Bayesian Machine Learning

31/05/21 - 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**

0 Remarks

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**

1. Variational Inference for probabilistic models

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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

Posterior distribution

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- **Approximate inference.** Approximate $P_X(Z) \approx \hat{P}_X(Z)$
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1. Variational Inference for probabilistic models

Variational Inference : Definition

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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

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Posterior

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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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Fixed by **model** — **Likelihood**

Fixed by **us** — **Prior**

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

Evidence — Fixed by **data**

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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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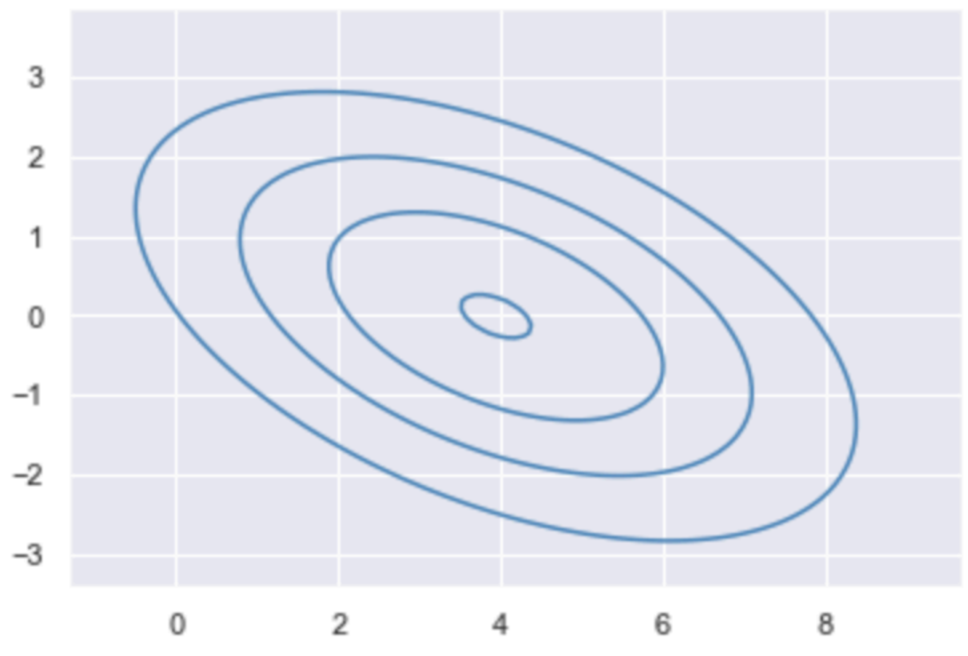
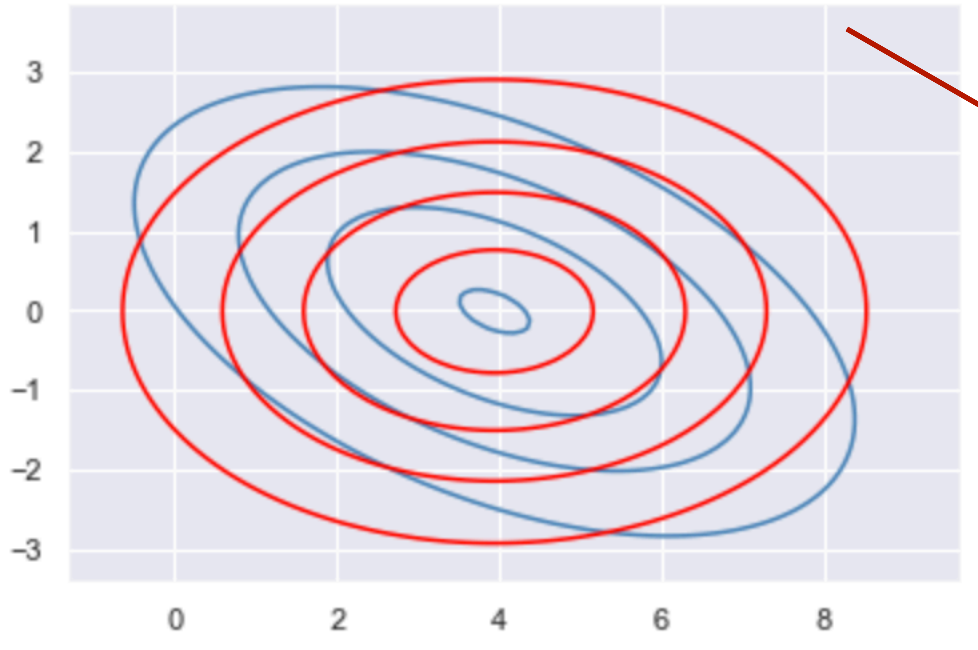
Example : Normal distribution

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



Mean Field

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



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

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Optimization algorithm : coordinate descent

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

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&\ldots \\
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\end{aligned}\right\}$$

Repeat until convergence with

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Optimal solution in Mean Field

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

$$\Longleftrightarrow$$

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

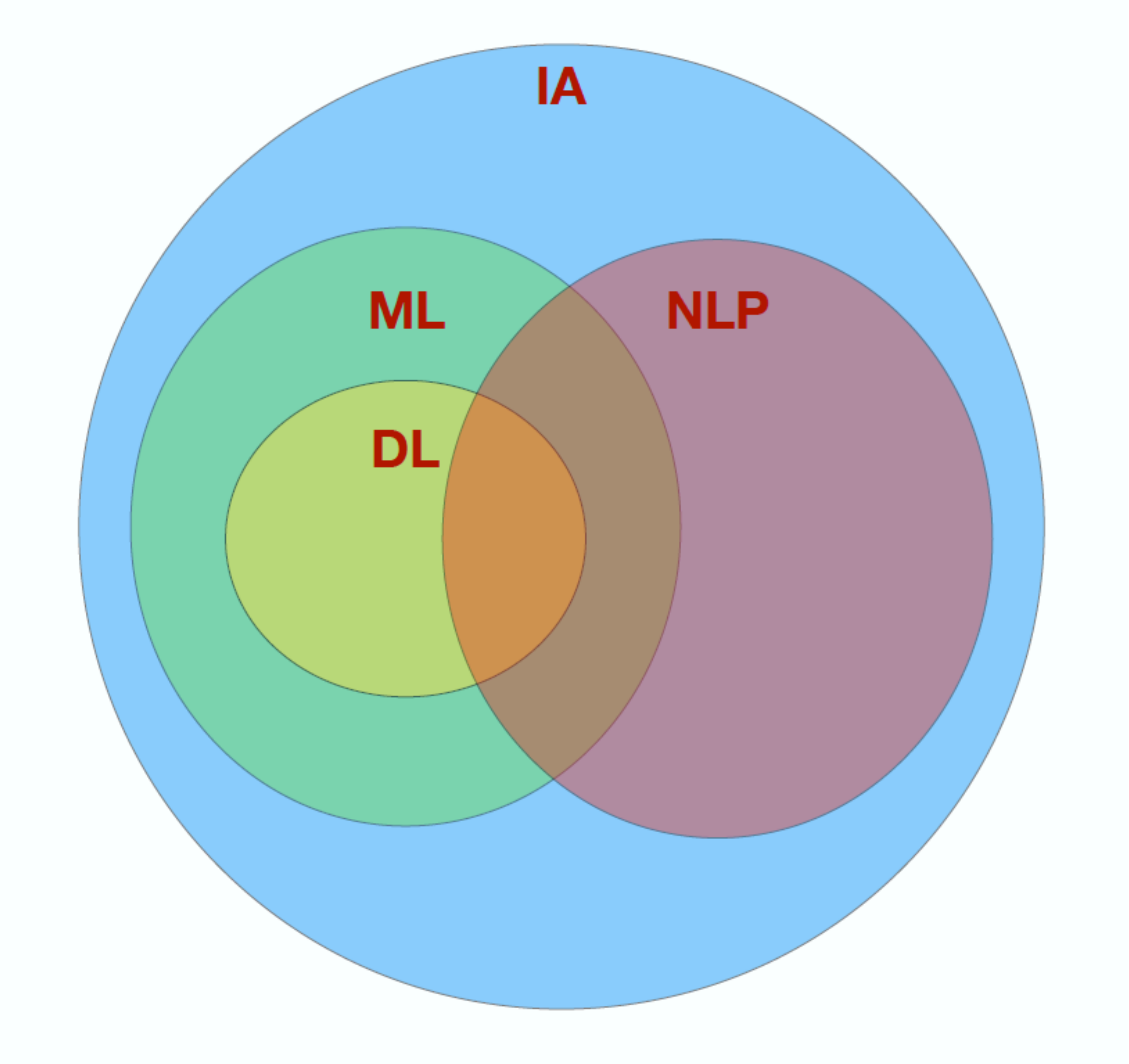
We will see in section 3 an example with the model LDA

2 Introduction to NLP

2. Introduction to NLP

Preprocessing : Tokenization

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



2. Introduction to NLP

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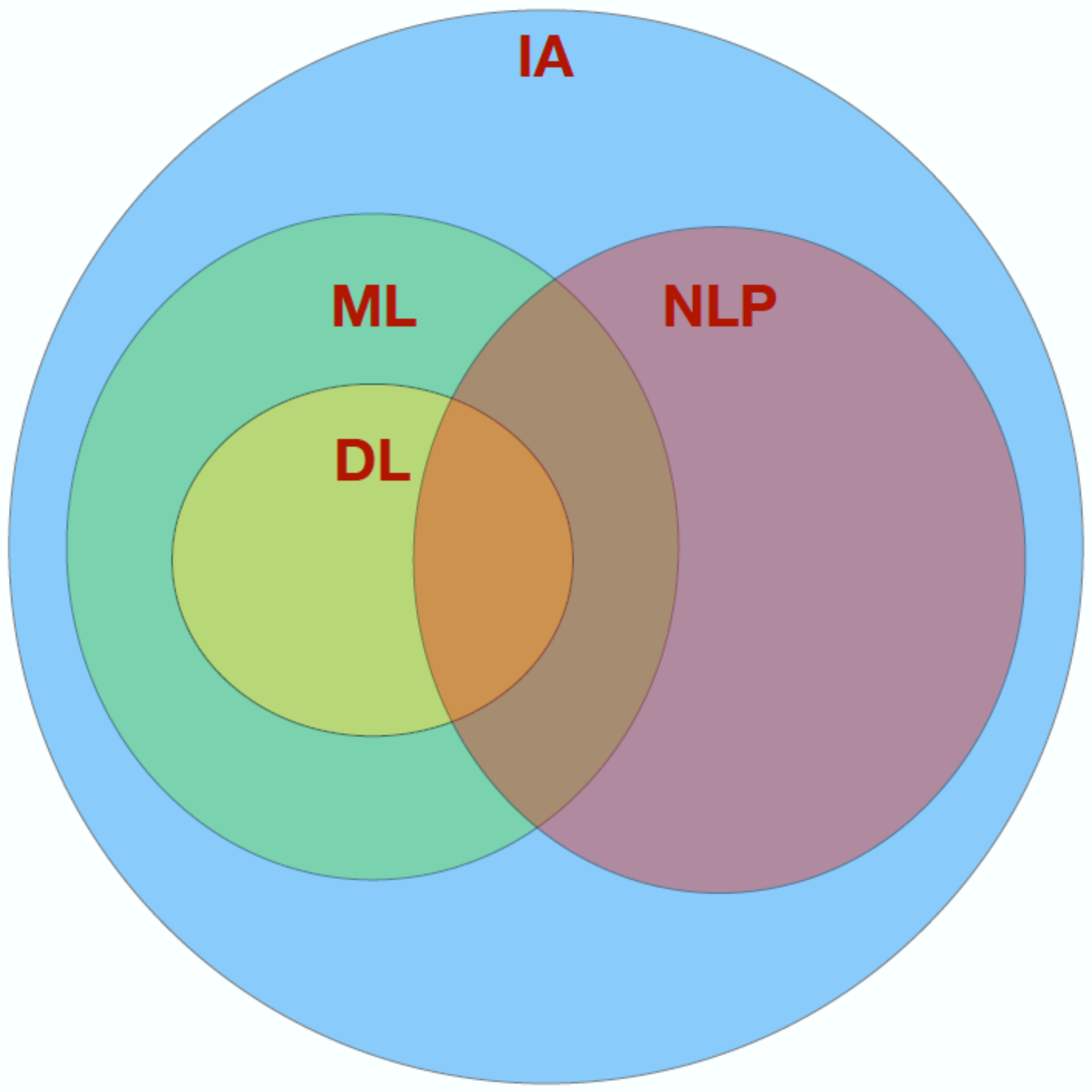

Some intuitions : we want to perform some learning tasks with textual data

- 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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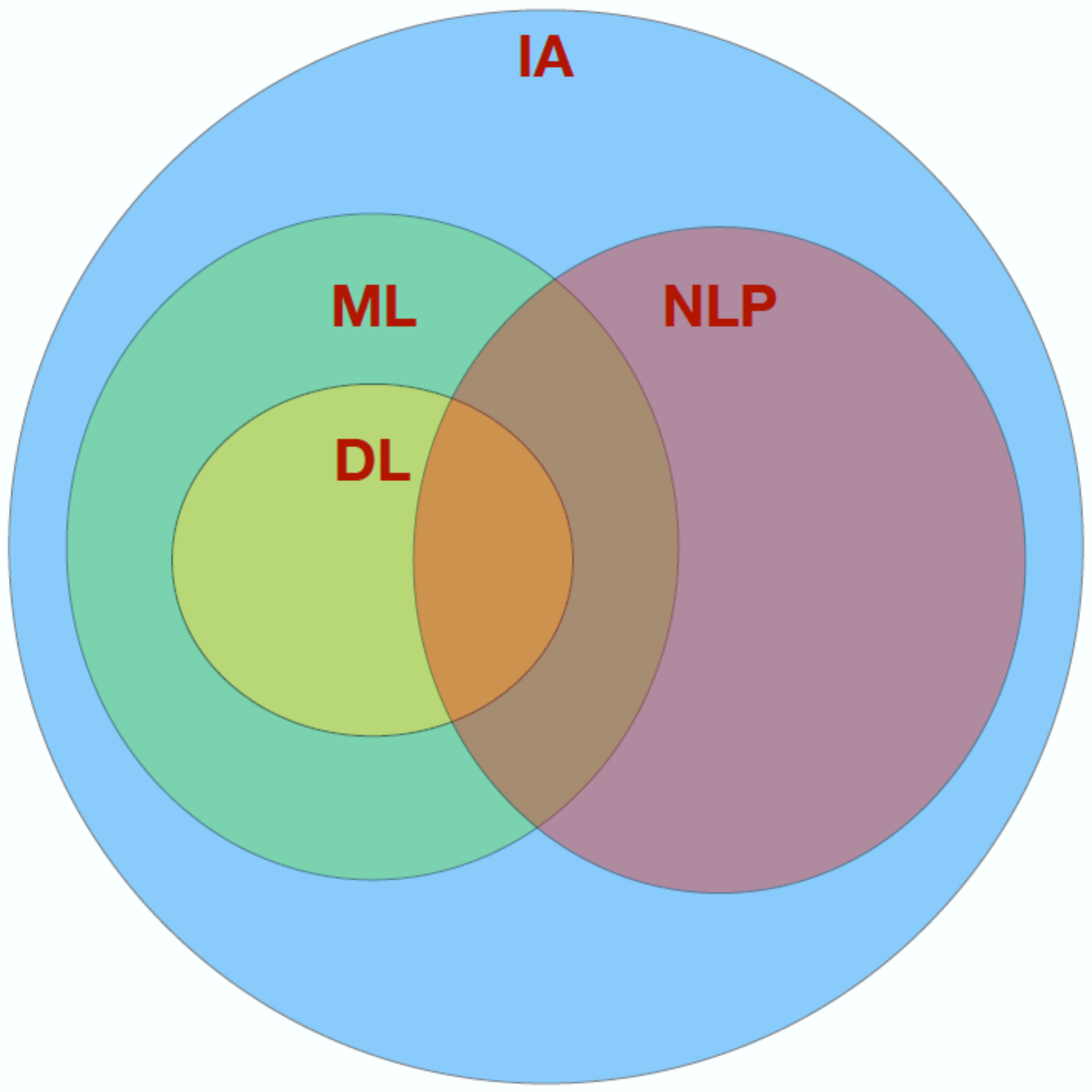

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- **Text** : sequence of words
- **Word** : sequence of logical characters
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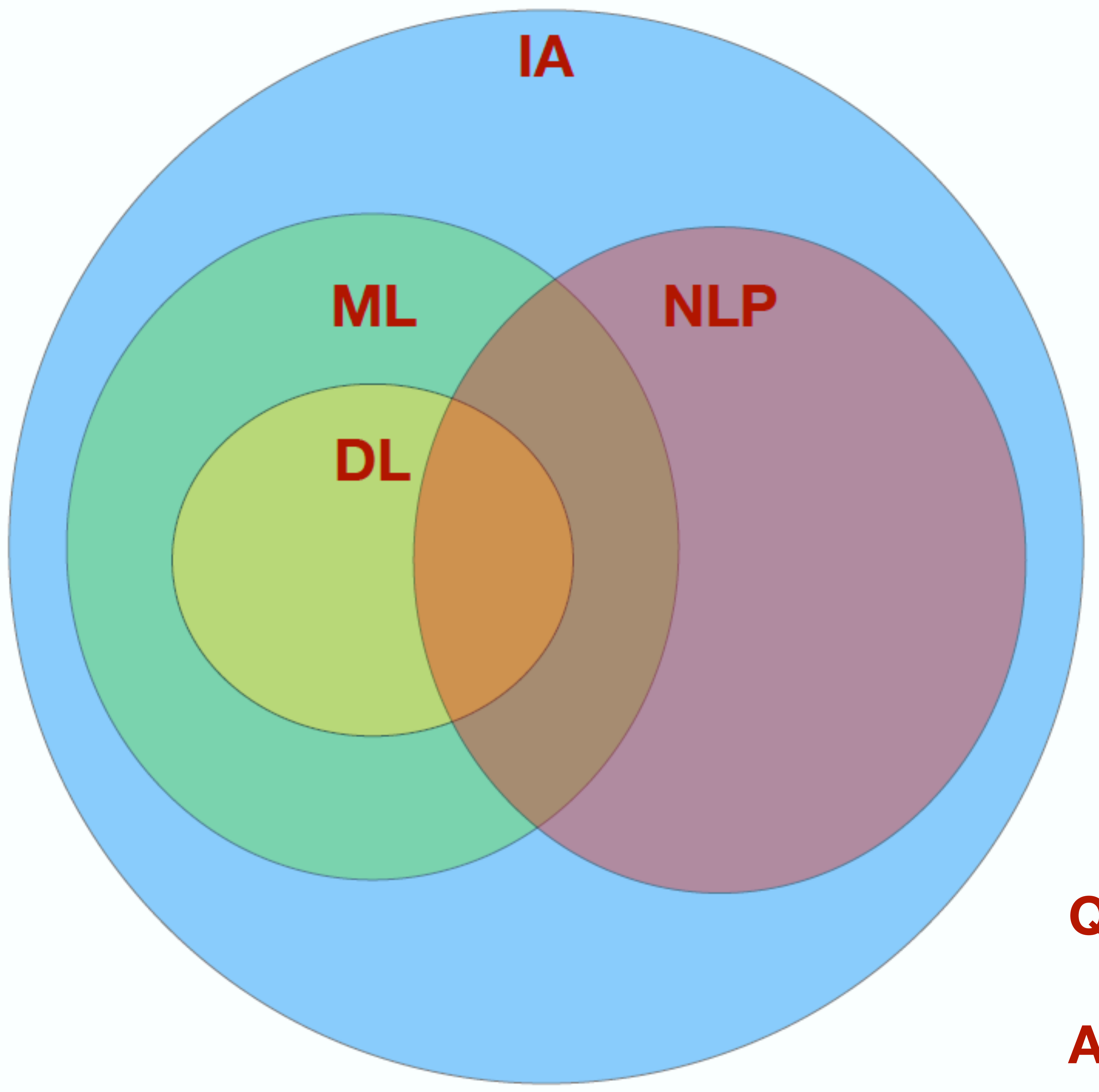

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Question : how to find the limits of a word?

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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Example : wait, waiting, waited, waits → wait

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

Example : study, studying, studies → 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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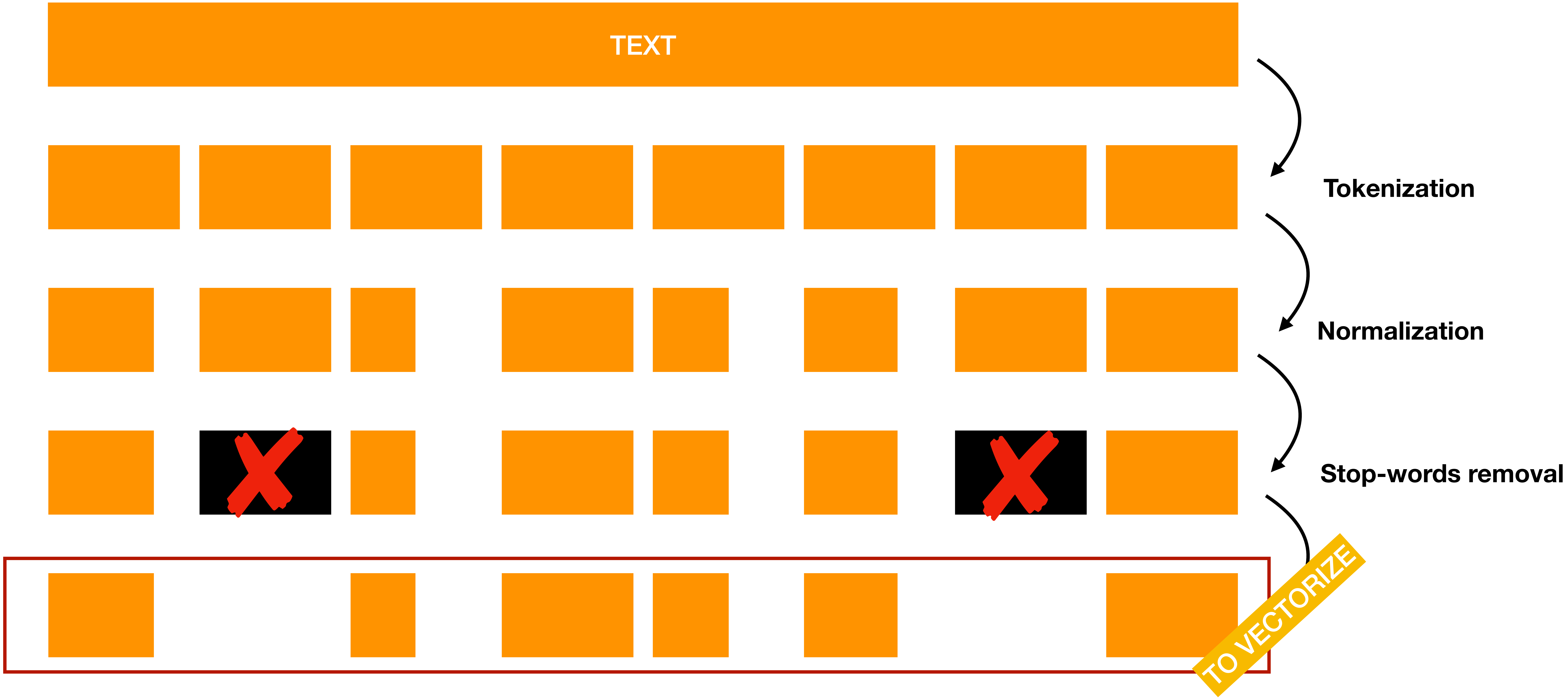
2. Introduction to NLP

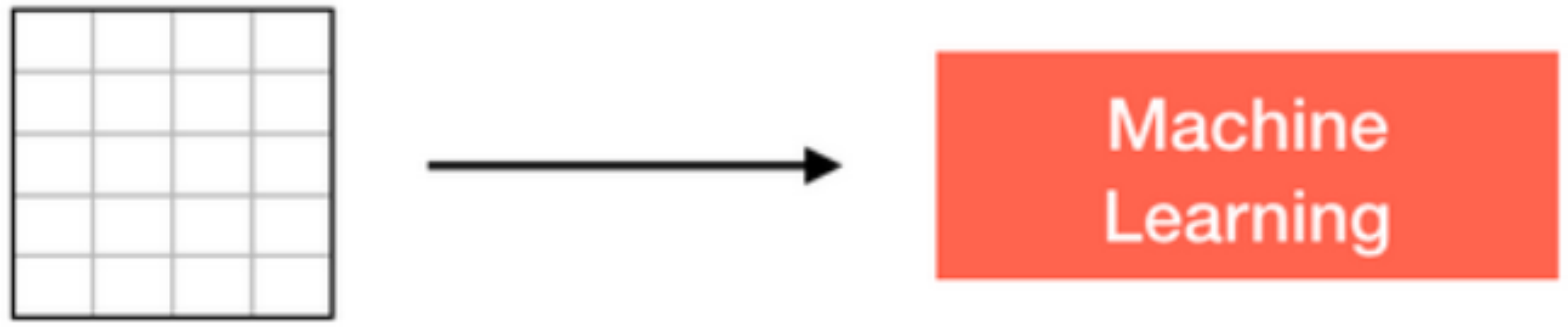
Preprocessing : overview



2. Introduction to NLP

Processing : Textual data into tabular data

For tabular data :



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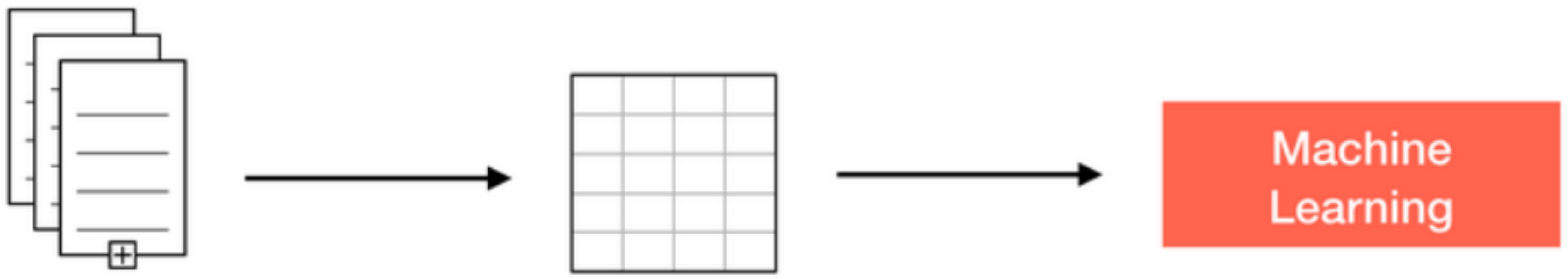

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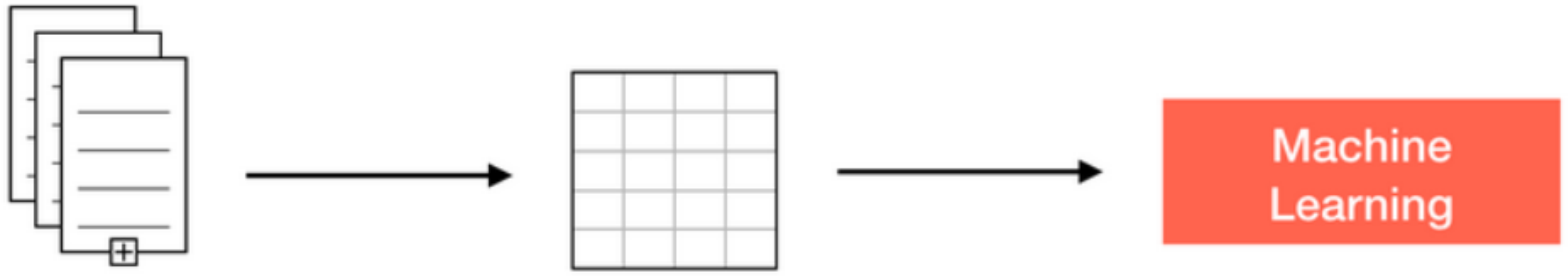
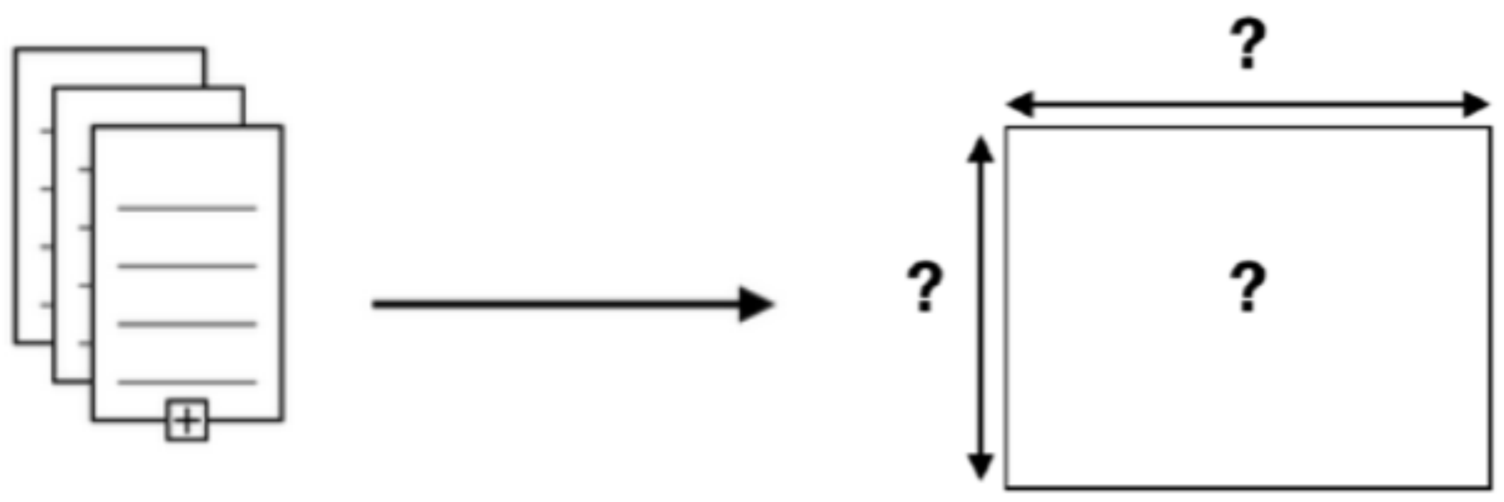


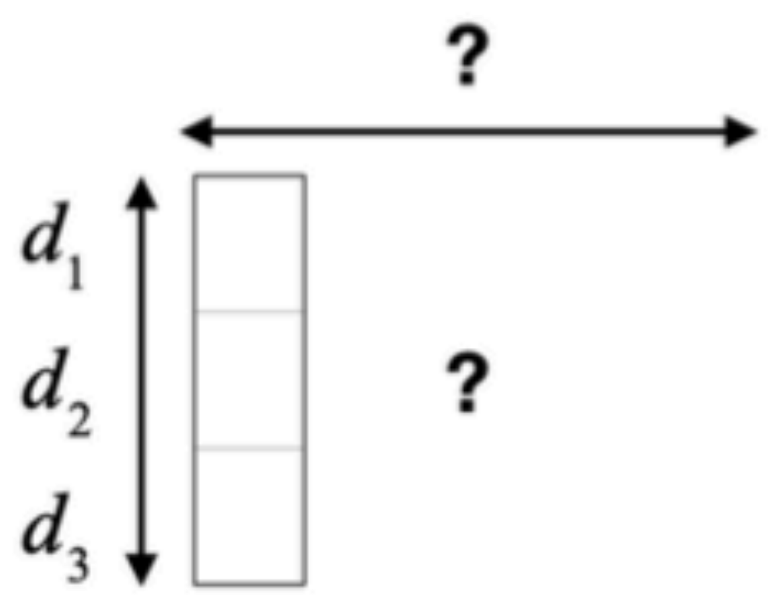
Problems :



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



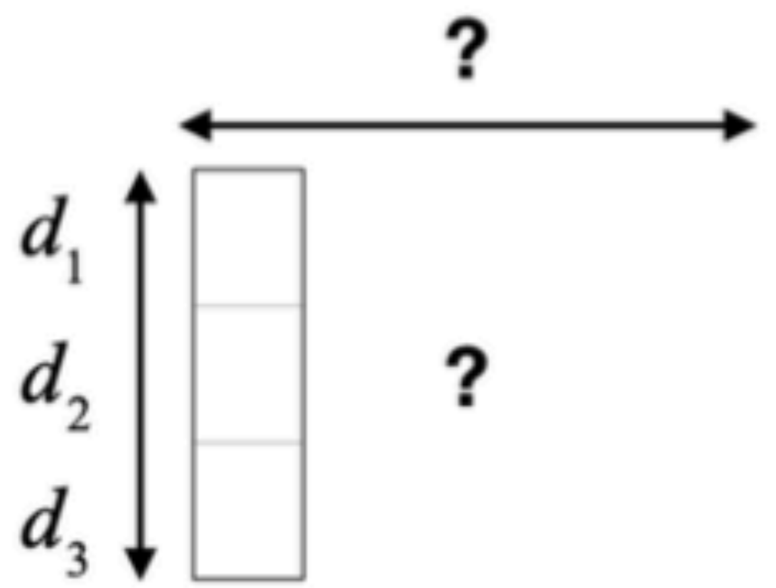
2. Introduction to NLP

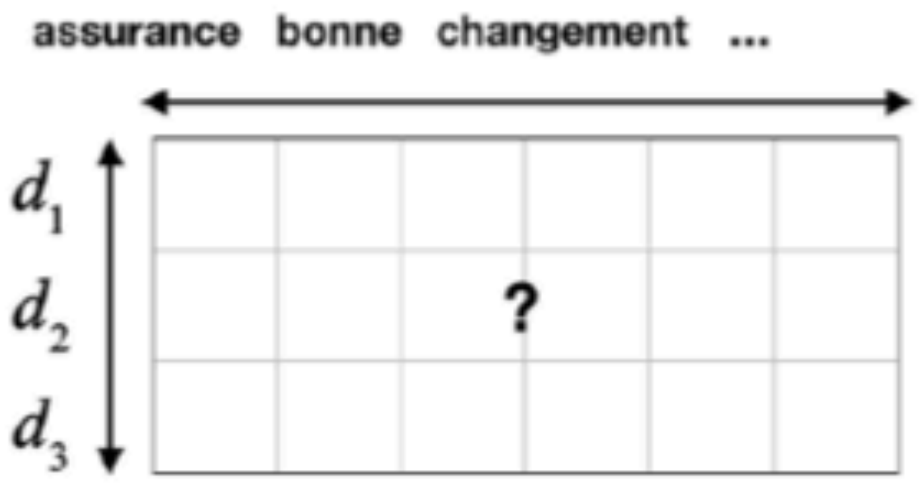
Processing : Textual data into tabular data

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
    }
```





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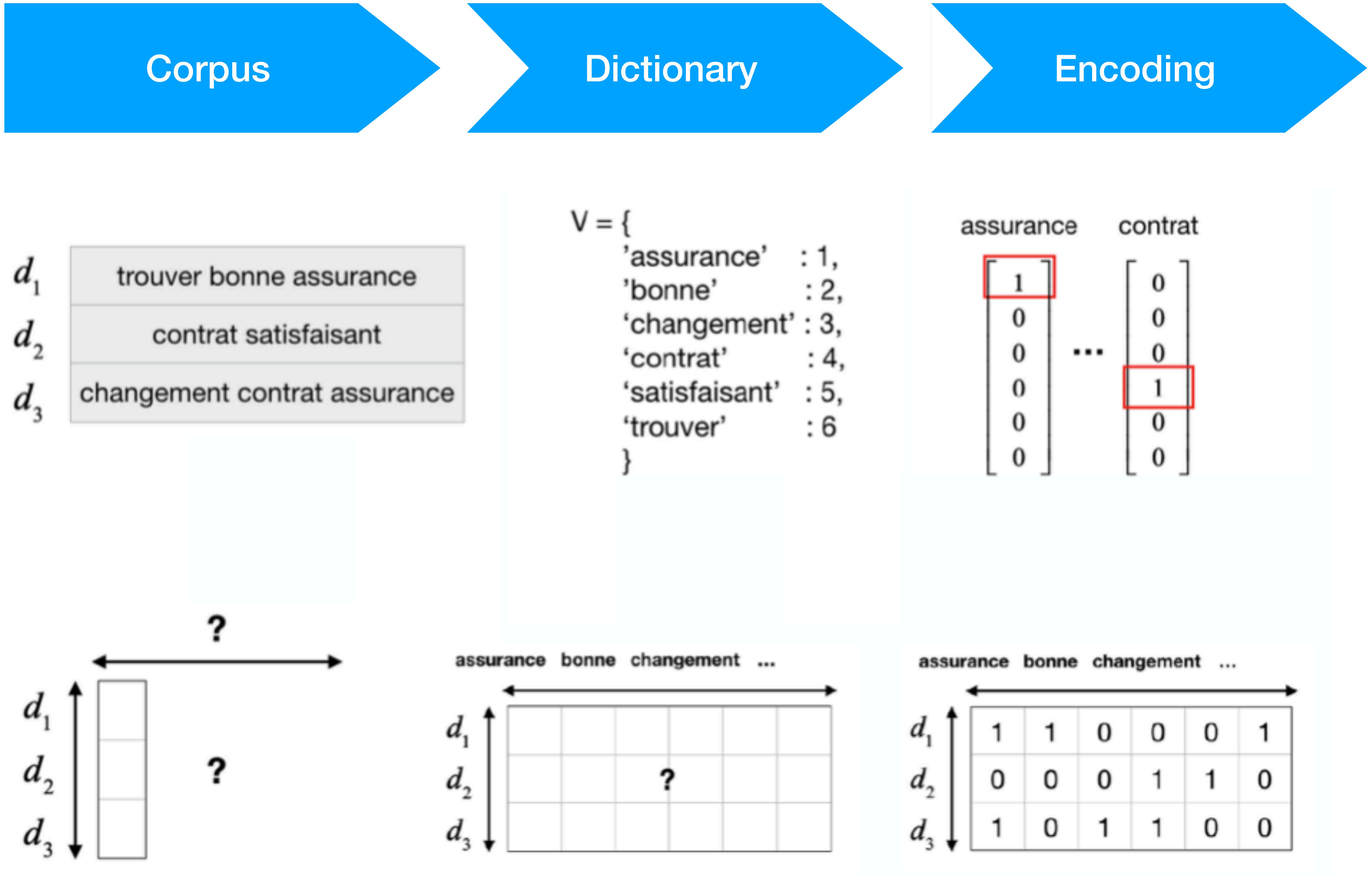

Bag-of-Words approach

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) :**

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

  - **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

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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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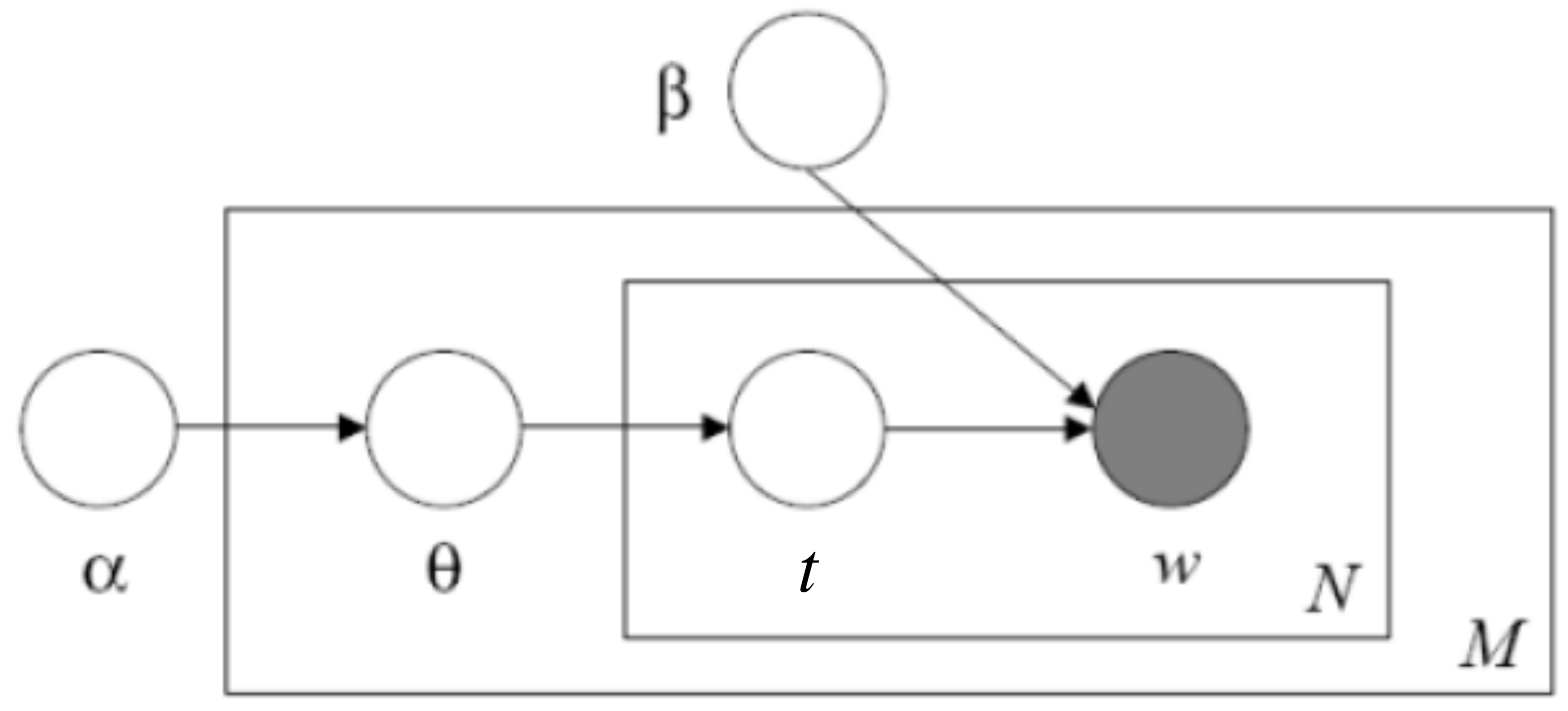
Idea :

- 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



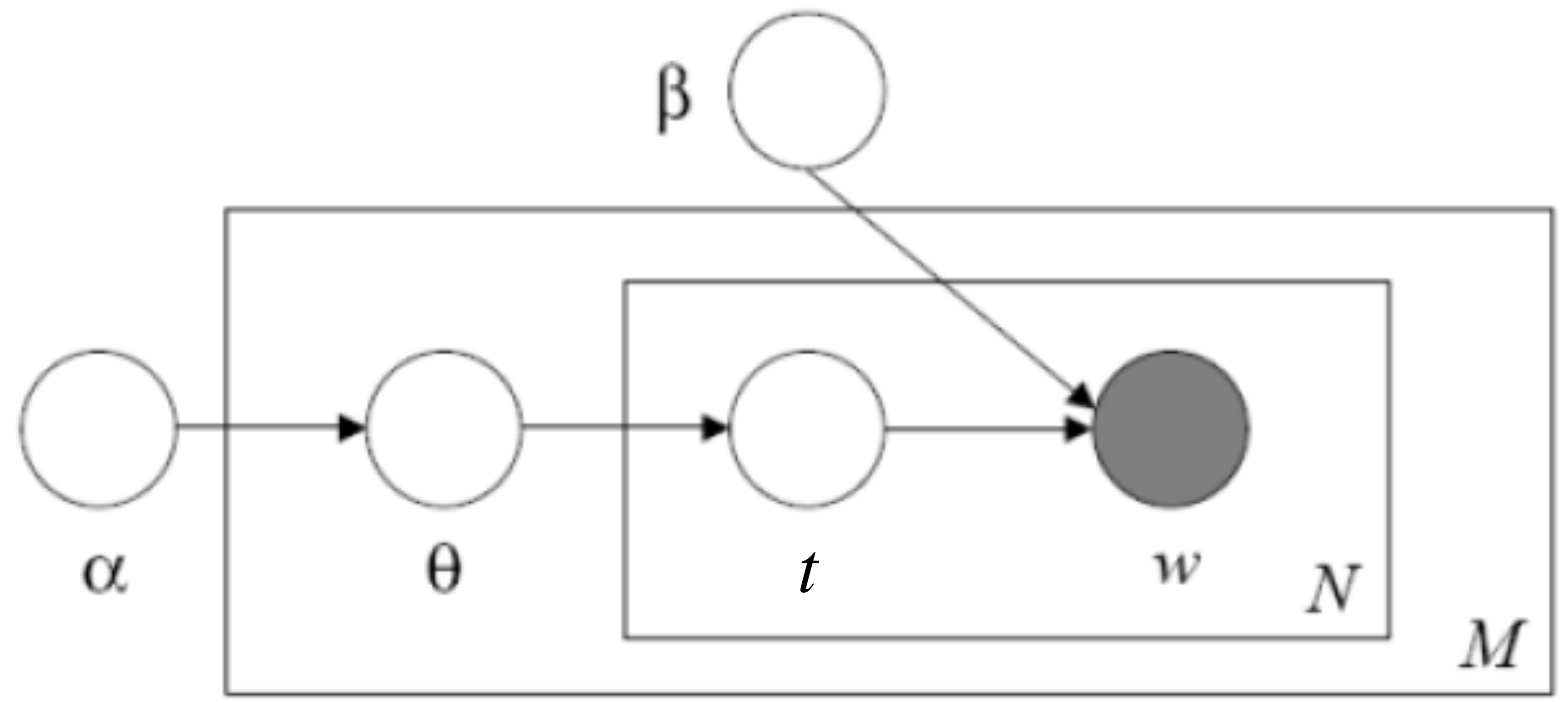
$$P(\theta, t, w \,|\, \alpha, \beta) = P(\theta \,|\, \alpha) \cdot P(t \,|\, \theta) \cdot P(w \,|\, t, \beta)$$

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

3. Latent Dirichlet Allocation

LDA : high-level view

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



~ Dirichlet ~ Multinomial ~ Multinomial

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

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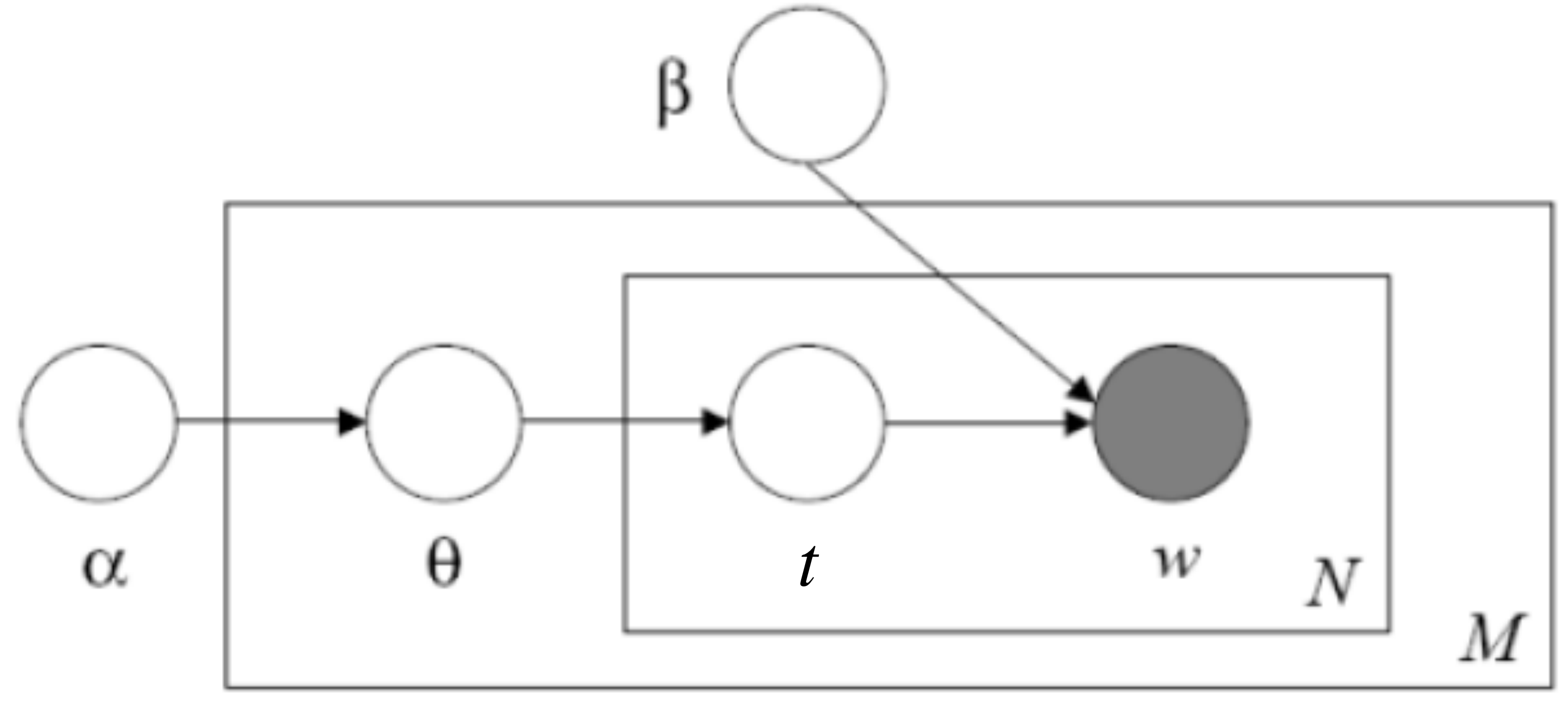
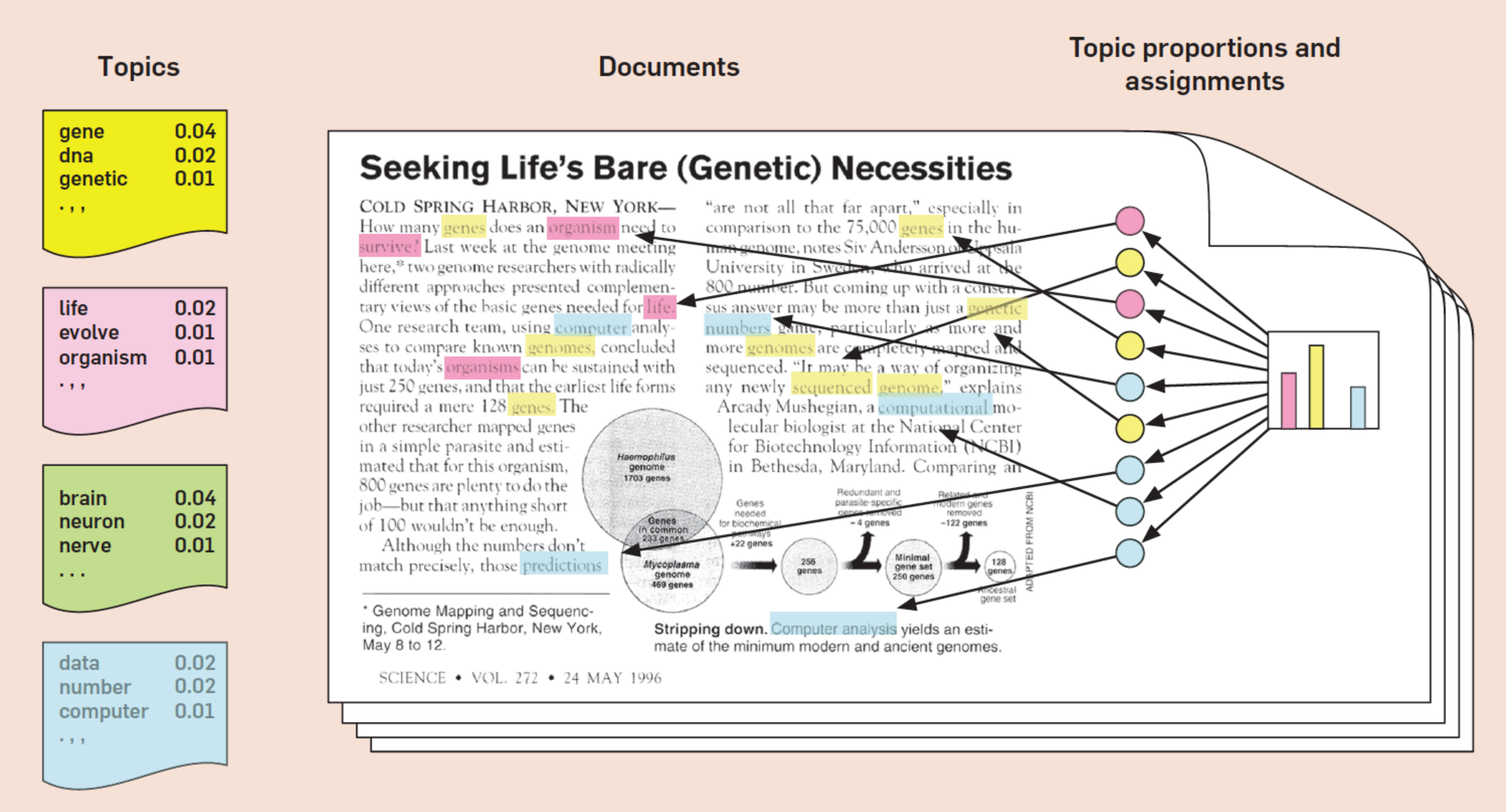


~ Dirichlet ~ Multinomial ~ Multinomial

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

$$= \prod_{d \in [M]} \underbrace{P(\theta_d \mid \alpha)}_{\sim \text{ Dirichlet}} \cdot \prod_{n \in [N]} \underbrace{P(t_{d,n} \mid \theta_d)}_{\sim \text{ Multinomial}} \cdot \underbrace{P(w_{d,n} \mid t_{d,n}, \beta)}_{\sim \text{ Multinomial}}$$

Example :



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

Assumption on the generation of texts :

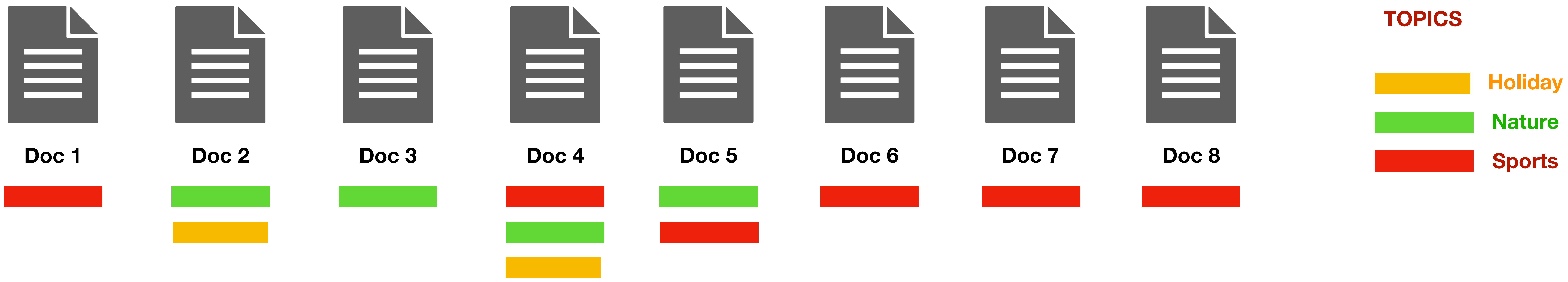
For each of M documents d,

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

3. Latent Dirichlet Allocation

LDA : Dirichlet distribution

Dirichlet distribution (dimension 3) :



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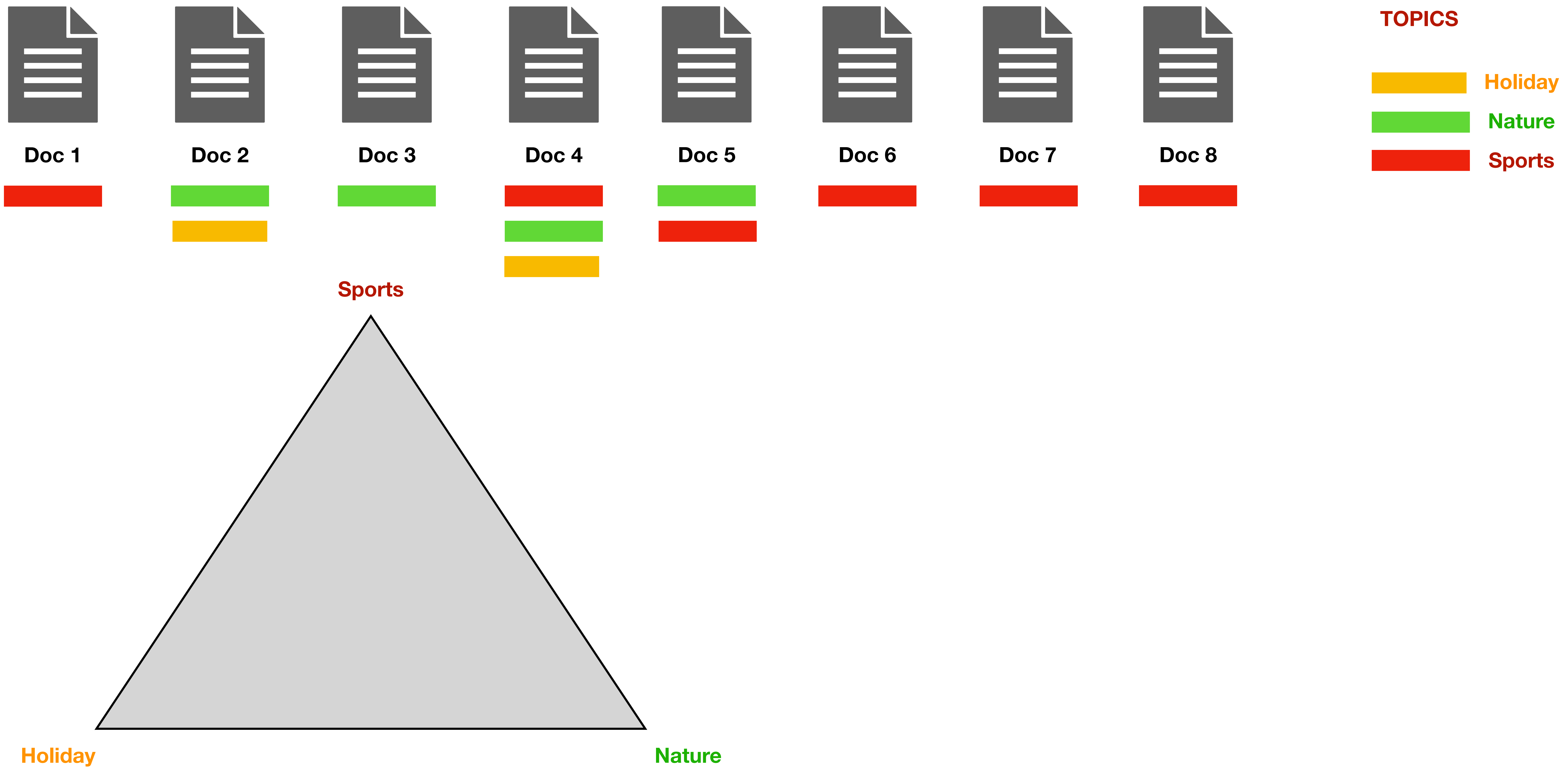
Dirichlet distribution (dimension 3) :



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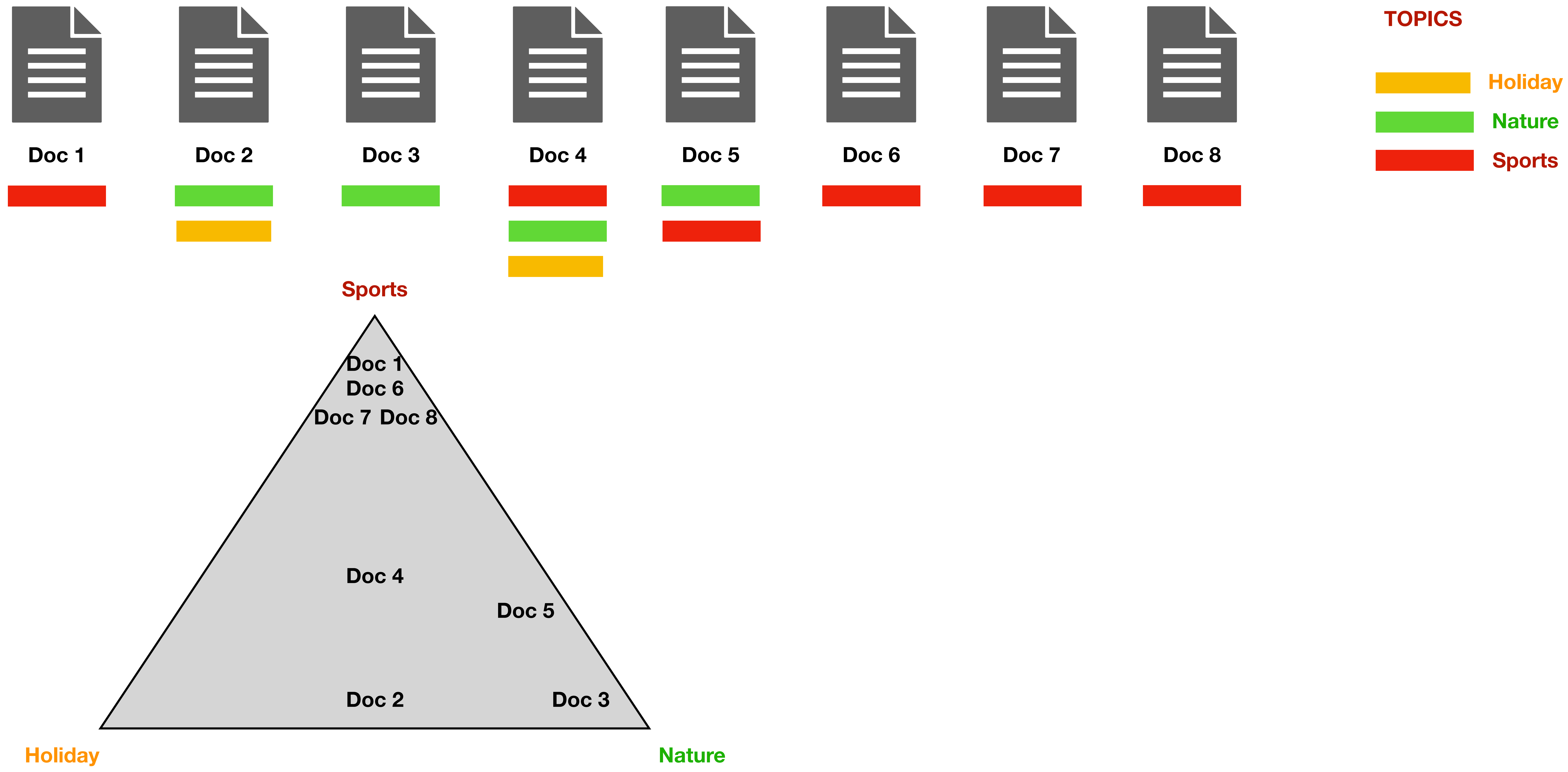

3. Latent Dirichlet Allocation

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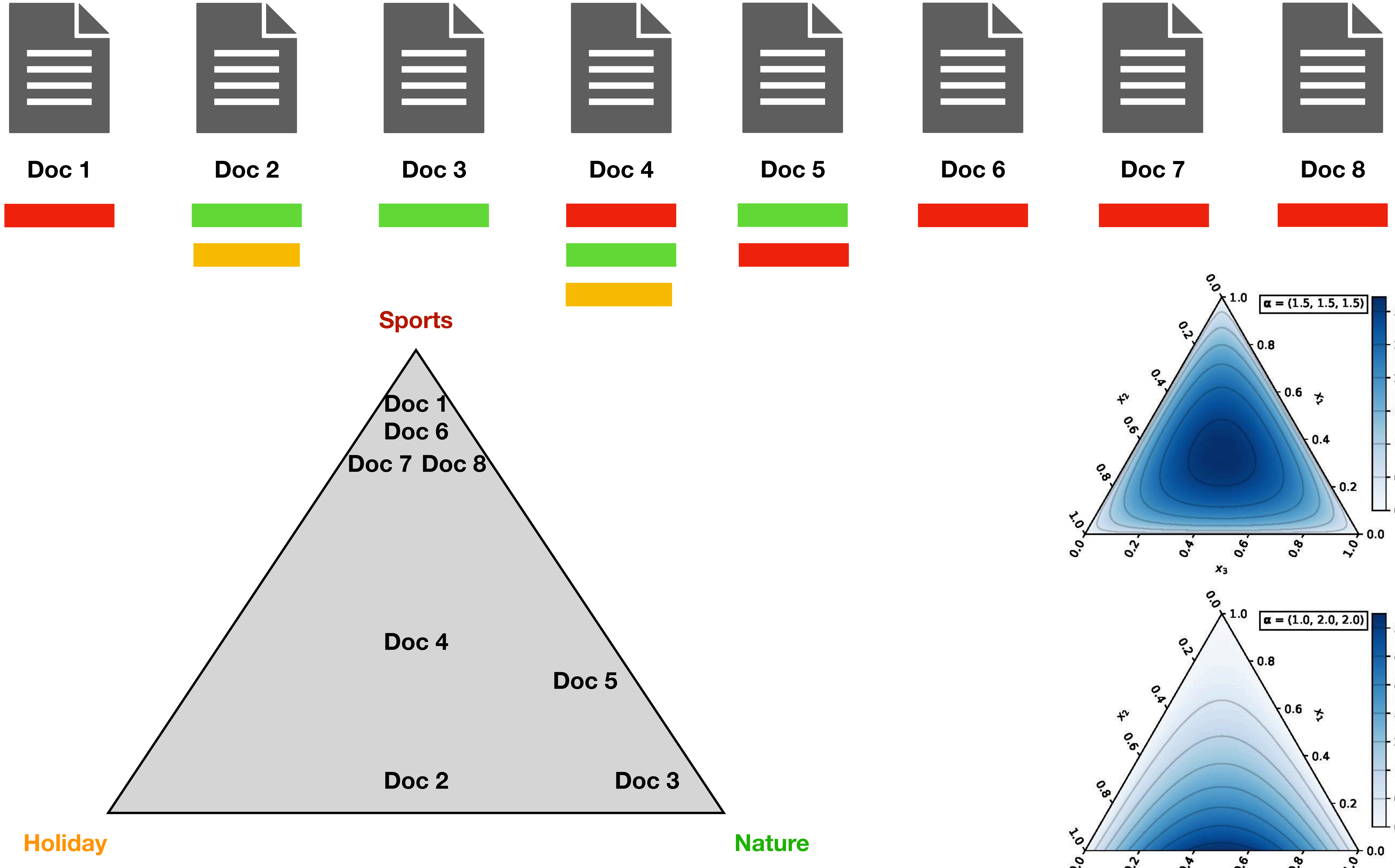
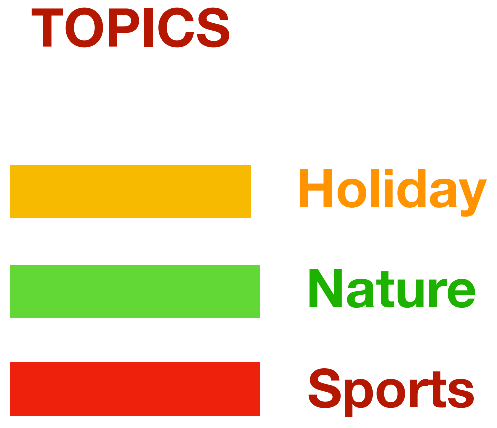
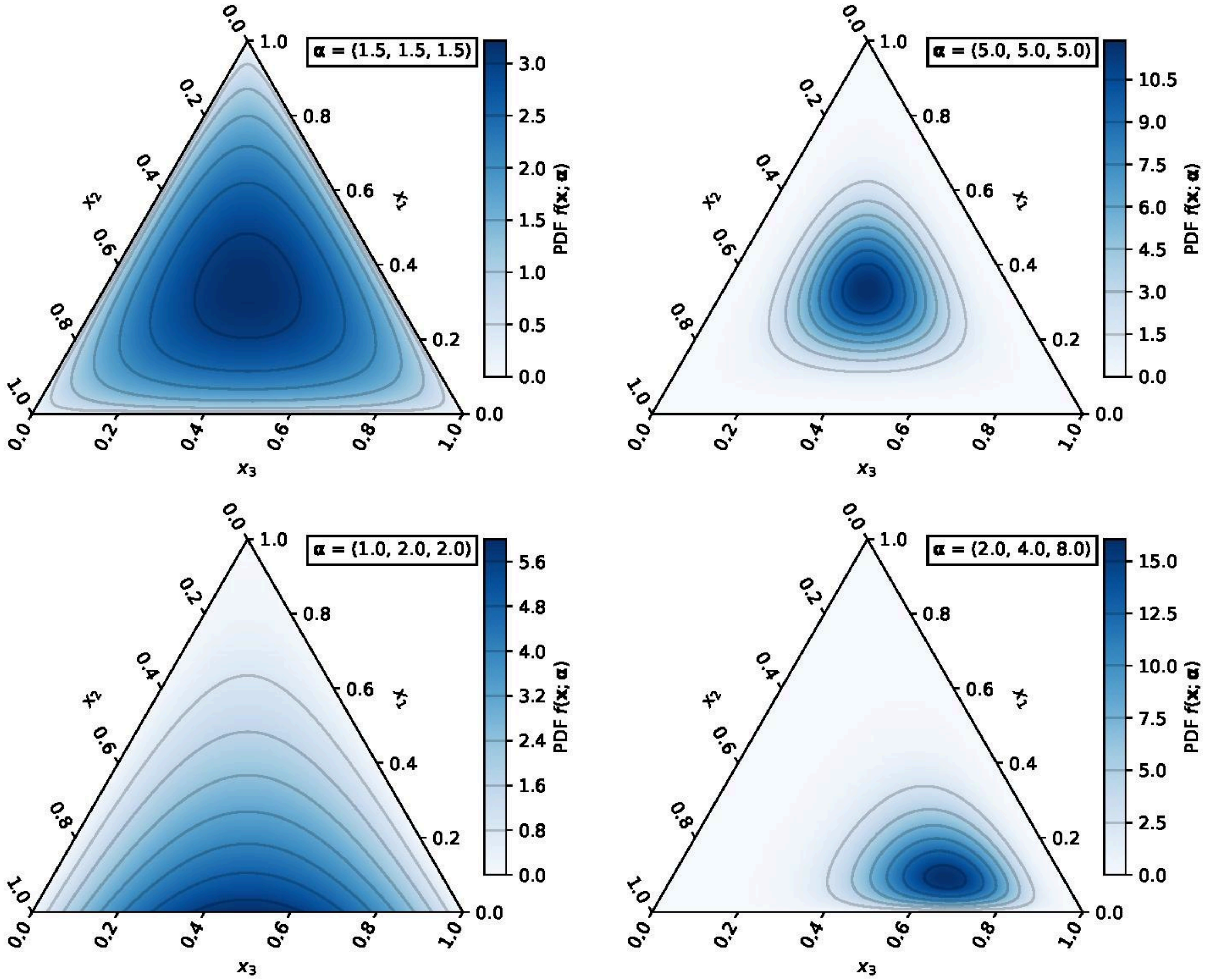
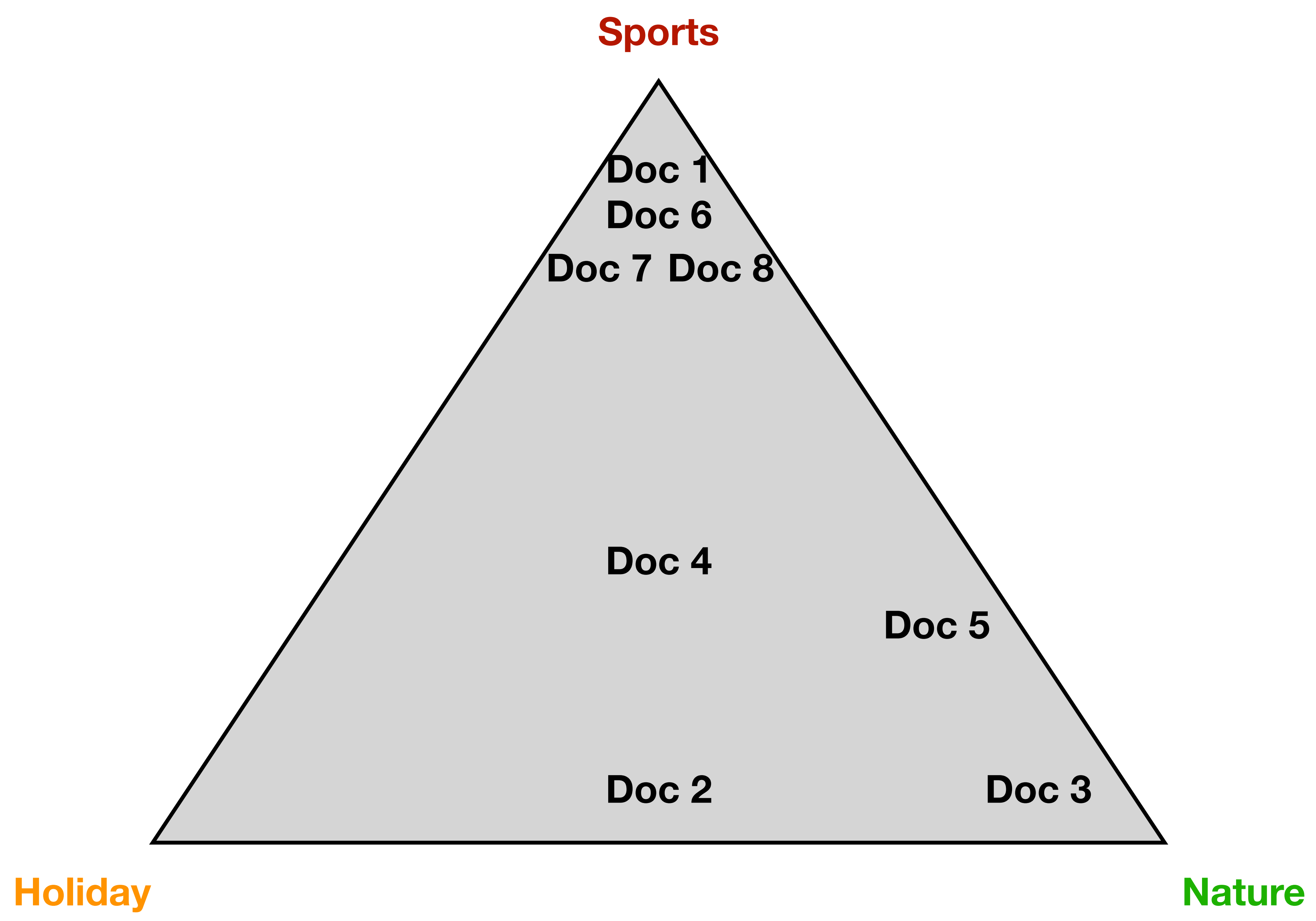






3. Latent Dirichlet Allocation

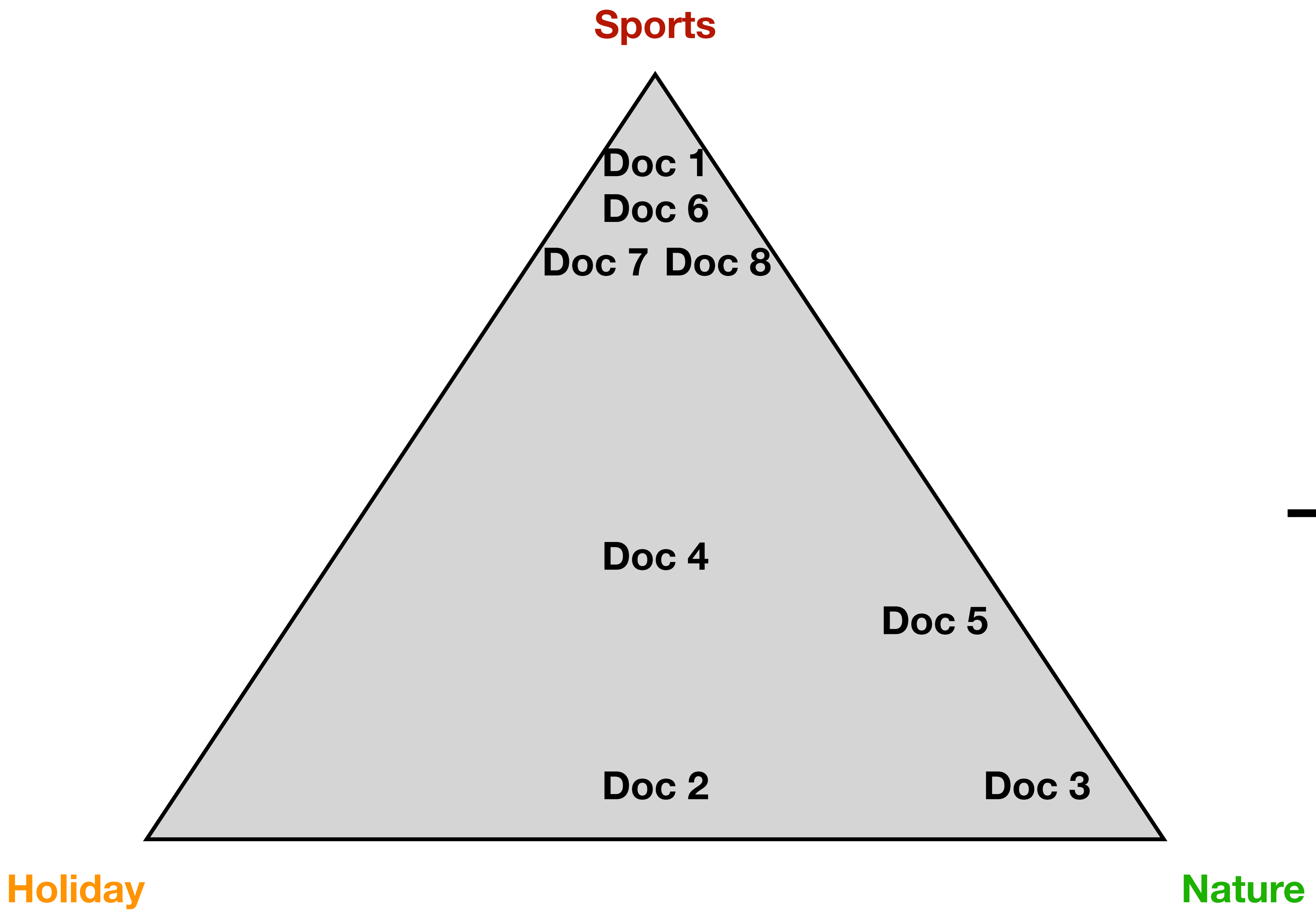
LDA : Multinomial distribution



Dirichlet distribution
« distribution of distribution »

3. Latent Dirichlet Allocation

LDA : Multinomial distribution

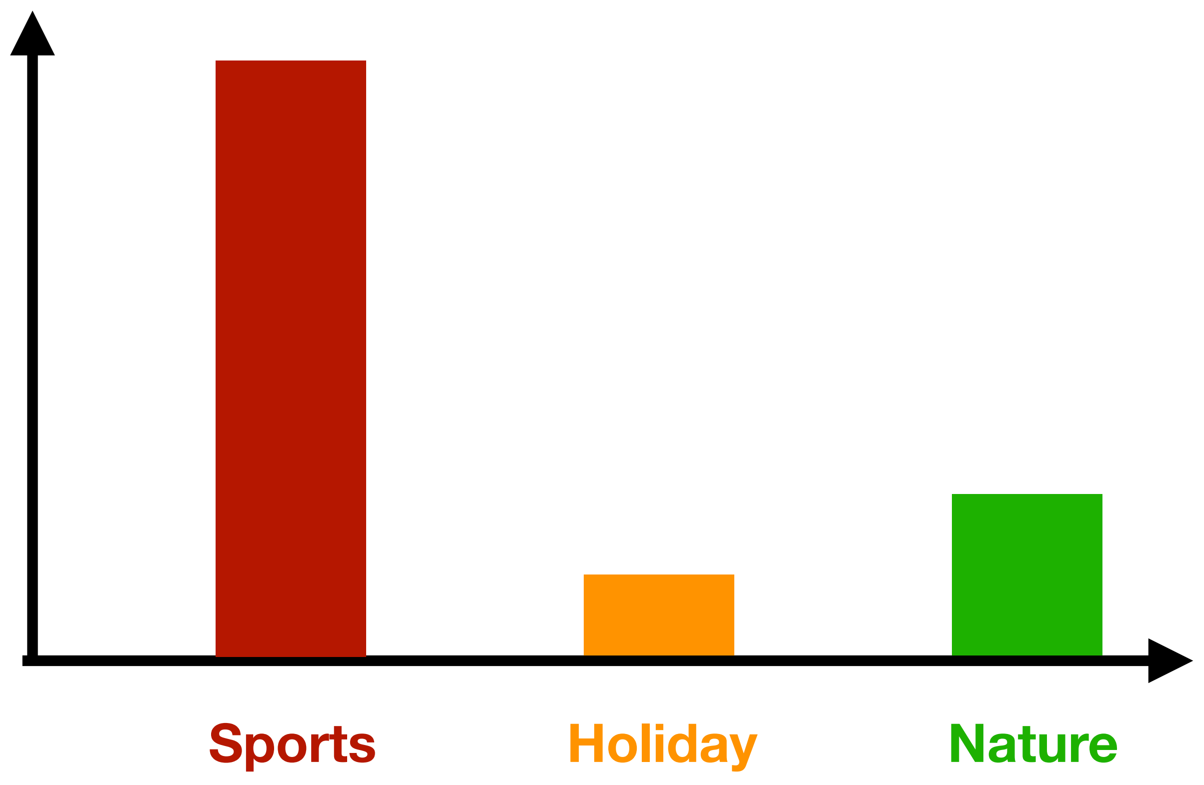


Dirichlet distribution
« distribution of distribution »

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

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

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

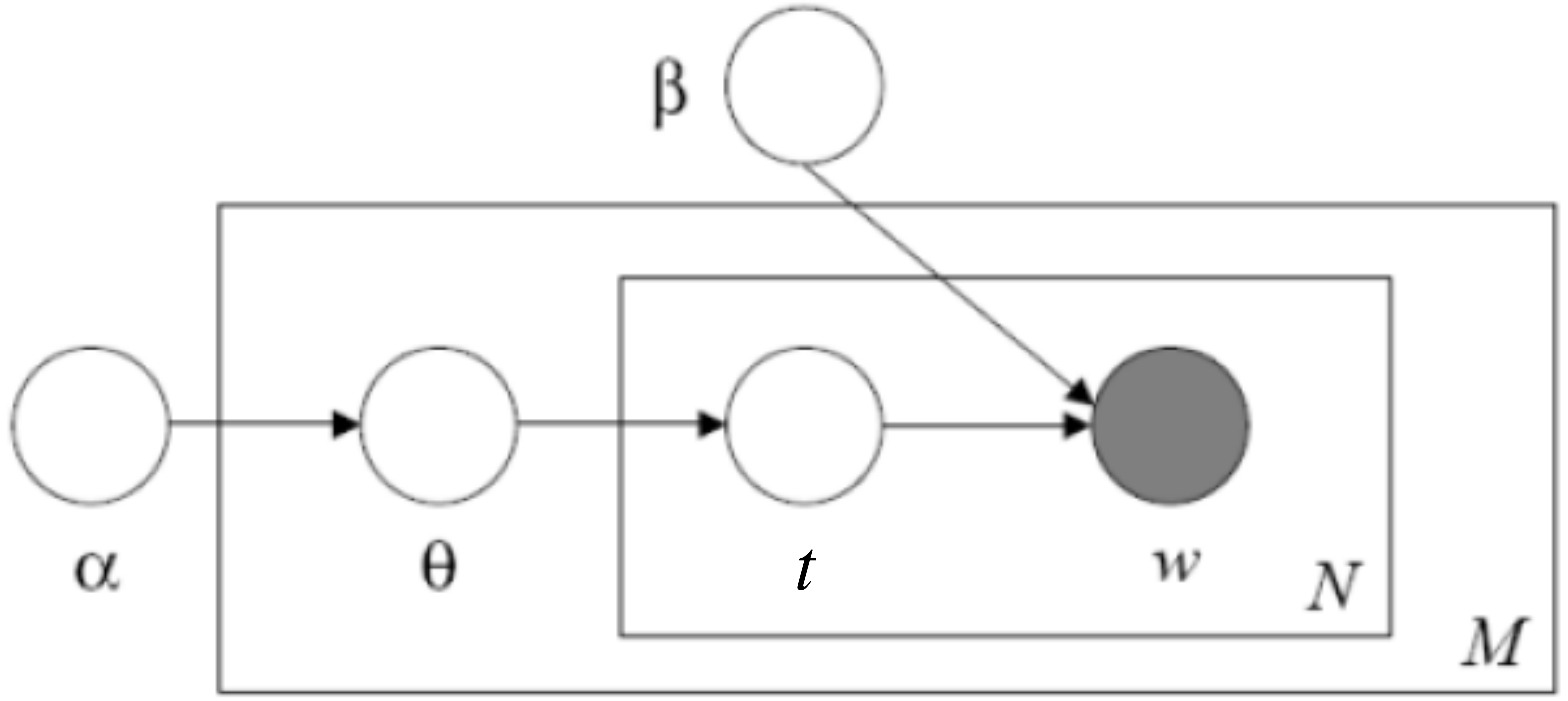


Multinomial distribution

3. Latent Dirichlet Allocation

LDA : E-step ; calibration of theta and Z

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



~ Dirichlet ~ Multinomial ~ Multinomial

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

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

E step :

Objective :

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

Optimal solution :

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

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

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

For θ,

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

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

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

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

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LDA : E-step ; calibration of theta and t

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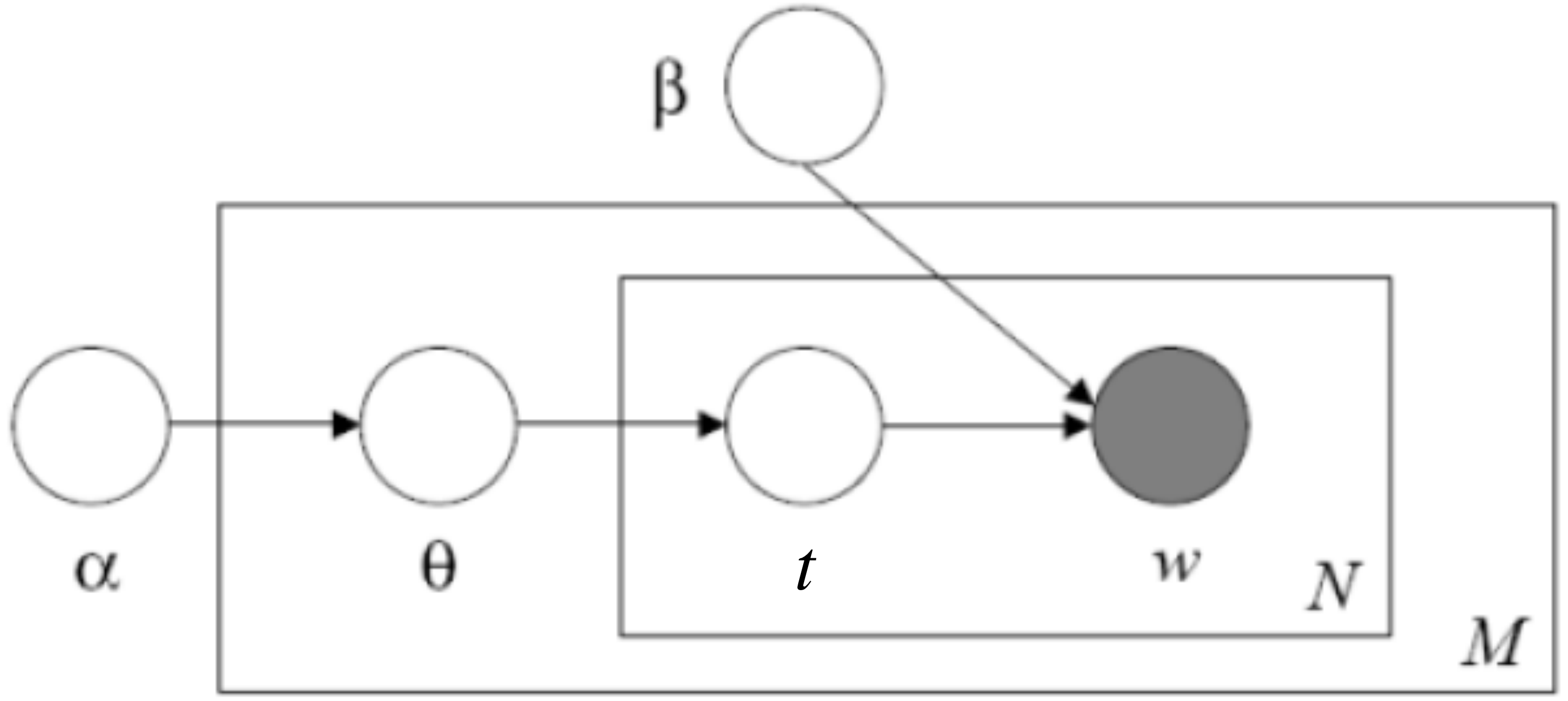

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for t,

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

$\perp t$

$$= E_{Q(\theta)} \left[\sum_d \sum_n \sum_k 1_{\{t_{d,n} = k\}} \left(\log \theta_{d,k} + \log \beta_{k, w_{d,n}} \right) \right] + const$$

$$= \sum_d \sum_n \sum_k 1_{\{t_{d,n} = k\}} \left(E_{Q(\theta)} \left[\log \theta_{d,k} \right] + \log \beta_{k, w_{d,n}} \right) + const$$

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

E step :

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LDA : M-step

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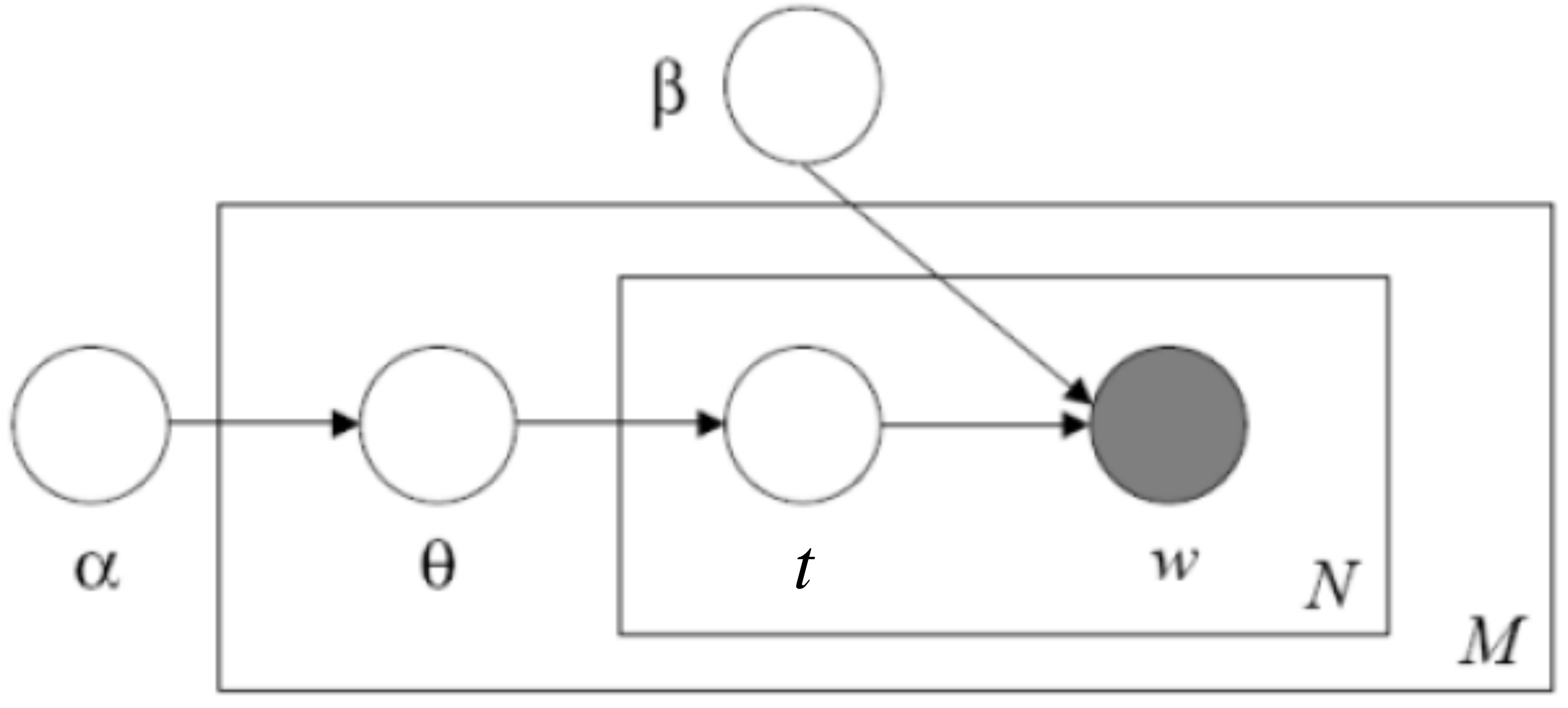

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M step :

Objective :

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

$$\| \qquad\qquad \perp\!\!\!\perp \theta, t$$

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

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 Applications and examples : notebook

Application and examples

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

EPITA - École pour l'informatique et les techniques avancées (2020 - ...)

- Master of Science in Artificial Intelligence Systems : **Bayesian Machine Learning** by François HU
  - **Training session / prerequisite :** [Statistics with python], [Data]
  - **Lecture 1** : [Bayesian statistics]
  - **Practical work 1** : [Conjugate distributions] [Correction]
  - **Lecture 2** : [Latent Variable Models and EM-algorithm]
  - **Practical work 2** : [Probabilistic K-means and probabilistic PCA] [Correction Part1]
  - **Lecture 3** : [Variational Inference and intro to NLP]
  - **Practical work 3** : [Topic Modeling with LDA] [No correction]
  - **Lecture 4** : (soon available)
  - **Practical work 4** : (soon available)
  - **Lecture 5** : (soon available)

TODO

! Road map

Bayesian statistics (03/05/21)

1

Bayesian perspective :

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

Hard to compute !

θ parameters

X observations

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

Conjugate distribution

Exemple :
Naive Bayes classifier,
Linear regression, ….

Pros :
- exact posterior

Cons :
- conjugate prior maybe inadequate

Latent variable models (17/05/21)

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 :
- fewer parameters / simpler models
- hidden variable sometimes meaningful
- clustering / dimensionality reduction

Cons :
- harder to work with
- requires math
- only local maximum or saddle point
- EM : the posterior of T could be intractable

Variational Inference (07/06/21)

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 :
- Useful when the posterior is intractable
- Suited to large dataset

Cons :
- can never generate exact result

Markov Chain Monte Carlo (14/06/21)

4

Extensions (28/06/21)

5