Answer : In French/English, we can separate words by spaces and punctuation

Example : **When should I start my job search ?** → **['When', 'should', 'I', 'start', 'my', 'job', 'search']**

2. Introduction to NLP

Preprocessing : Normalization & stop-words

Stemming : keep the root of a term by cutting off the end or the beginning of the word

Example : wait, wait**ing**, wait**ed**, wait**s** → wait

there exists many text-preprocessing packages in python : nltk, spacy, …

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Lemmatization : keep the root of a term by transforming the words into its root words

Example : study, study**ing**, studi**es** ⟶ study **(In stemming :** stud)

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Stop-words : set of words frequently used in a language and which do not bring any important meaning

Example : the, a, of, is, at, which, …

Aim : Remove these stop-words

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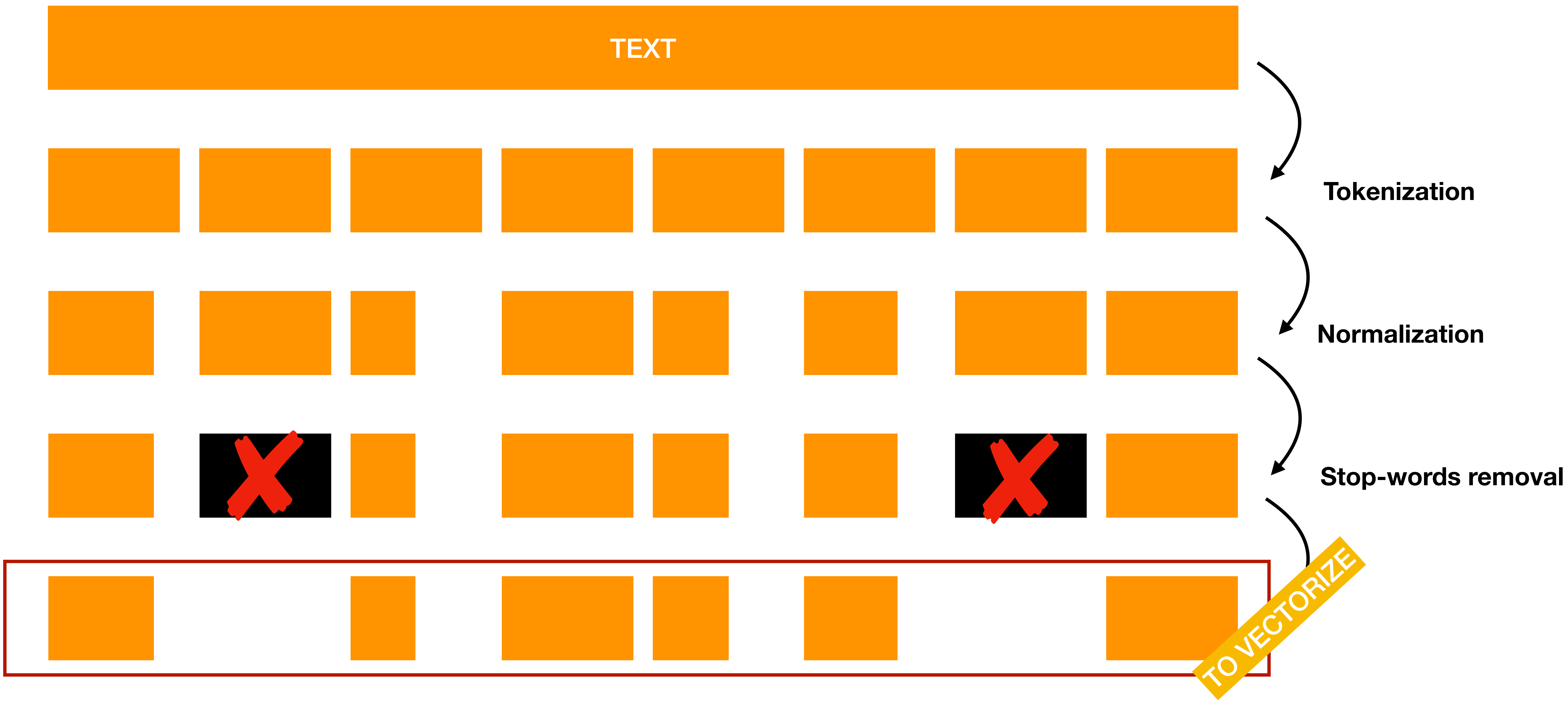
2. Introduction to NLP

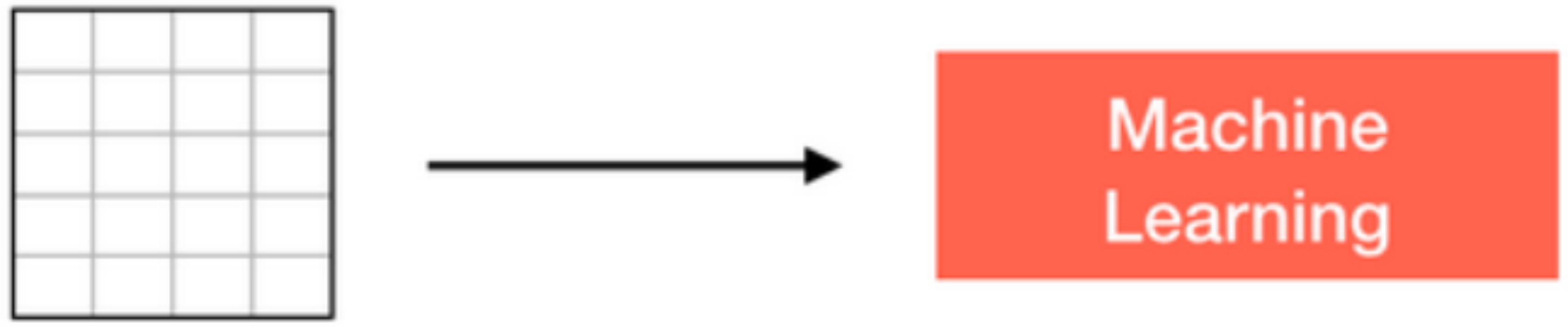
Preprocessing : overview



2. Introduction to NLP

Processing : Textual data into tabular data

For tabular data :



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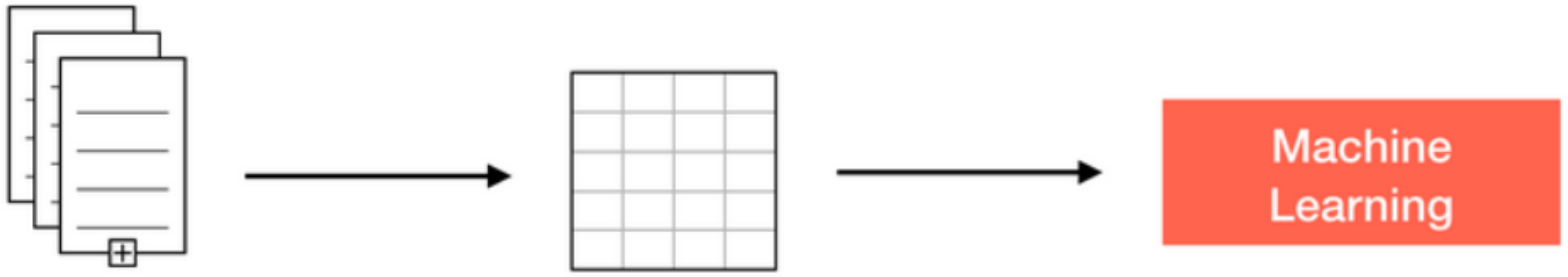

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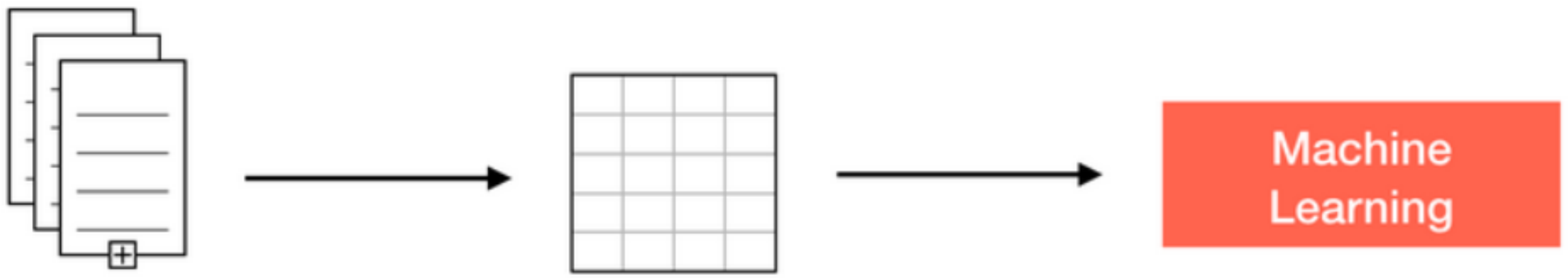
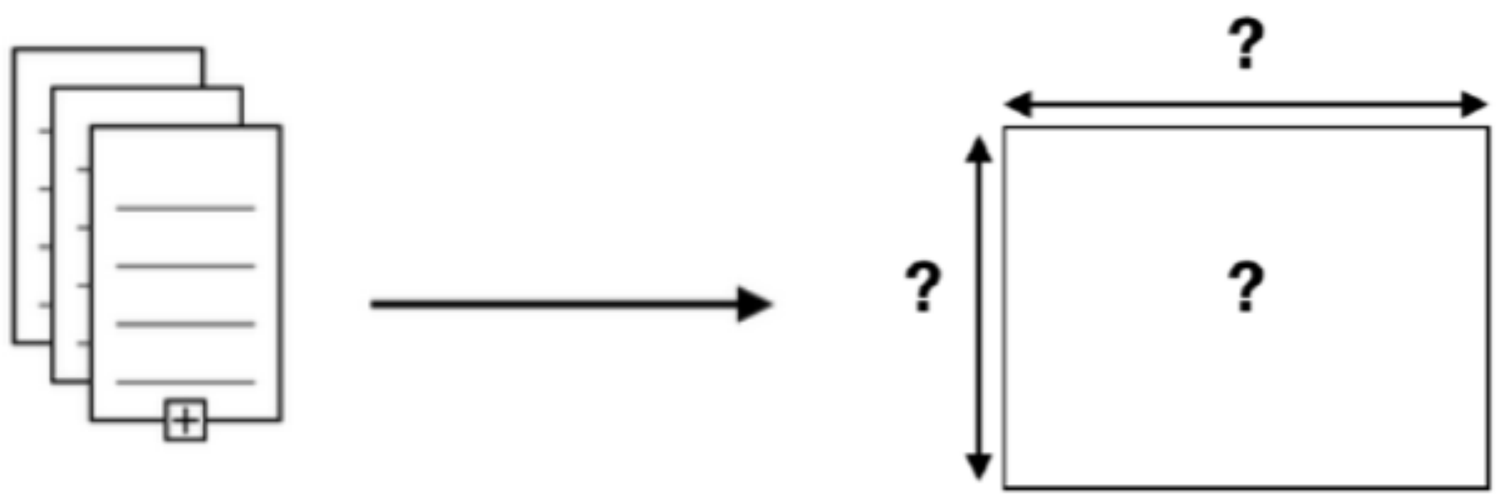


Problems :

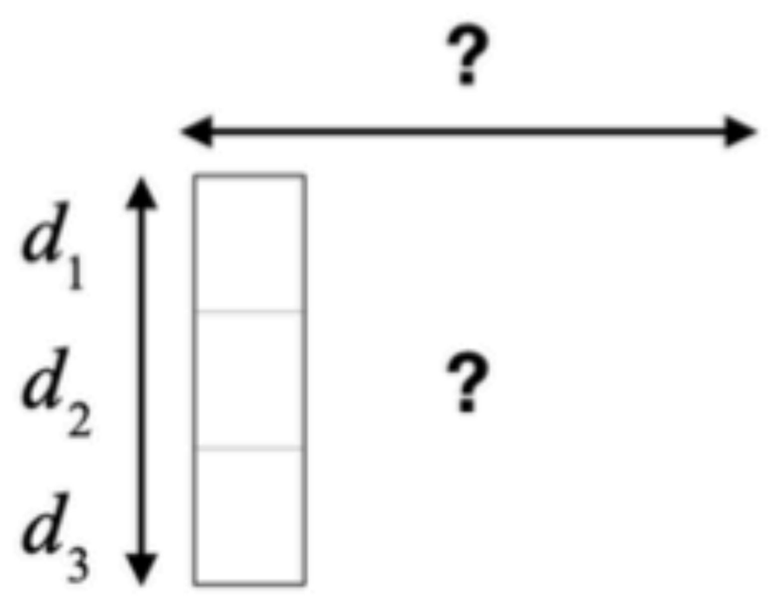


2. Introduction to NLP

Processing : Textual data into tabular data

Corpus

d_1	trouver bonne assurance
d_2	contrat satisfaisant
d_3	changement contrat assurance



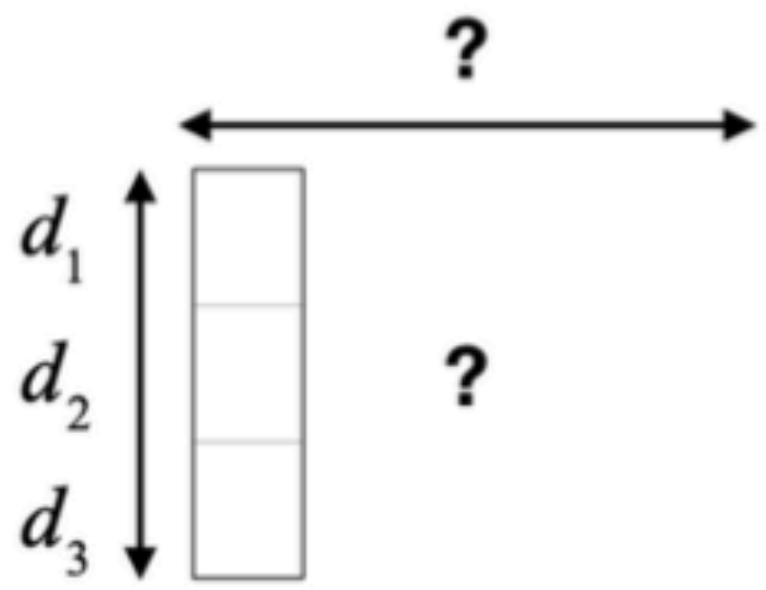
2. Introduction to NLP

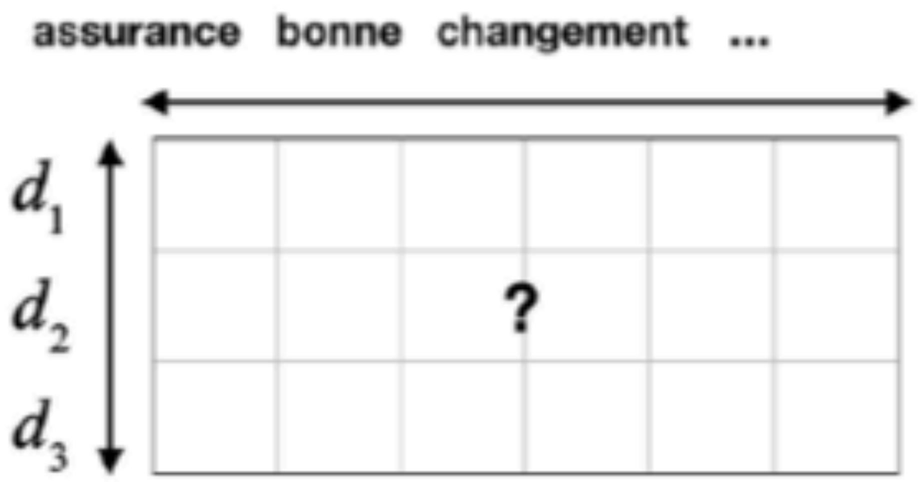
Processing : Textual data into tabular data

Corpus → Dictionary

d_1	trouver bonne assurance
d_2	contrat satisfaisant
d_3	changement contrat assurance

V = {
    'assurance'   : 1,
    'bonne'   : 2,
    'changement' : 3,
    'contrat'   : 4,
    'satisfaisant' : 5,
    'trouver'   : 6
    }





2. Introduction to NLP

Processing : Textual data into tabular data

Corpus → **Dictionary** → **Encoding**

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d_2	contrat satisfaisant
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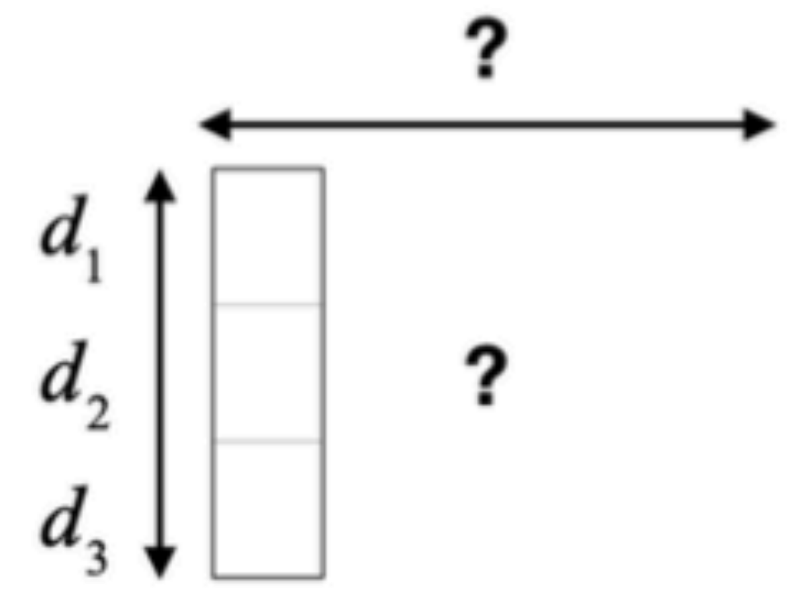
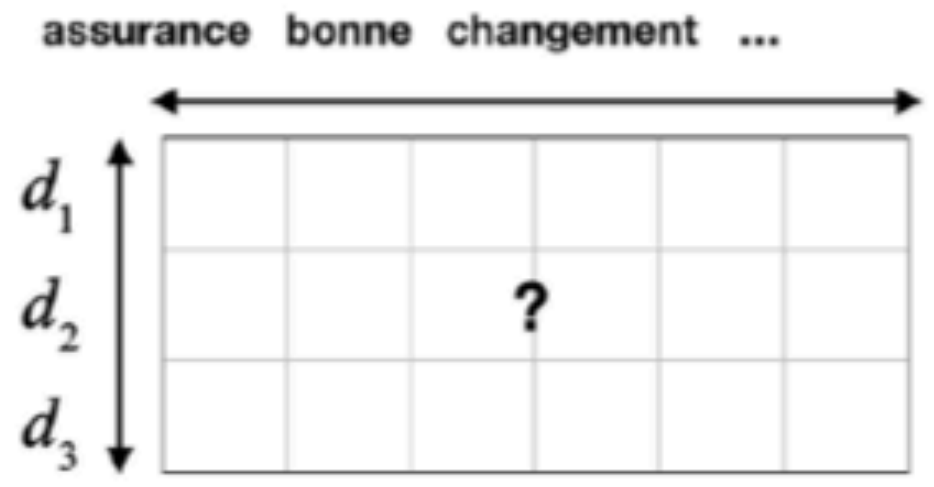
$$\begin{array}{ccc} \text{assurance} & & \text{contrat} \\ \begin{bmatrix} \boxed{1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} & \cdots & \begin{bmatrix} 0 \\ 0 \\ 0 \\ \boxed{1} \\ 0 \\ 0 \end{bmatrix} \end{array}$$





	assurance	bonne	changement	...		
d_1	1	1	0	0	0	1
d_2	0	0	0	1	1	0
d_3	1	0	1	1	0	0

Bag-of-Words approach

2. Introduction to NLP

Some important considerations on vectorization

trouver	contrat	assurance	...
1	0	1	...
0	1	0	...
0	1	1	...

Bag-of-Words (BoW) approach

- based on term frequency
- problem : don't keep the word orders
- solution : n-grams approach

trouver	assurance	contrat assurance	...
1	1	0	...
0	0	0	...
0	1	1	...

n-grams approach

- based on sequence of *n* words frequency
- problem : too many features / too sparse
- solution : stop-words and some n-grams removal (too **high** or too **low** frequencies)

trouver	assurance	contrat assurance	...
0.10	0.41	0	...
0	0	0	...
0	0.41	0.10	...

TF-IDF approach

- Based on the product of two values :
  - **Term frequency (TF) :**

$$\mathrm{TF}(\mathrm{t}, \mathrm{d}) = \text{frequency of } \mathrm{t} \text{ in } \mathrm{d}$$

  - **Inverse Document Frequency (IDF):**

$$IDF(t, D) = \log \frac{\#\text{documents}}{\#\text{documents with terme t}}$$

3 Application on textual data with LDA

3. Latent Dirichlet Allocation

Topic modeling

Topic modeling : a statistical model for **finding out the hidden « topics »** that occur in a collection of documents

3. Latent Dirichlet Allocation

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Motivations : This method is also used in

- create **recommendation systems** (used by e-tailers, search engines, …)
- text **categorization**
- **data mining** processes
- in bioinformatics: **extracting hidden knowledge** from biological data (DNA molecules)

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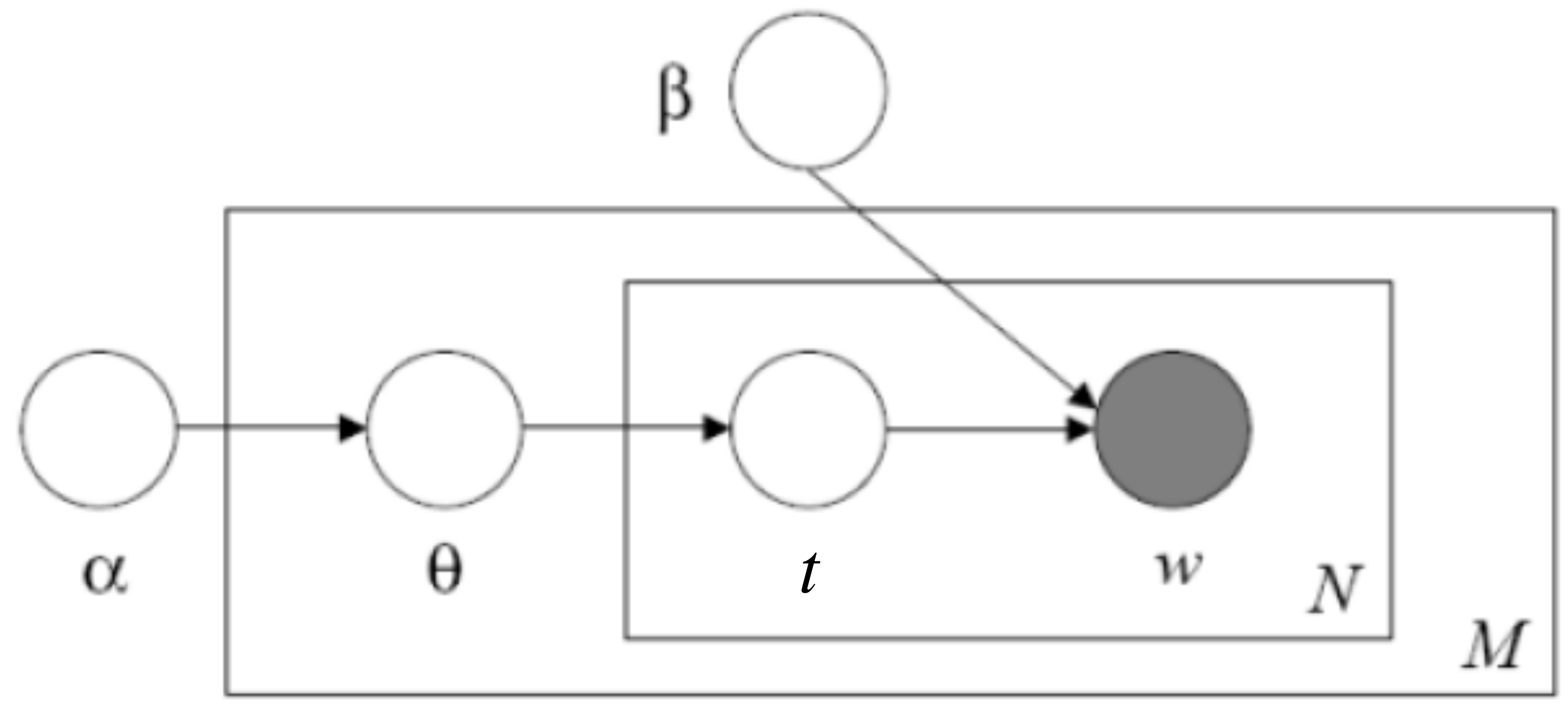
Idea :

- Every **document** consists of a mix of **topics**
- Every **topics** consists of a mix of **words**

3. Latent Dirichlet Allocation

LDA : high-level view

Latent Dirichlet Allocation (LDA) : (popular) topic modeling based on Bayesian inference with the following PGM



$$P(\theta, t, w \,|\, \alpha, \beta) = P(\theta \,|\, \alpha) \cdot P(t \,|\, \theta) \cdot P(w \,|\, t, \beta)$$

$$= \prod_{d \in [M]} P(\theta_d \,|\, \alpha) \cdot \prod_{n \in [N]} P(t_{d,n} \,|\, \theta_d) \cdot P(w_{d,n} \,|\, t_{d,n}, \beta)$$

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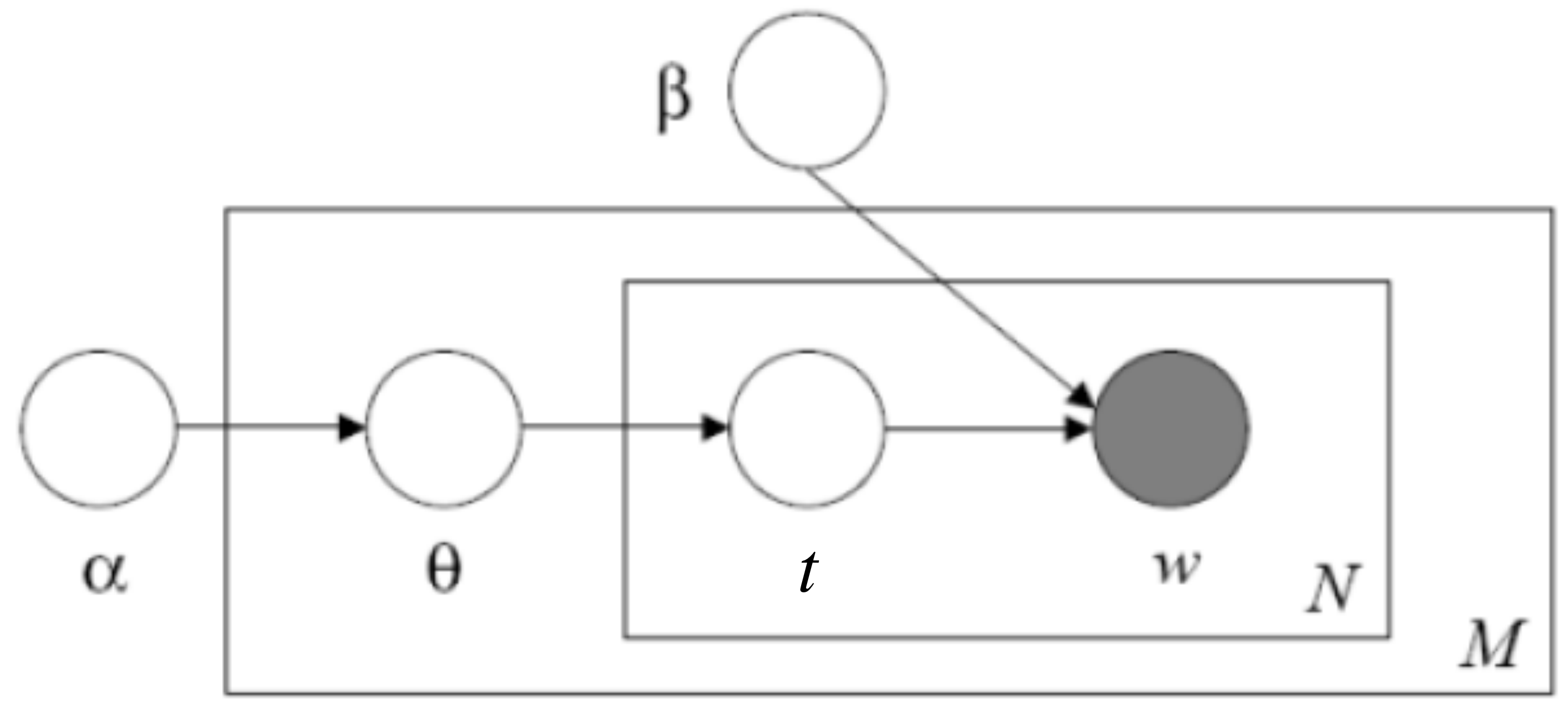

~ Dirichlet ~ Multinomial ~ Multinomial

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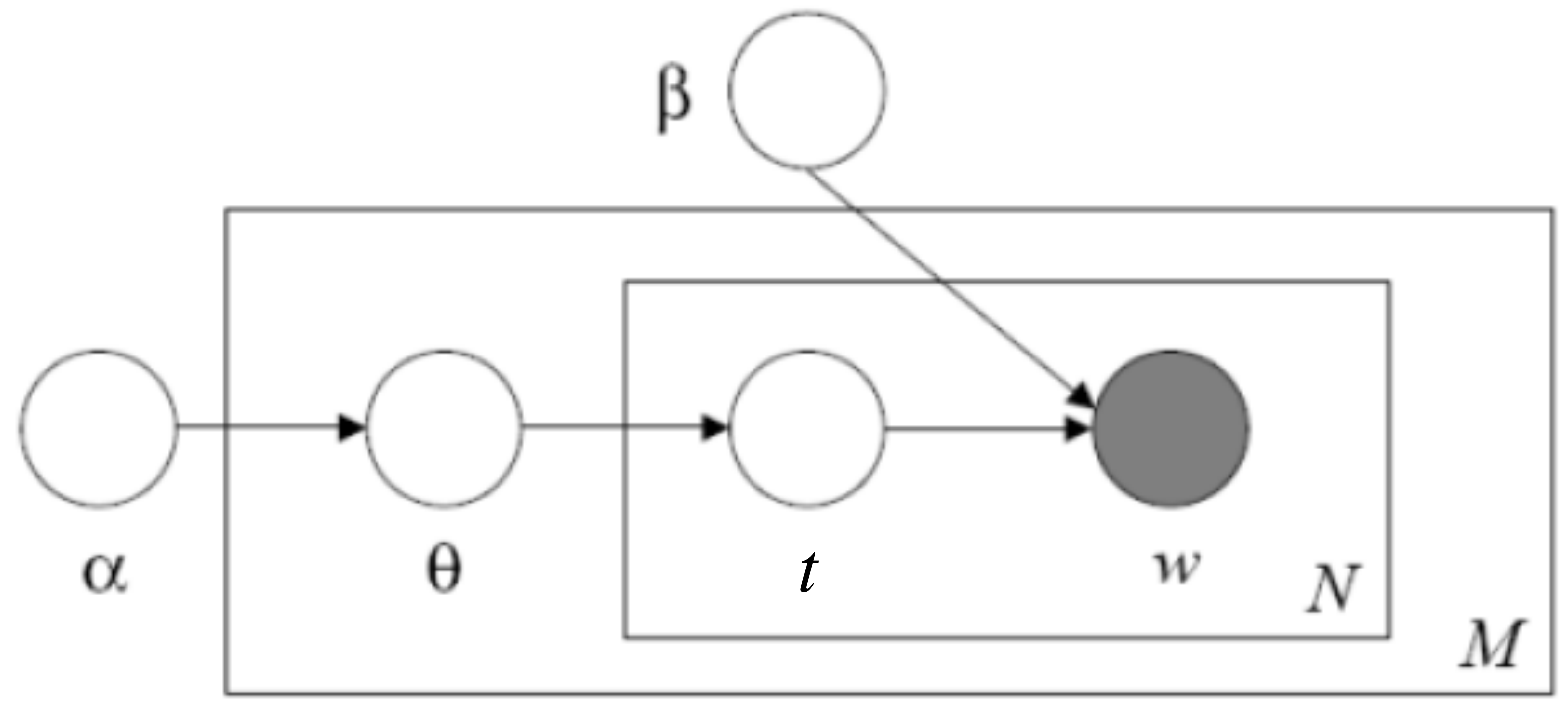

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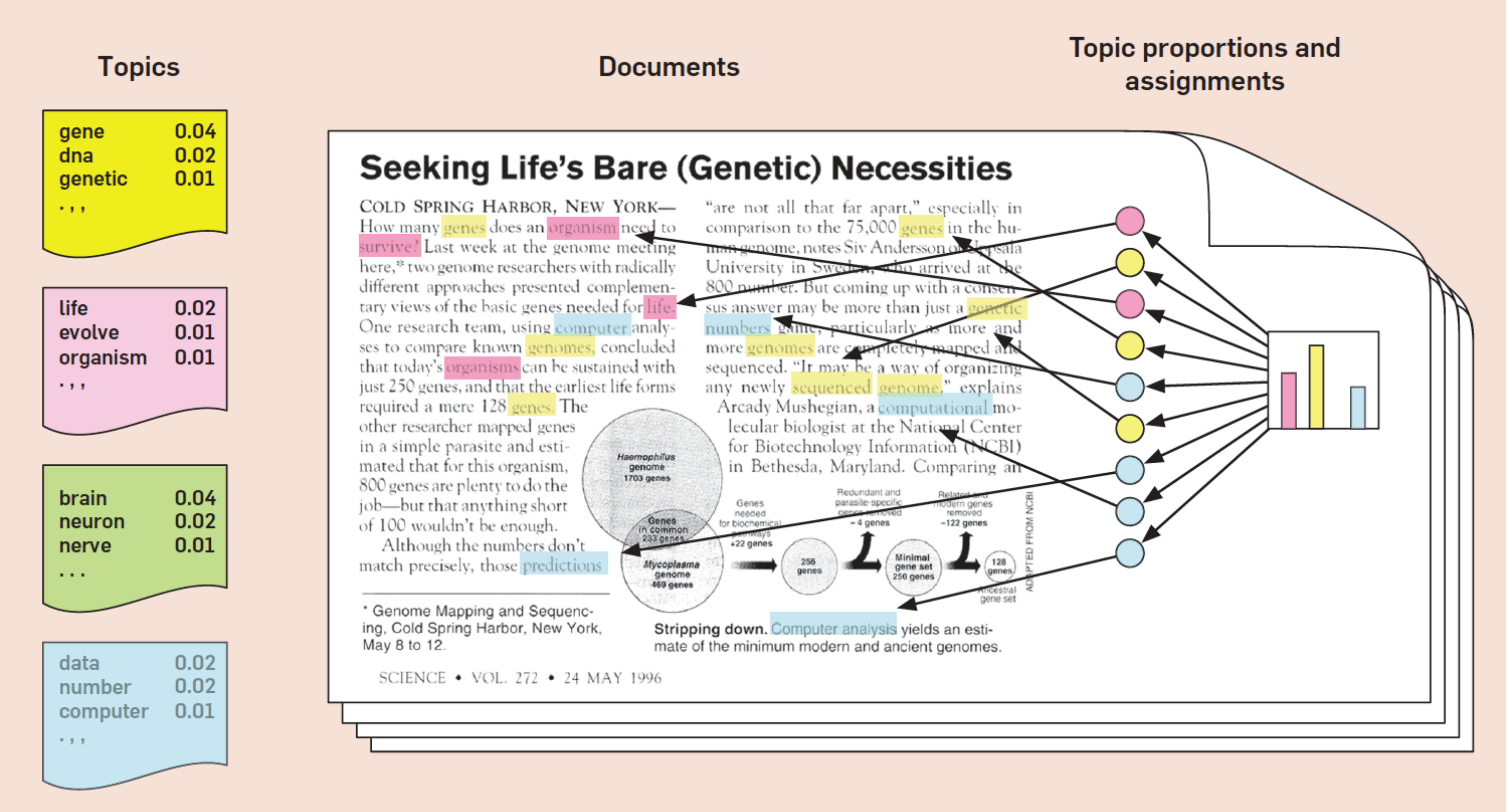
Example :



source : Blei, D.M. (2012). Probabilistic topic models. Communications of the ACM, 55(4), 77-84.

Assumption on the generation of texts :

For each of M documents d,

- Choose the **topic distribution** $\theta_d \sim \mathrm{Dirichlet}(\alpha)$
- For each of N words w,
  - choose a **topic** $t \sim \mathrm{Multinomial}(\theta_\mathrm{d})$
  - choose a **word** $w \sim \mathrm{Multinomial}(\beta)$

3. Latent Dirichlet Allocation

LDA : Dirichlet distribution

Dirichlet distribution (dimension 3) :

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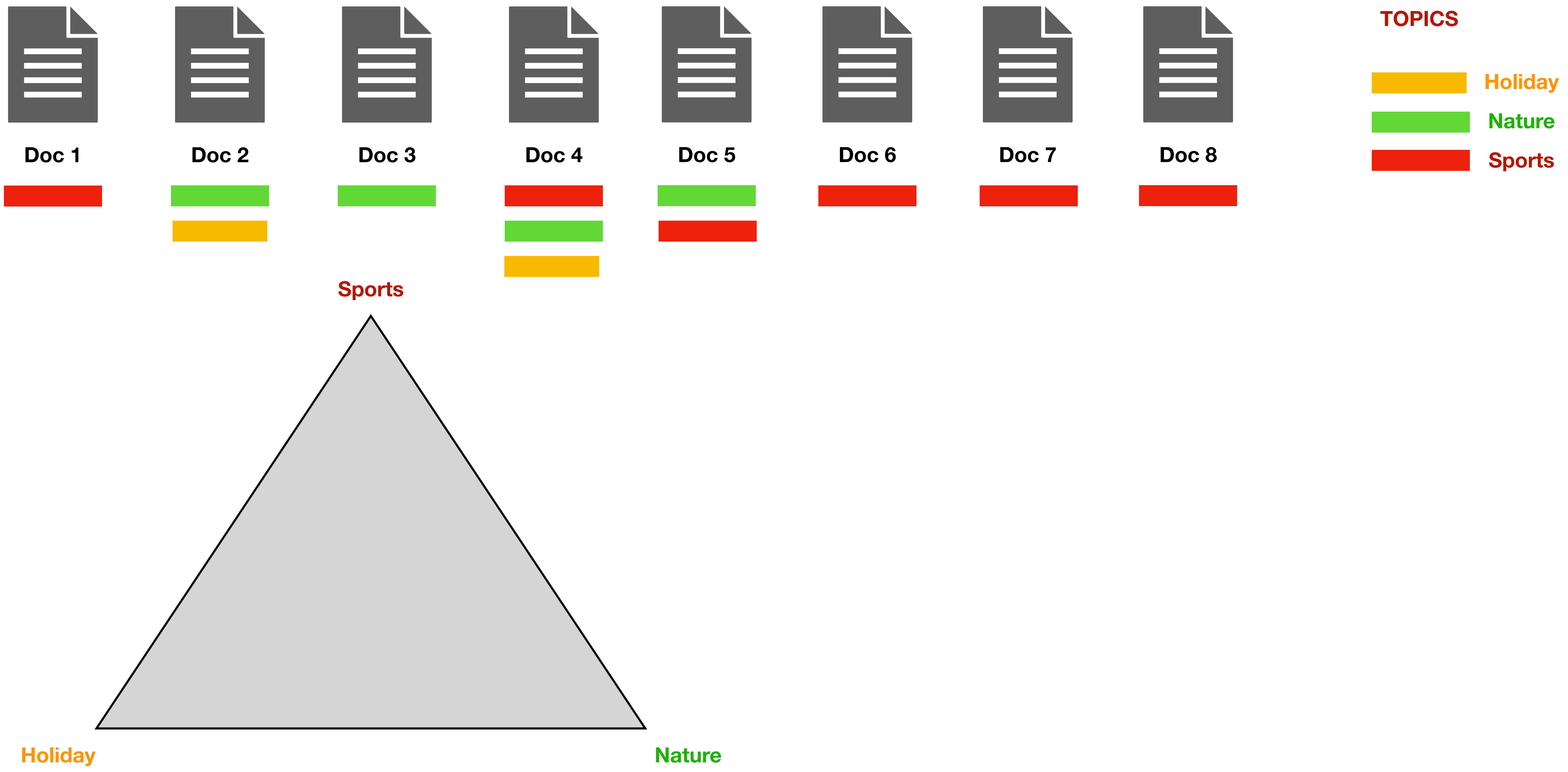
Dirichlet distribution (dimension 3) :



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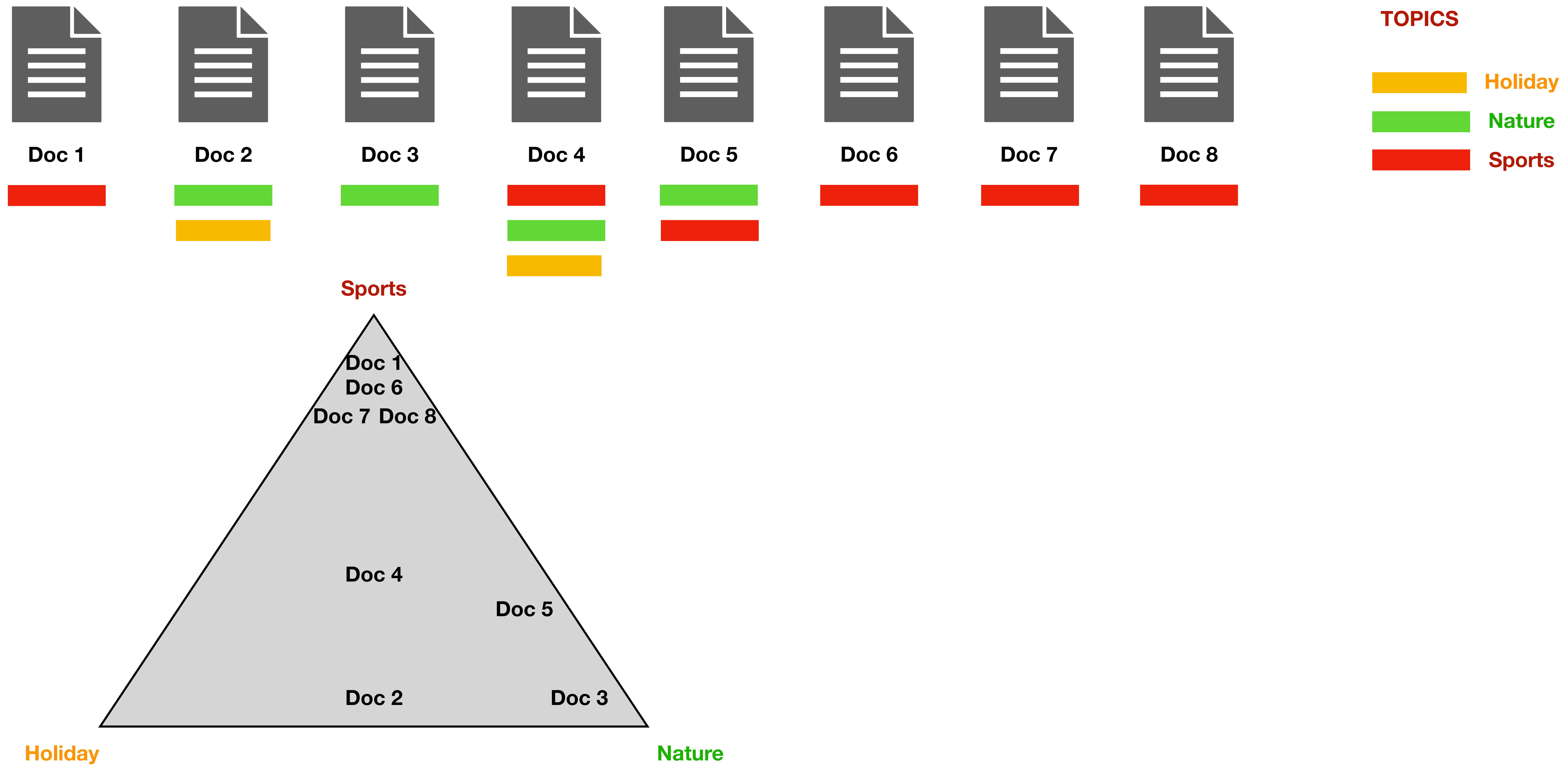
Dirichlet distribution (dimension 3) :



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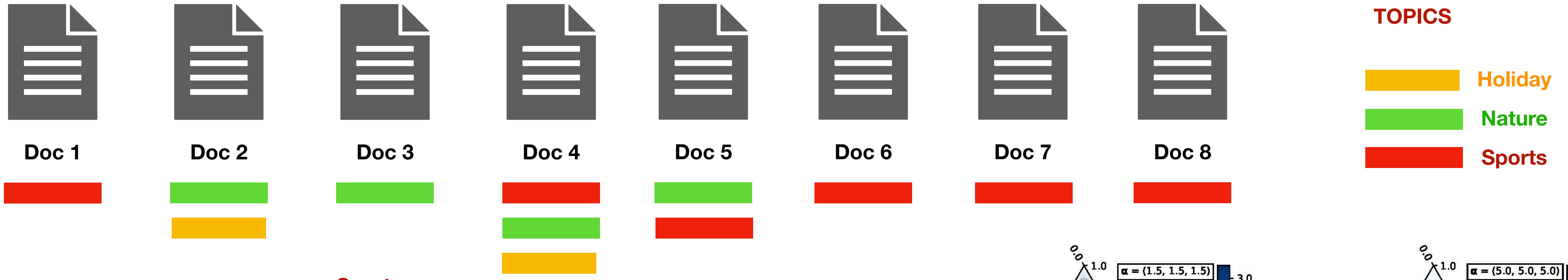

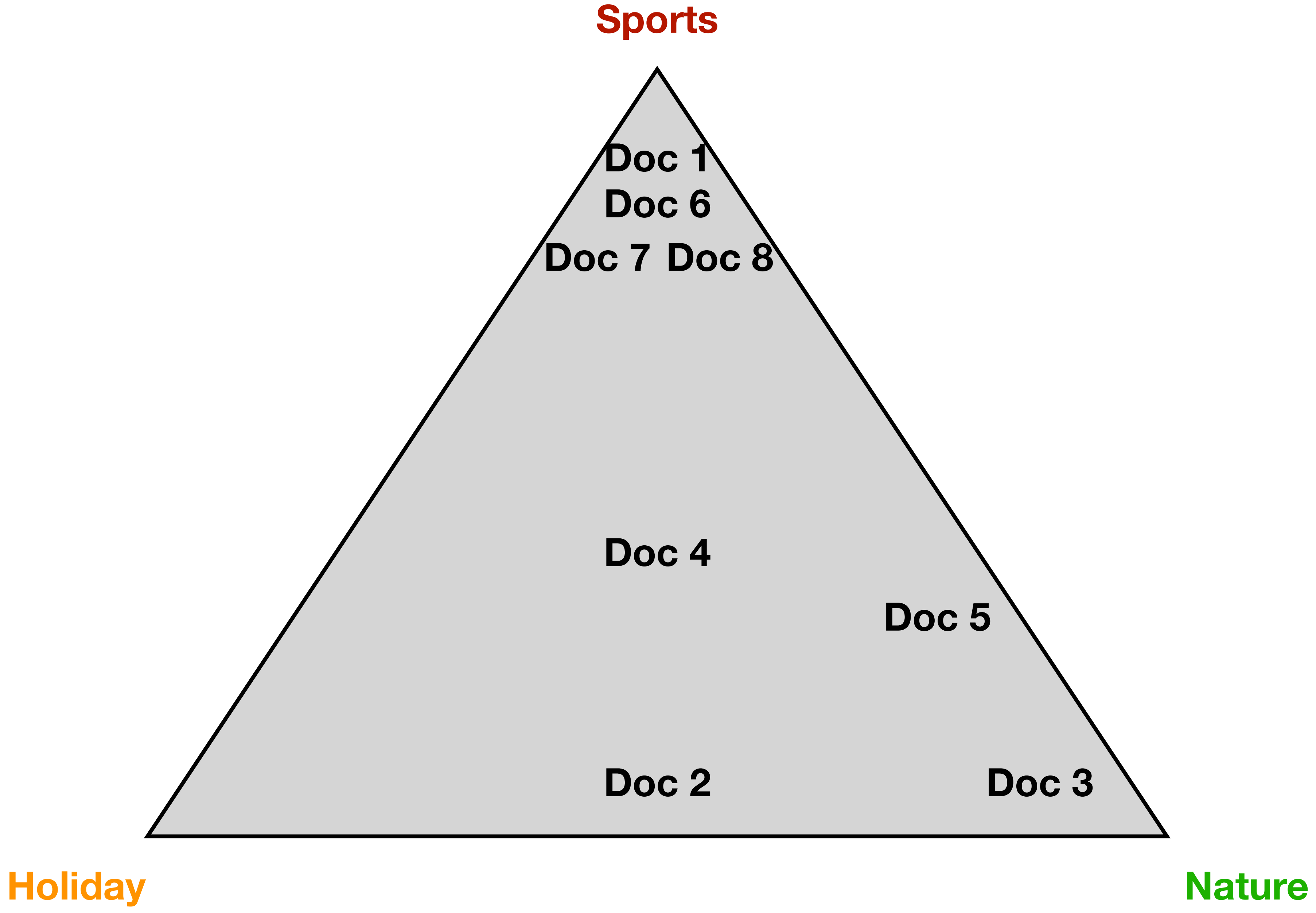

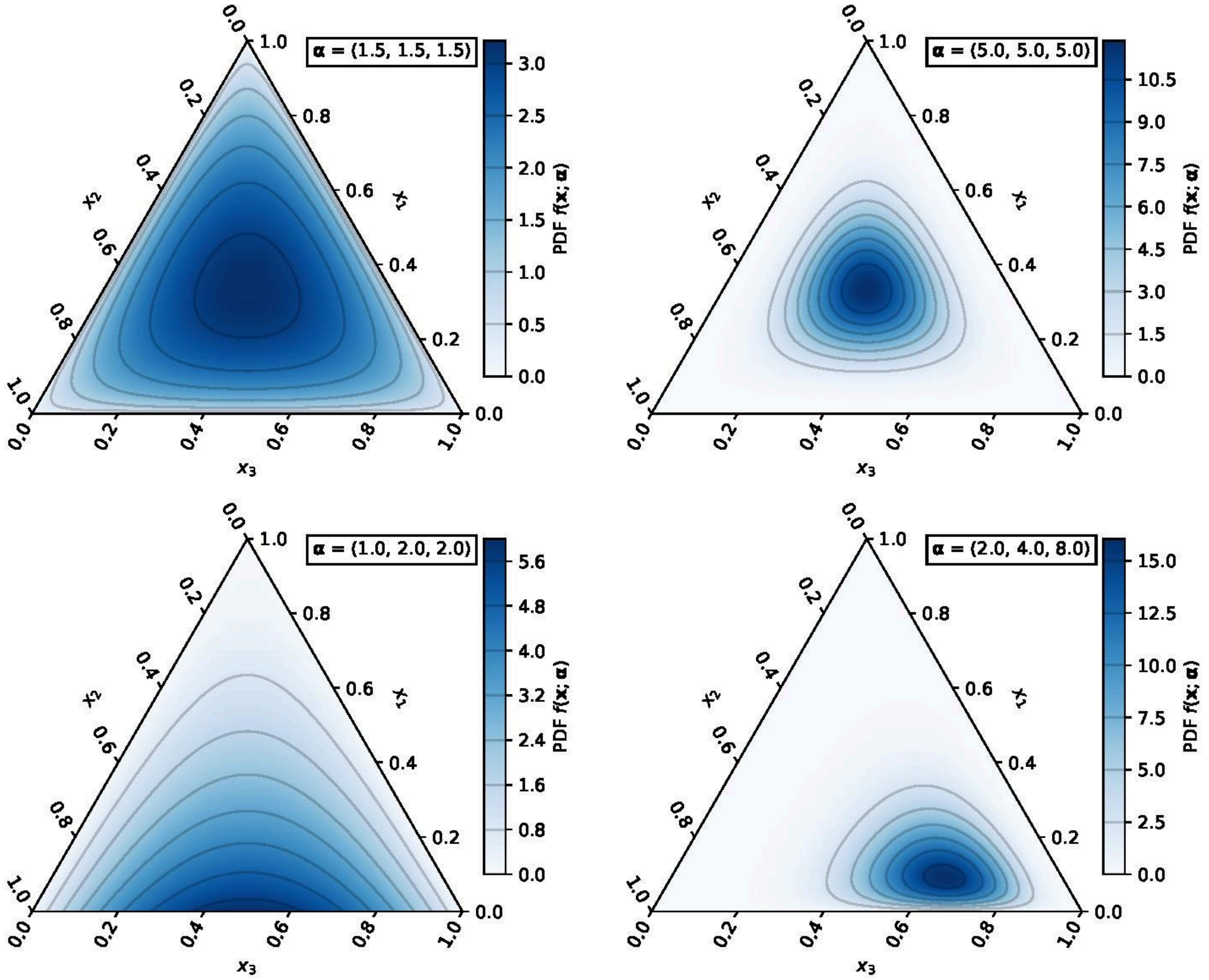

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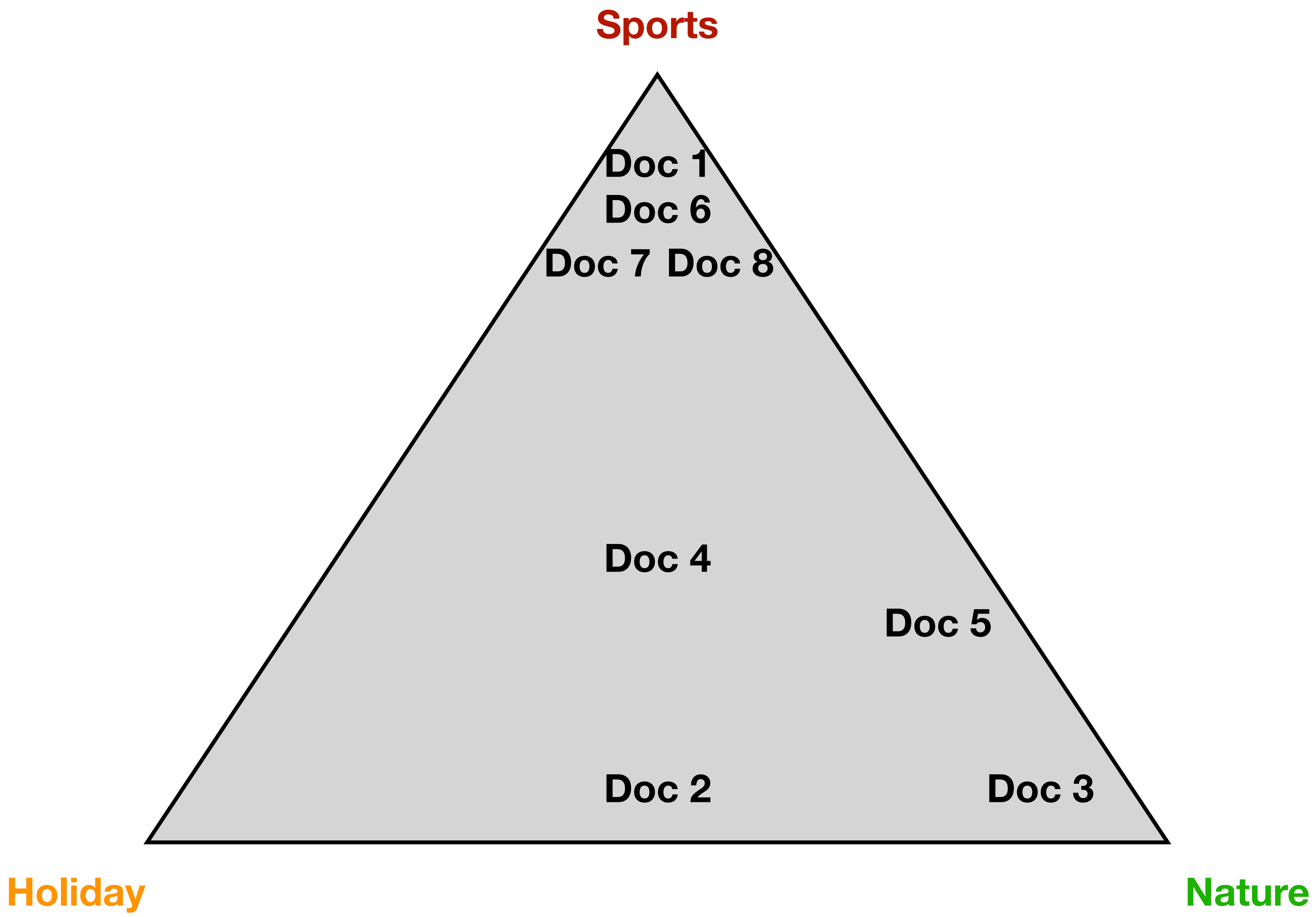
LDA : Multinomial distribution



Dirichlet distribution
« distribution of distribution »

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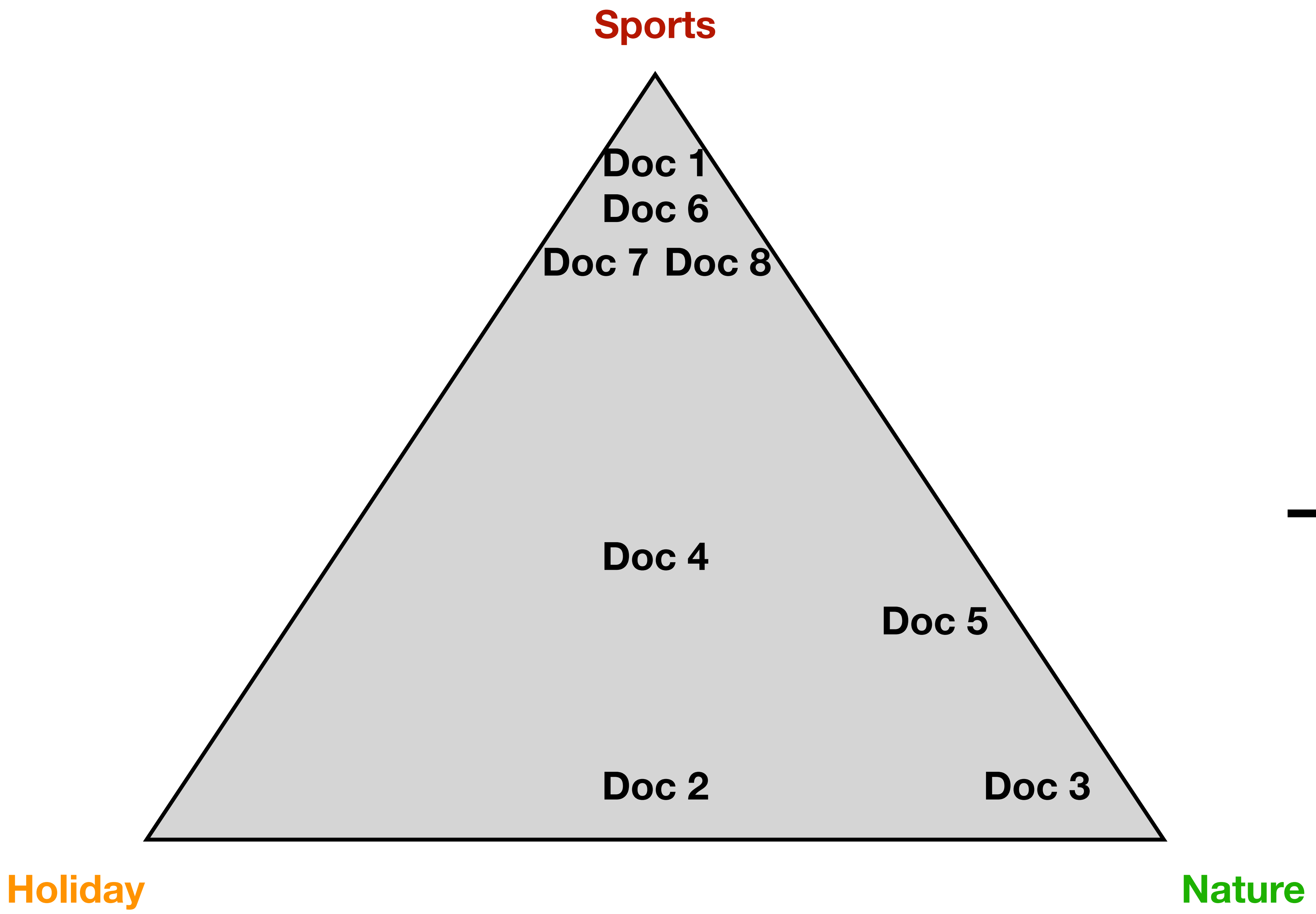
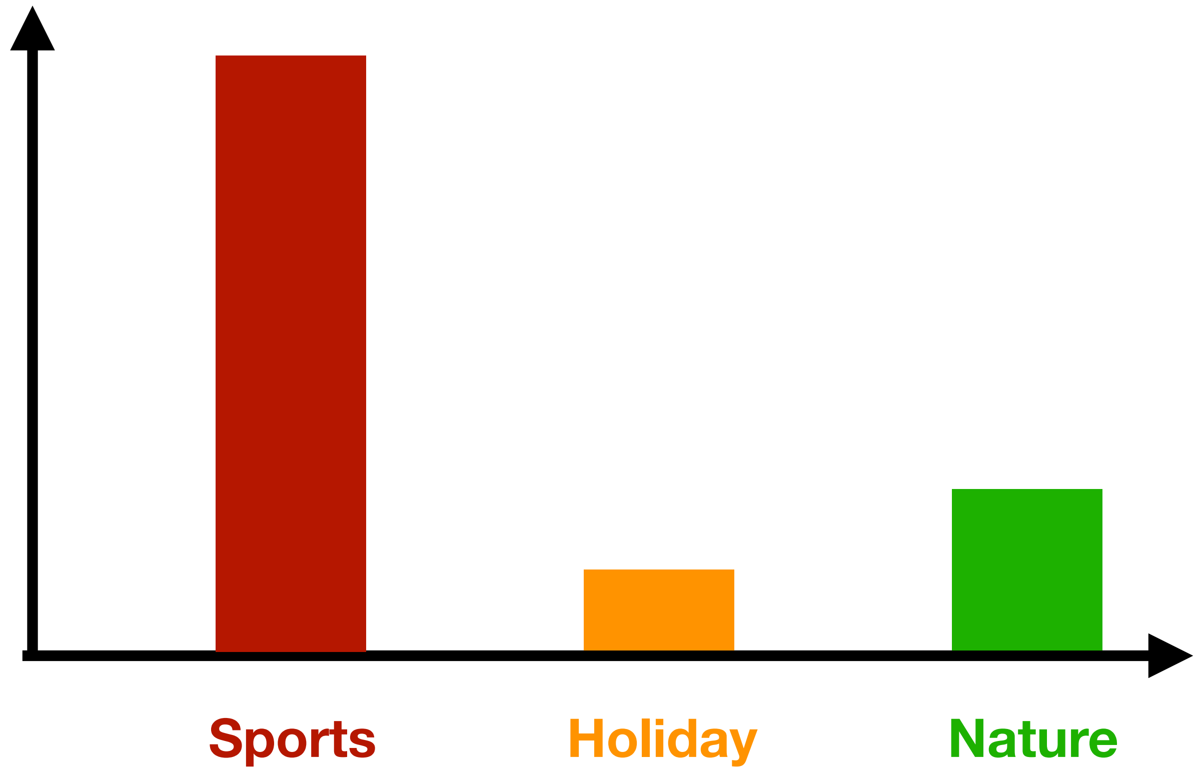


Dirichlet distribution
« distribution of distribution »

$$\theta_{\text{sports}} = P(\text{sports} \mid \alpha) = 0.7$$

$$\theta_{\text{holiday}} = P(\text{holiday} \mid \alpha) = 0.1$$

$$\theta_{\text{nature}} = P(\text{nature} \mid \alpha) = 0.2$$



Multinomial distribution

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LDA : E-step ; calibration of theta and t

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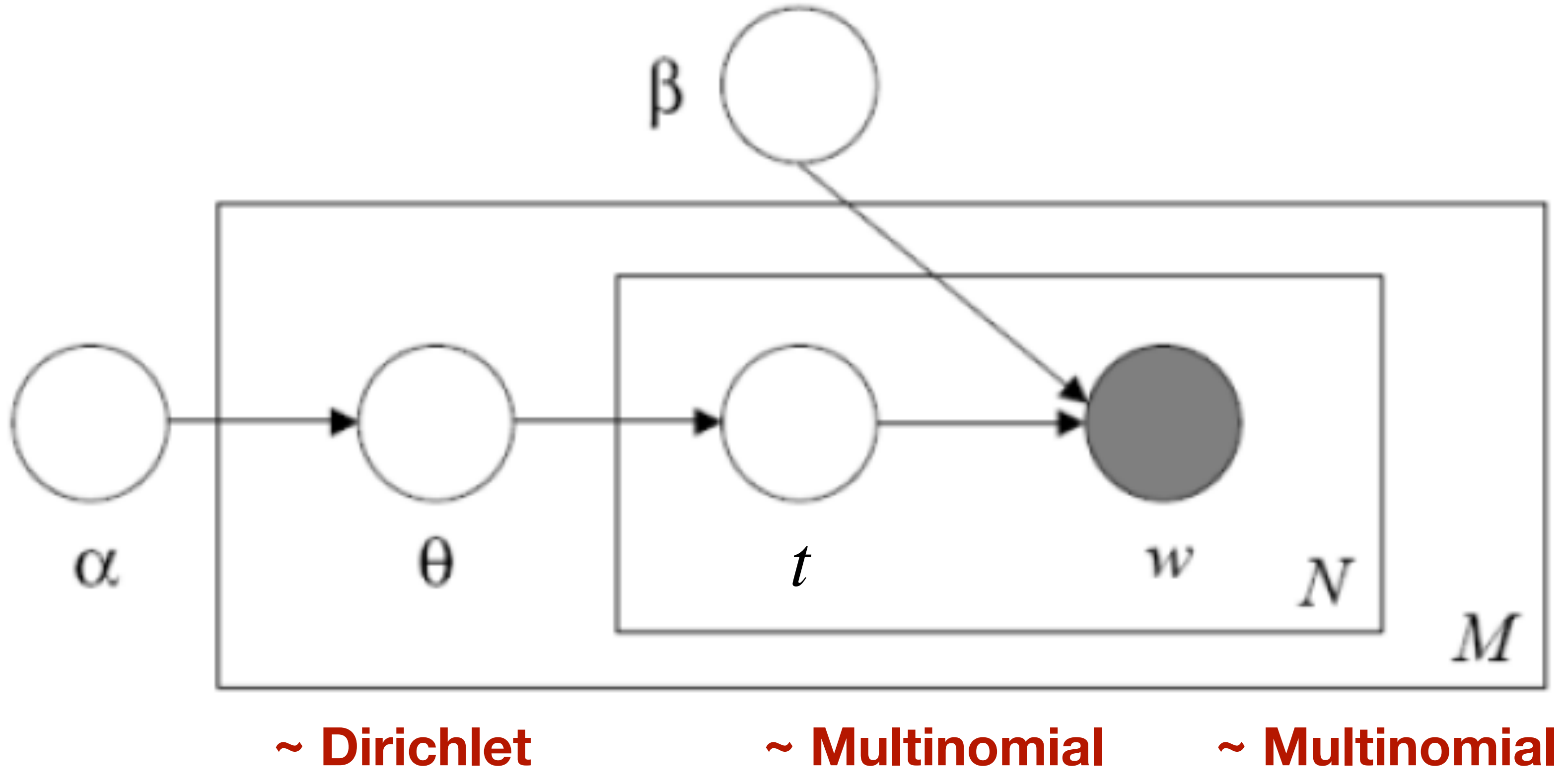

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$$= \prod_{d \in [M]} \mathrm{Dir}(\theta_{\mathrm{d}} \mid \alpha) \cdot \prod_{n \in [N]} \mathrm{Multi}(\mathrm{t}_{\mathrm{d,n}} \mid \theta_{\mathrm{d}}) \cdot \mathrm{Multi}(\mathrm{w}_{\mathrm{d,n}} \mid \mathrm{t}_{\mathrm{d,n}})$$

$$\propto \prod_{d \in [M]} \prod_{k \in [K]} \theta_{d,k}^{\alpha_t - 1} \cdot \prod_{n \in [N]} 1_{k = t_{d,n}} \cdot \theta_{d,t_{d,n}} \cdot \beta_{t_{d,n}, w_{d,n}}$$

E step :

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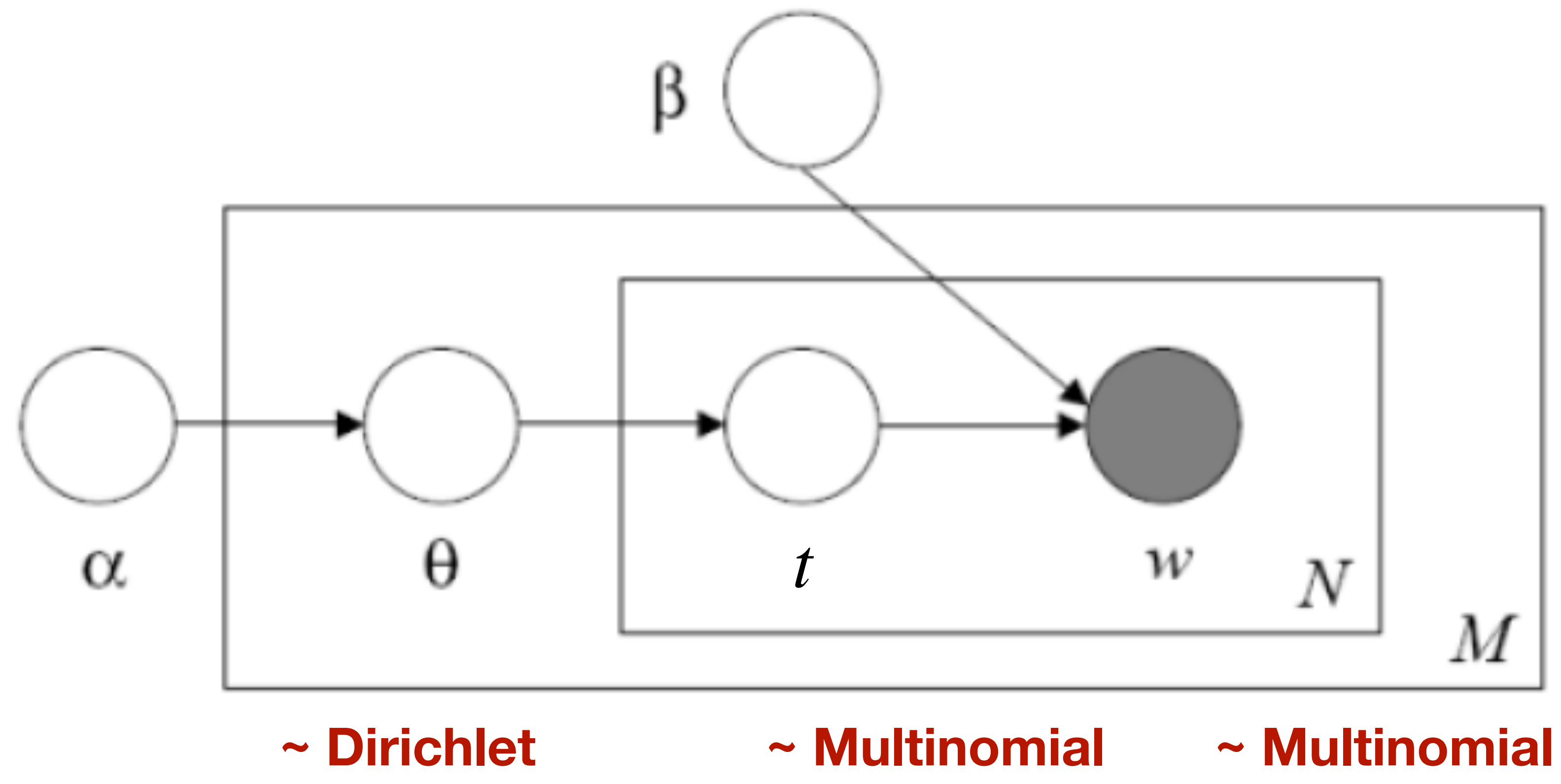

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E step :

Objective :

$$\hat{P} = \arg \min_{Q(\theta),\, Q(t)} D_{KL}(\, Q(\theta) \times Q(t) \,||\, P(\theta, t \,|\, w)\,)$$

Optimal solution :

$$\log \hat{P}(\theta) = \mathbb{E}_{Q(t)} \left[\log P(\theta, t, w) \right] + \mathrm{const}$$

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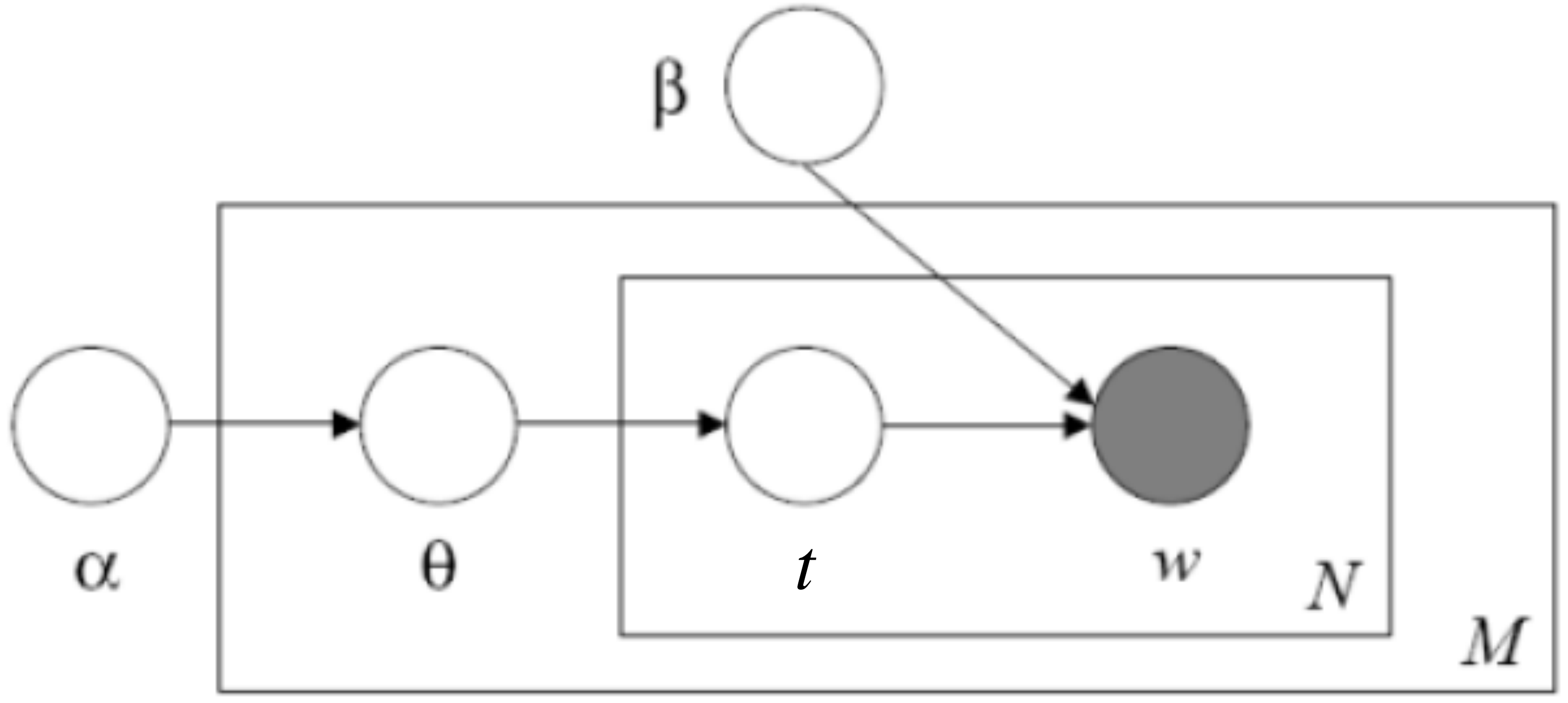

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$$\log P(\theta, t, w \,|\, \alpha, \beta) = \sum_{d \in [M]} \left[\sum_{k \in [K]} (\alpha_k - 1) \log \theta_{d,k} + \sum_{n \in [N]} \sum_{k \in [K]} 1_{\{k = t_{d,n}\}} \left(\log \theta_{d, t_{d,n}} + \log \beta_{t_{d,n}, w_{d,n}} \right) \right] + \text{const}$$

For θ,

$$\log \hat{p}(\theta) = E_{Q(t)} \left[\log P(\theta, t, w) \right] + \text{const}$$

$\perp\!\!\!\perp \theta$

$$= E_{Q(t)} \left[\sum_{d \in [M]} \left(\sum_{k \in [K]} (\alpha_k - 1) \log \theta_{d,k} + \sum_{n \in [N]} \sum_{k \in [K]} 1_{k = t_{d,n}} \left(\log \theta_{d, \cancel{t_{d,n}}\, k} \right) \right) \right] + \text{const}$$

$$= \sum_{d \in [M]} \sum_{k \in [K]} \left[(\alpha_k - 1) + \sum_{n \in [N]} \underbrace{E_{Q(t_{d,n})} \left[1_{t_{d,n} = k} \right]}_{\gamma_{d,n}(k)} \right] \times \log \theta_{d,k} + \text{const}$$

$$\boxed{\hat{p}(\theta) \propto \prod_{d \in [M]} \prod_{k \in [K]} \theta_{d,k}^{\alpha_k + \sum_n \gamma_{d,n}(k) - 1} \Rightarrow \hat{p}(\theta_d) \propto \mathrm{Dir}\left(\theta_d \,|\, \alpha + \textstyle\sum_n \gamma_{d,n}(k)\right)}$$

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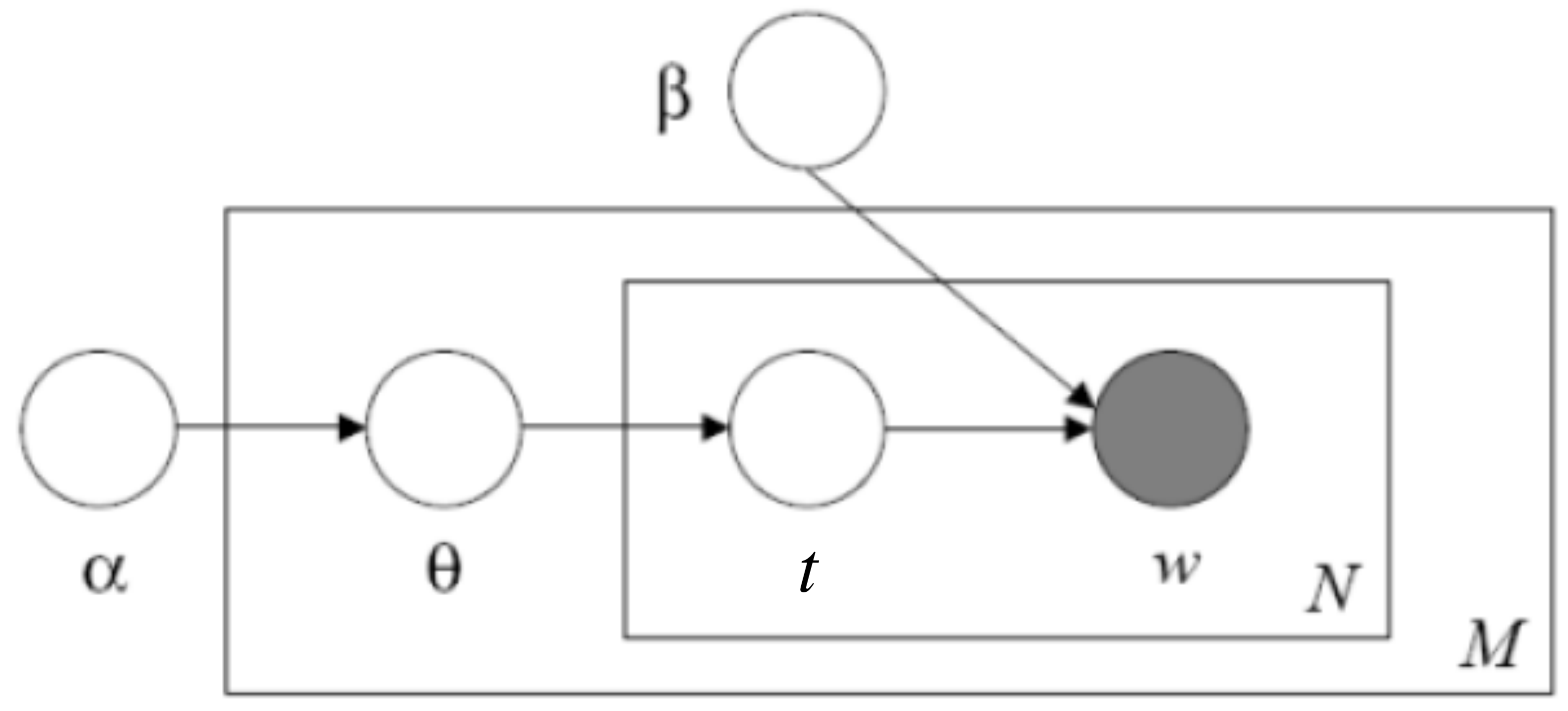

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$\perp\!\!\!\perp t$

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$$\boxed{\hat{p}(t) = \prod_d \prod_n \hat{p}(t_{d,n}) \Rightarrow \hat{p}(t_{d,n} = k) = \frac{\beta_{k, w_{d,n}} e^{E_{Q(\theta)}[\log \theta_{d,k}]}}{\sum_{k'} \beta_{k', w_{d,n}} e^{E_{Q(\theta)}[\log \theta_{d,k}]}}}$$

E step :

Objective :

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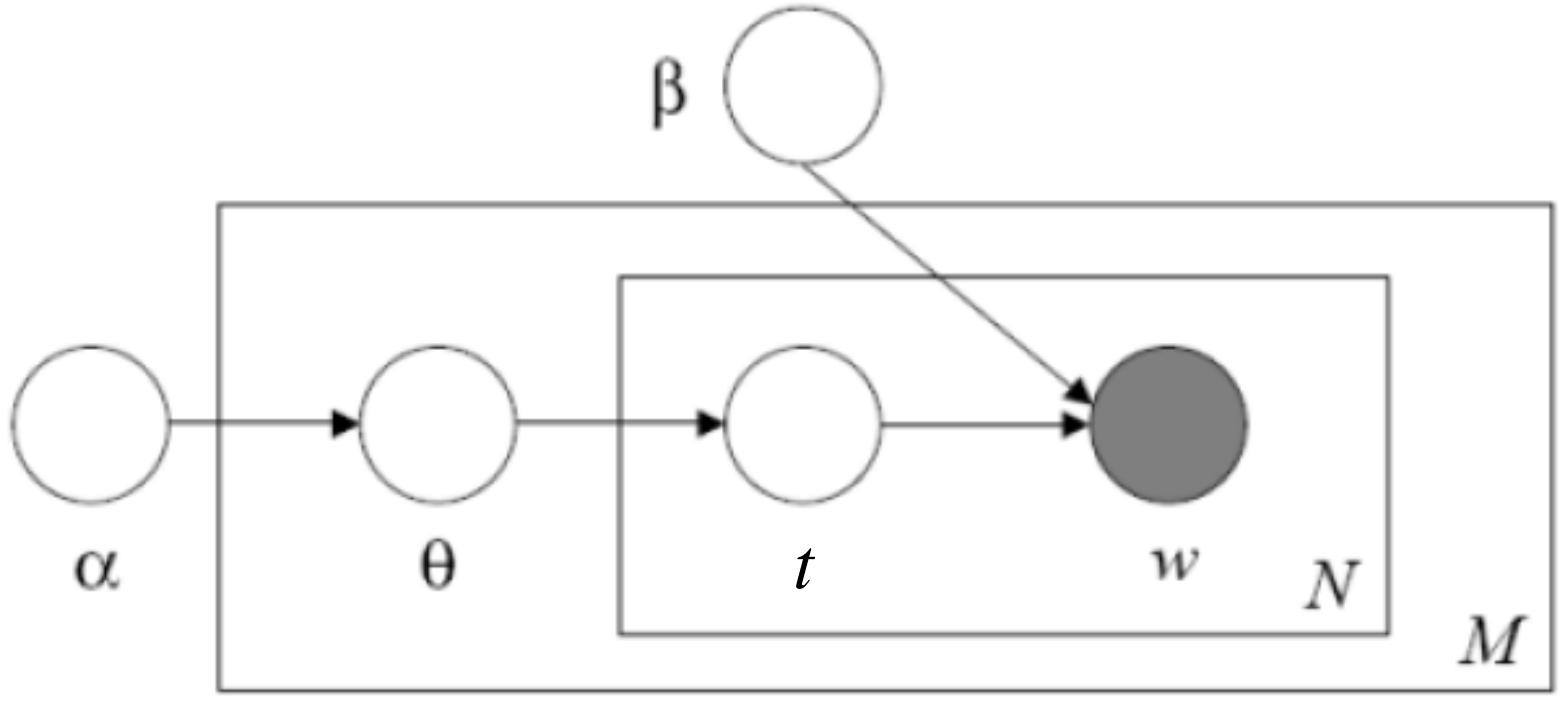

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M step :

Objective :

$E_{Q(\theta), Q(t)} \log P(\theta, t, w)$ to maximize w.r.t. β

$$\| $$

$$= E_{Q(\theta), Q(t)} \left[\sum_d \sum_n \sum_k \mathbb{1}_{\{t_{d,n} = k\}} \left(\log \beta_{k, w_{d,n}} \right) \right] + \underbrace{\text{const}}^{\perp\!\!\!\perp\, \theta, t}$$

with the following constraint : $\begin{cases} \beta_{k,w} \geq 0 \\ \sum_w \beta_{k,w} = 1 \text{ for all } k \in [K] \end{cases}$

Let's compute the Lagrange

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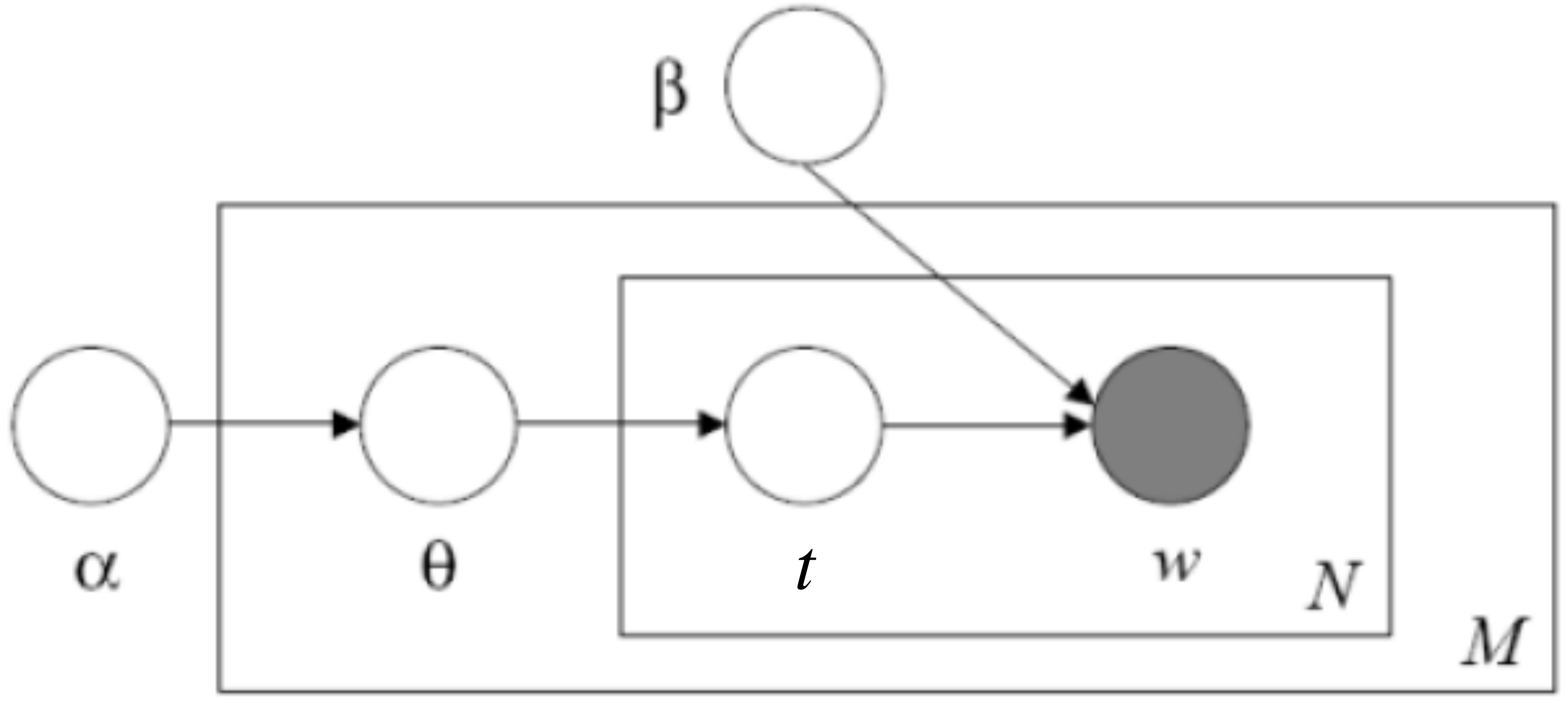

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$$\parallel$$

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with the following constraint : $\begin{cases} \beta_{k,w} \geq 0 \\ \sum_w \beta_{k,w} = 1 \text{ for all } k \in [K] \end{cases}$

Let's compute the Lagrange

Reminder : in order to max $f(x)$ with $g(x) = 0$ constraint :

denote the Lagrangian function : $L(x, \lambda) = f(x) - \lambda g(x)$

and find the stationary point.

$$L(x, \lambda) = \sum_d \sum_n \sum_k \gamma_{d,n}(k) \left(\log \beta_{k,w_{d,n}} \right) - \sum_k \lambda_k \left(\sum_w \beta_{k,w} - 1 \right)$$

$$\frac{\partial L}{\partial \beta_{k,w}}(x, \lambda) = 0 \iff \boxed{\beta_{k,w} = \frac{\sum_{d,n,k} \gamma_{d,n}(k)\, \mathbb{1}_{\{w_{d,n}=w\}}}{\sum_{w',d,n,k} \gamma_{d,n}(k)\, \mathbb{1}_{\{w_{d,n}=w'\}}}}$$

left as exercise

4 Application and examples : notebook

Application and examples

website : https://curiousml.github.io/

- Master of Science in Artificial Intelligence Systems : **Bayesian Machine Learning** by François HU
  - **Lecture 1** : Bayesian statistics [Lecture]
  - **Lecture 2** : Latent Variable Models and EM-algorithm [Lecture]
  - **Lecture 3** : Variational Inference and intro to NLP [Soon available]
  - **Lecture 4** : Markov Chain Monte Carlo [Soon available]
  - **Lecture 5** : [Oral presentations]
  - **Training session / prerequisite :** Statistics with python [Notebook], [Data]
  - **Practical work 1** : Conjugate distributions [Notebook] [Correction]
  - **Practical work 2** : Probabilistic K-means and probabilistic PCA [Notebook]
  - **Practical work 3** : Topic Modeling with LDA [Notebook]
  - **Practical work 4** : MCMC samples [Soon available]

TODO

! Road map

Bayesian statistics

1

Bayesian perspective :

Likelihood

Prior distribution

$$P(\theta|X) = \frac{P(X,\theta)}{P(X)} = \frac{P(X|\theta)\cdot P(\theta)}{P(X)}$$

Posterior distribution

Evidence

Hard to compute !

θ parameters

X observations

Exemple :
Naive Bayes classifier,
Linear regression, ….

MAP : $\arg\max_{\theta} P(X|\theta)\cdot P(\theta)$

Conjugate distribution

Pros :	Cons :
- exact posterior	- conjugate prior maybe inadequate

Latent variable models

2

Hidden variable models :

$$P(X|\theta) = \sum_{t \in T_{indexes}} P(X, T = t|\theta)$$

$$P(X,T|\theta) = P(X|T,\theta)P(T|\theta)$$

Exemple :
GMM, K-means, PCA/PPCA

Pros :	Cons :
- fewer parameters / simpler models - hidden variable sometimes meaningful - clustering / dimensionality reduction	- harder to work with - requires math - only local maximum or saddle point - EM : the posterior of T could be intractable

Variational Inference

3

Deterministic approximation of posterior :

$$p(Z|X) = \frac{P(X|Z)\cdot P(Z)}{P(X)}$$

Mean Field Approximation !

Exemple :
Topic modelling, LDA trained by VI

Pros :	Cons :
- Useful when the posterior is intractable - Suited to large dataset	- can never generate exact result

Markov Chain Monte Carlo

4

Extensions

5