



Bayesian Machine Learning

07/06/21 - 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

The diagram illustrates the components of the posterior distribution formula. A vertical green line is on the left. The formula is $P(Z|X) = \frac{P(X,Z)}{P(X)} = \frac{P(X|Z) \times P(Z)}{P(X)}$. The term $P(Z|X)$ is labeled 'Posterior' in green. The term $P(X,Z)$ is labeled 'Likelihood' in green, with a red arrow pointing to it from the text 'Fixed by model' in black. The term $P(X|Z)$ is labeled 'Evidence' in green, with a red arrow pointing to it from the text 'Fixed by data' in black. The term $P(Z)$ is labeled 'Prior' in green, with a red arrow pointing to it from the text 'Fixed by us' in black.

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

Fixed by **model**

Fixed by **us**

Fixed by **data**

Posterior

Likelihood

Prior

Evidence

1. Variational Inference for probabilistic models

Reminder

Posterior distribution

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

Diagram illustrating the components of the posterior distribution formula:

- Posterior** ($P(Z|X)$) is the result of the division.
- Likelihood** ($P(X|Z)$) is the numerator term, labeled "Fixed by **model**".
- Prior** ($P(Z)$) is the denominator term, labeled "Fixed by **us**".
- Evidence** ($P(X)$) is the denominator term, labeled "Fixed by **data**".

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 $\mathbb{E}_T [\log P(X, T|\theta)]$ with $Z = \{T, \theta\}$

1. Variational Inference for probabilistic models

Approximate inference

Posterior distribution

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

Fixed by **model** (Likelihood) Fixed by **us** (Prior)

Posterior Evidence Fixed by **data**

Methods we have seen so far

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

- **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

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Variational Inference (VI)

- Select a family of distributions \mathcal{Q}
- Find the « **best** » approximation $\hat{P}_X \in \mathcal{Q} : \ll P_X(Z) \approx \hat{P}_X(Z) \gg$

1. Variational Inference for probabilistic models

Variational Inference : KL-divergence

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- Fixed by model** points to **Likelihood** ($P(X|Z)$).
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- Evidence** points to $P(X)$.
- Fixed by data** points to $P(X)$.

Kullback-Leibler (KL) divergence

Consider P and Q two distributions

we want to compare the « differences » / divergence.

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

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

(ii) Find the **best** approximation : $\hat{P}_X = \arg \min_{Q \in \mathcal{Q}} D_{KL}(Q||P_X)$

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Variational Inference (VI)

- (i) Select a family of distributions \mathcal{Q} on $Z = (Z_1, \dots, Z_d)$
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Mean Field Approximation

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

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

1. Variational Inference for probabilistic models

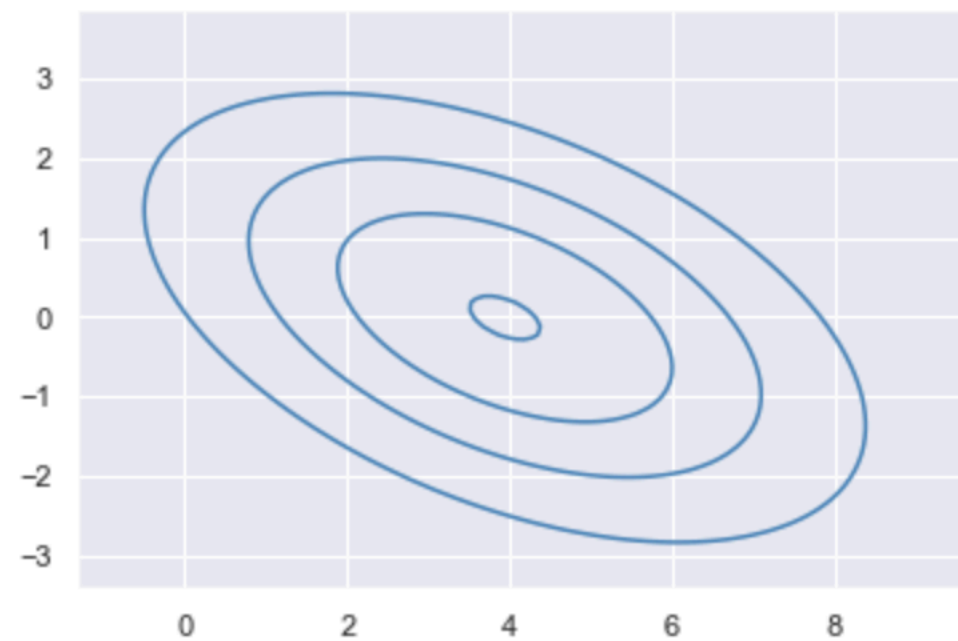
Variational Inference : Mean Field Approximation

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Example : Normal distribution

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



Mean Field

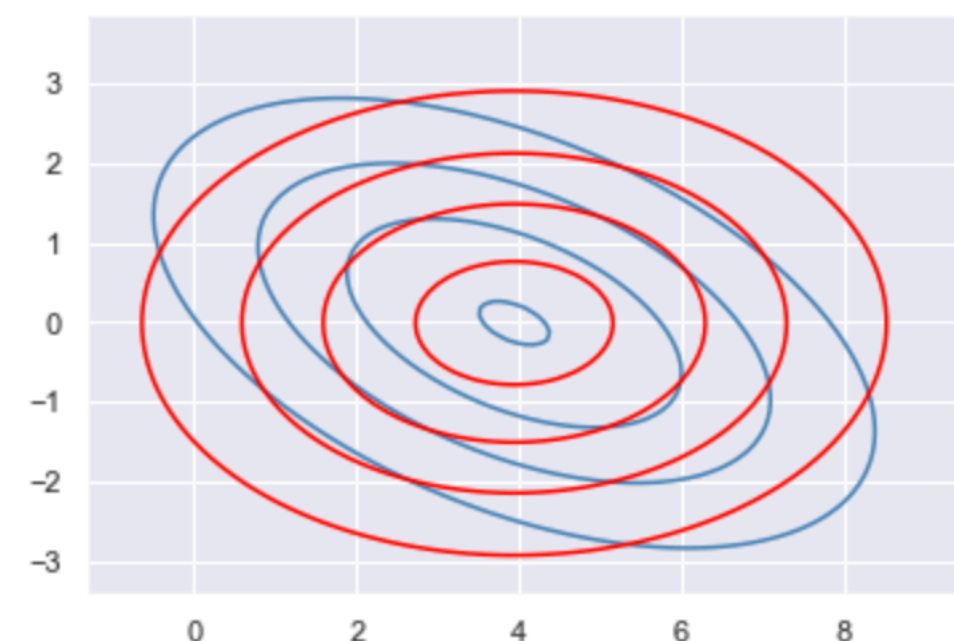


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$$P(z_1, z_2) \approx Q(z_1, z_2) = Q_1(z_1) \times Q_2(z_2) \text{ with } Q_i(z_i) = \mathcal{N}(z_i | \mu_i, \sigma_i^2)$$



1. Variational Inference for probabilistic models

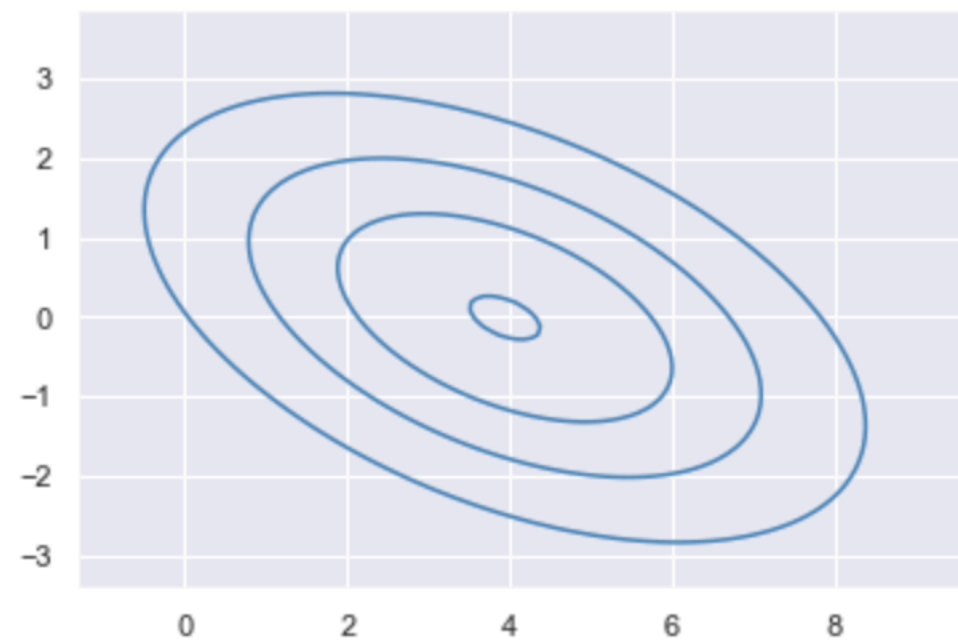
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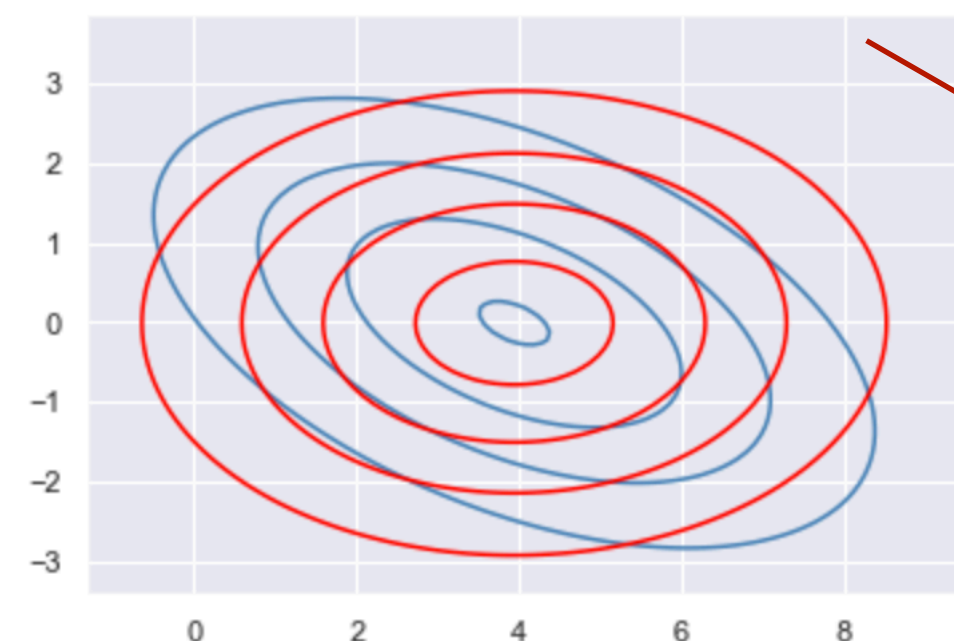


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$$\mathcal{N}_2\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}\right)$$

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Optimization algorithm : coordinate descent

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

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Optimization algorithm : coordinate descent

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

Coordinate
descent
↓

$$\hat{P}_1 = \arg \min_{Q_1} D_{KL}(Q_1 \times Q_2 \times \dots \times Q_d \parallel P)$$

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Variational Inference : Mean Field Approximation

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Variational Inference : Mean Field Approximation

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...

$$\hat{P}_d = \arg \min_{Q_d} D_{KL}(\hat{P}_1 \times \hat{P}_2 \times \dots \times Q_d || P)$$

Repeat until
convergence
with
 Q_1, \dots, Q_d
=
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Variational Inference : Mean Field Approximation

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=

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?

?

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Optimization algorithm : coordinate descent

Optimal solution in Mean Field

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Repeat until
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$$Q_1, \dots, Q_d$$

=

$$\hat{P}_1, \dots, \hat{P}_d$$

?

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

\Leftrightarrow

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

1. Variational Inference for probabilistic models

Variational Inference : Mean Field Approximation

Optimization algorithm : coordinate descent

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

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



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

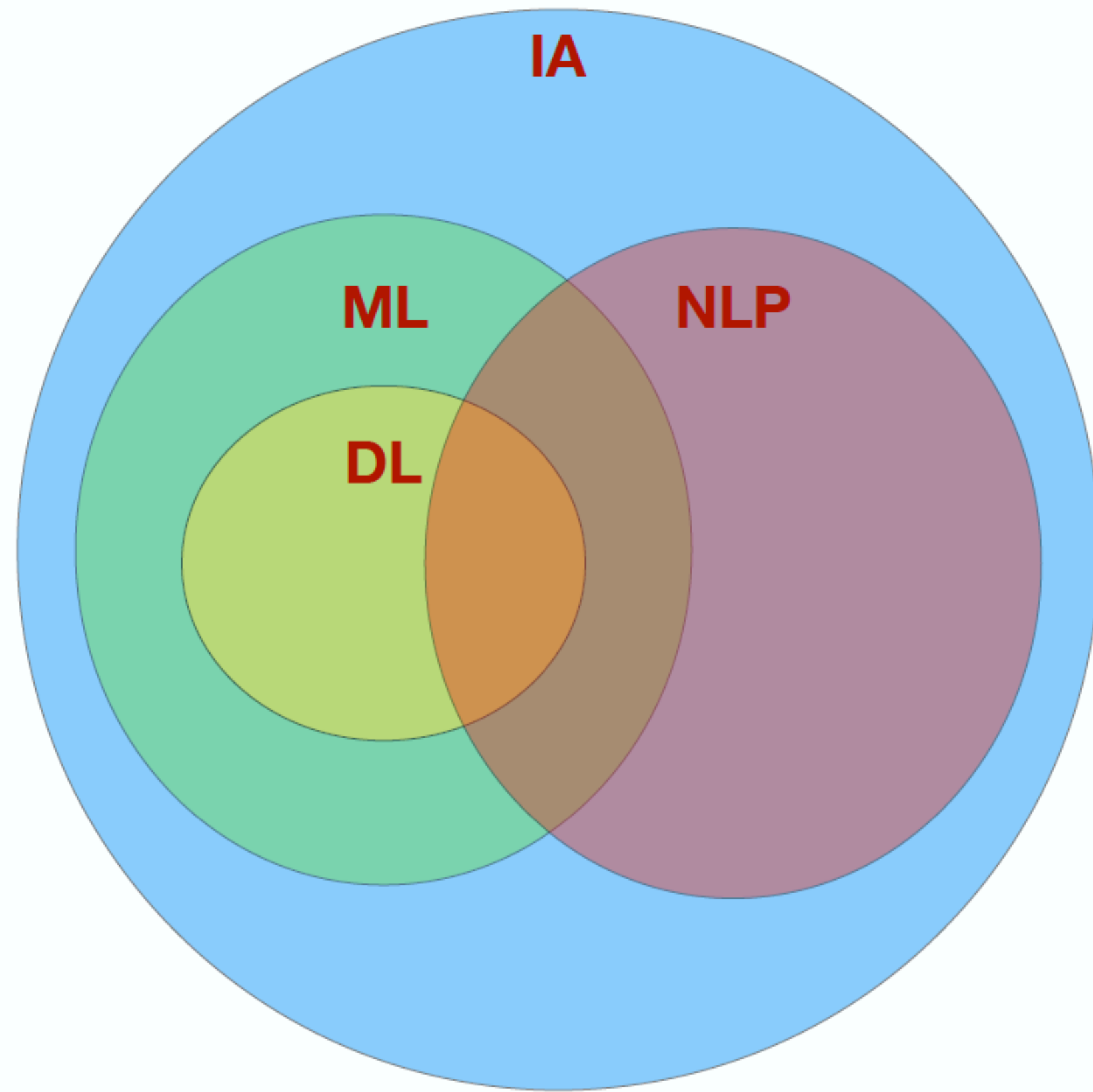
2

Introduction to NLP

2. Introduction to NLP

Preprocessing : Tokenization

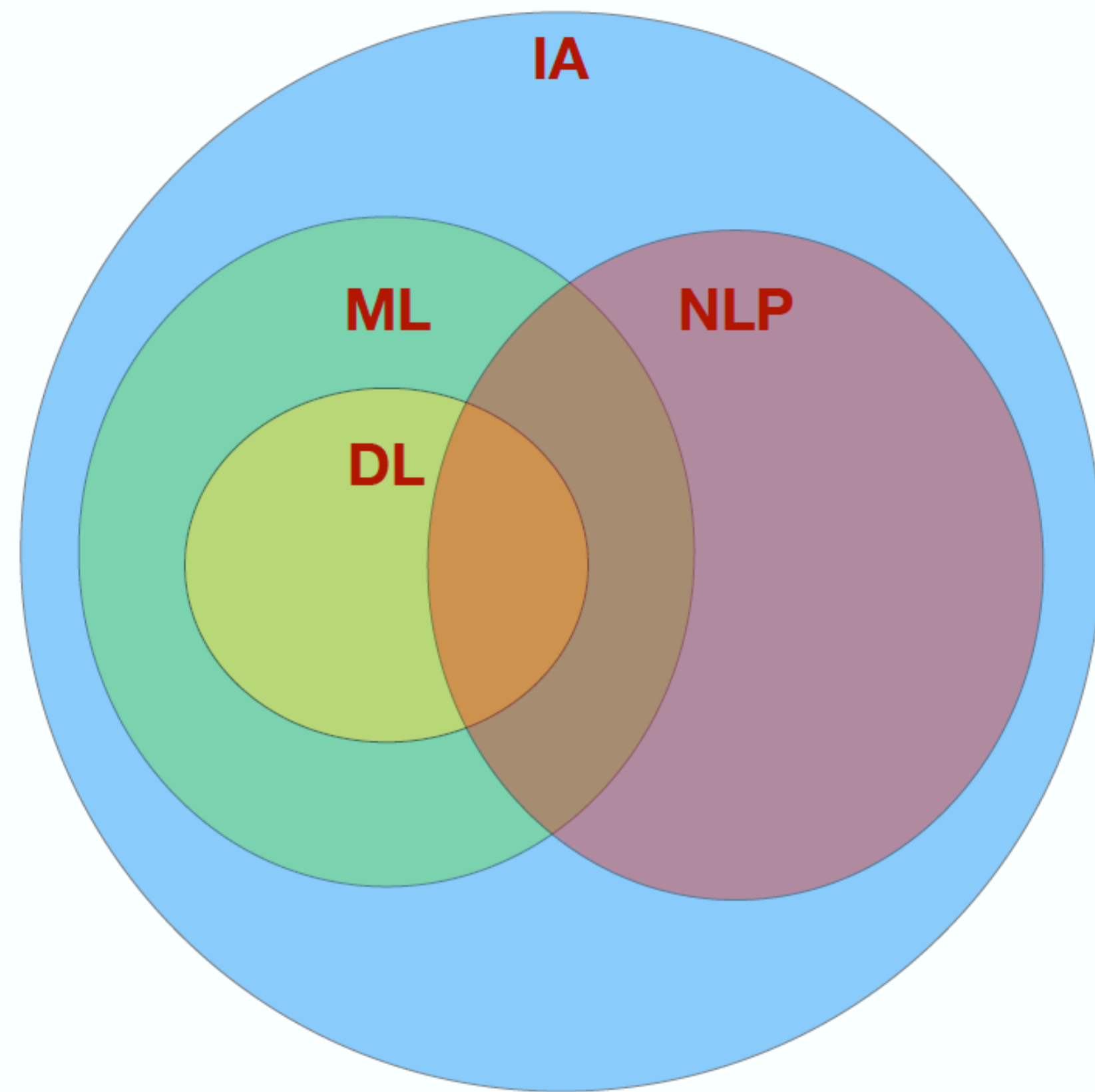
Natural Language Processing : The science of programming computers to understand human language



2. Introduction to NLP

Preprocessing : Tokenization

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



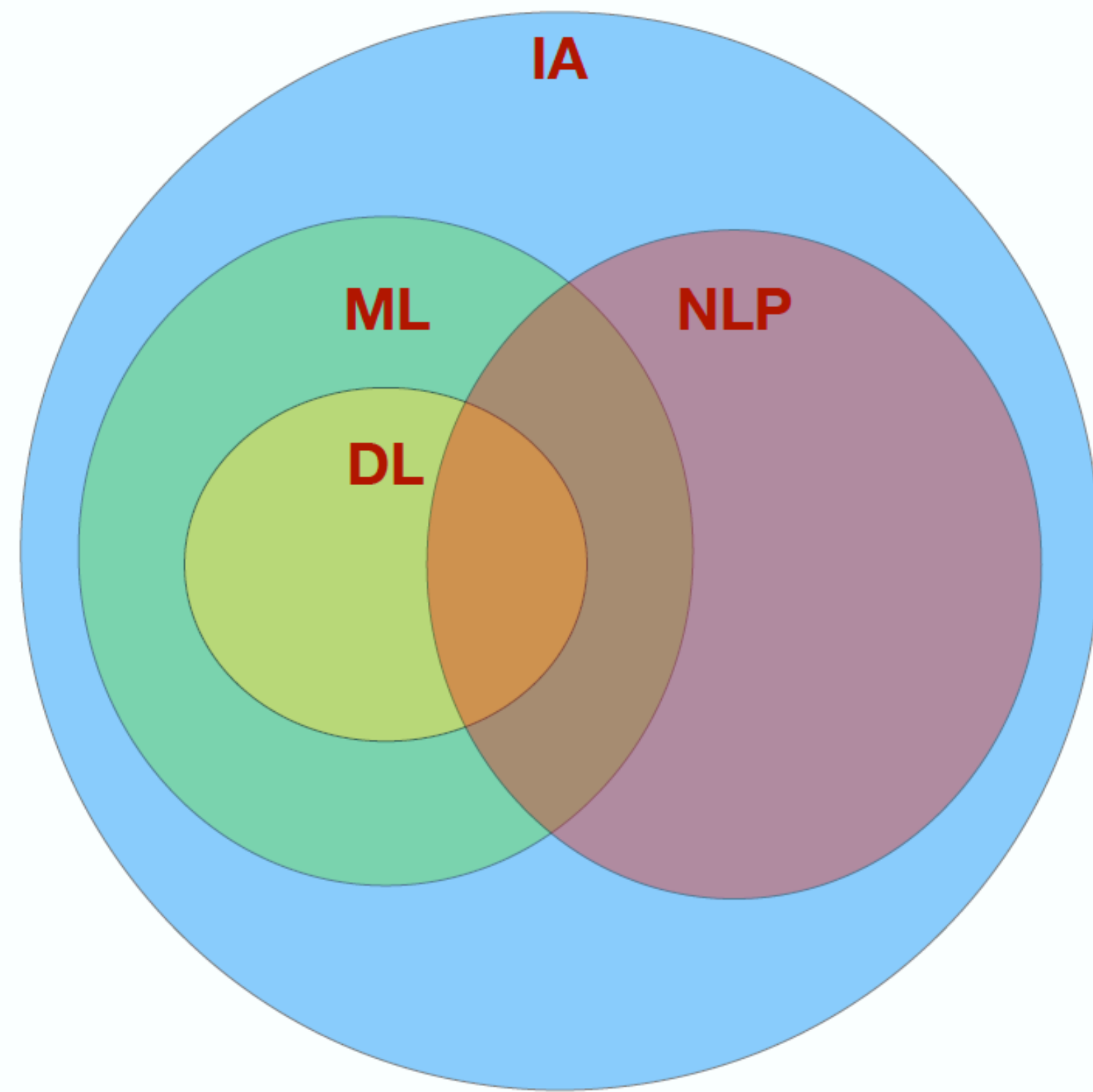
Some intuitions : we want to perform some learning tasks with textual data

- 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 ?**

2. Introduction to NLP

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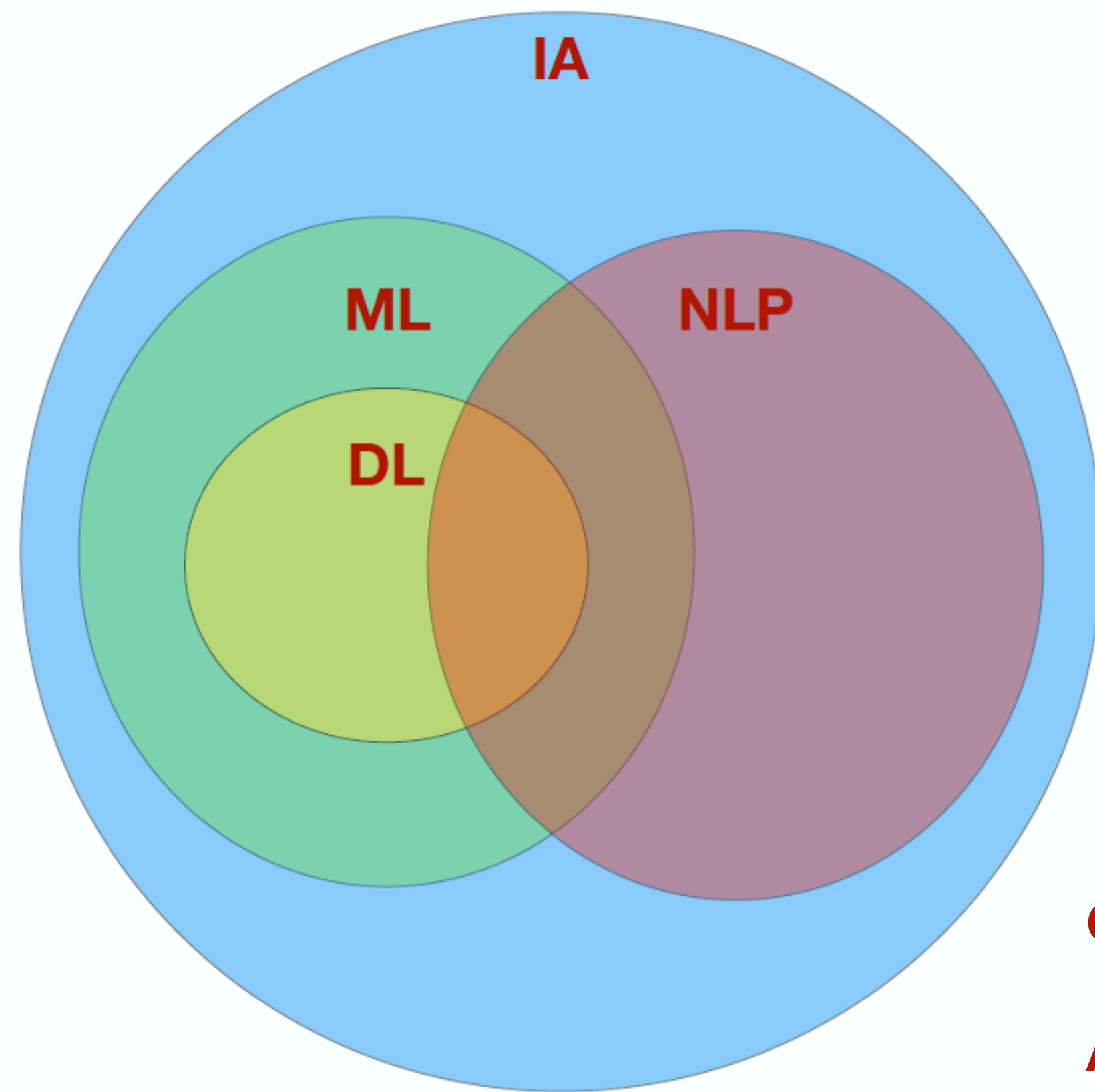
Definitions

- **Text** : sequence of words
- **Word** : sequence of logical characters
- **Tokenization** : process that separates a sequence (text) into a list of tokens (words)

2. Introduction to NLP

Preprocessing : Tokenization

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Definitions

- **Text** : sequence of words
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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 ? \longrightarrow ['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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Preprocessing : Normalization & stop-words

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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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2. Introduction to NLP

Preprocessing : Normalization & stop-words

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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** \longrightarrow study (**In stemming** : stud)

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

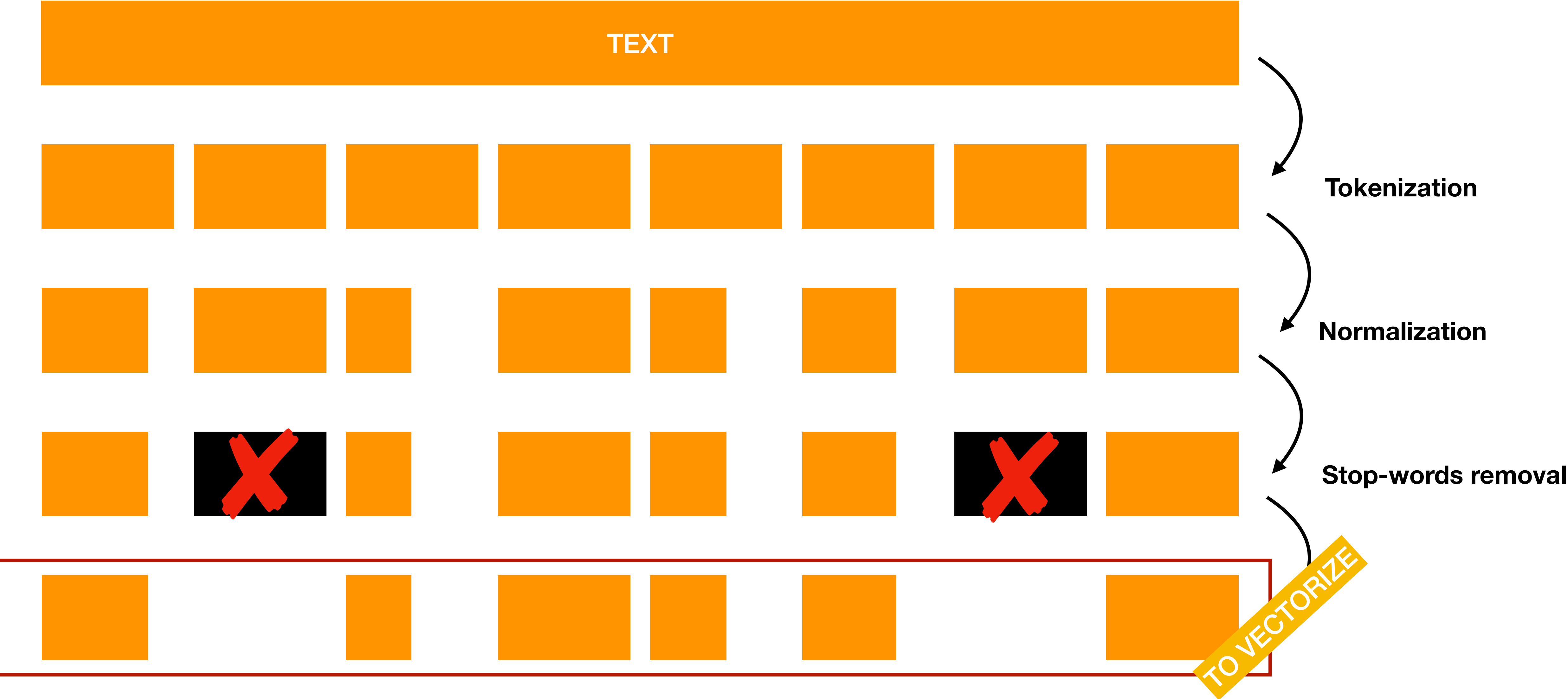
Example : the, a, of, is, at, which, ...

Aim : Remove these stop-words

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

2. Introduction to NLP

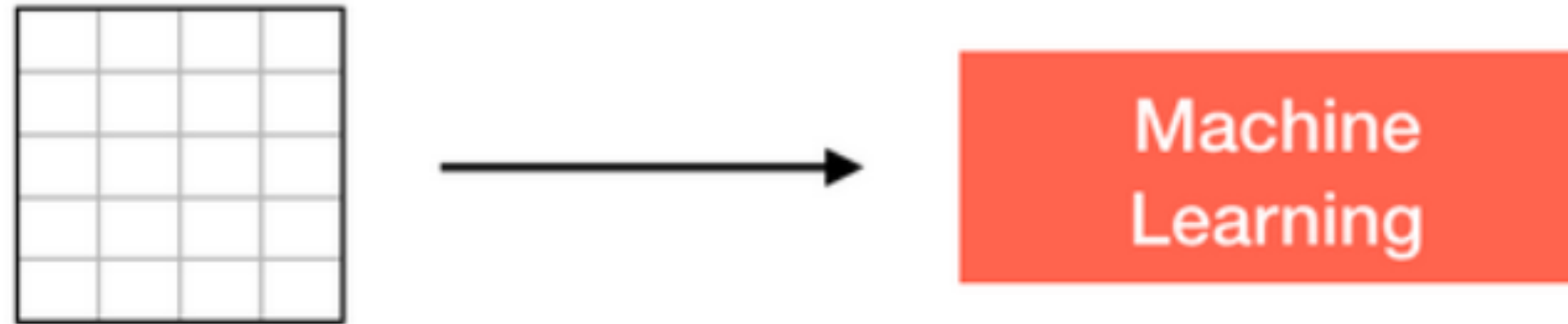
Preprocessing : overview



2. Introduction to NLP

Processing : Textual data into tabular data

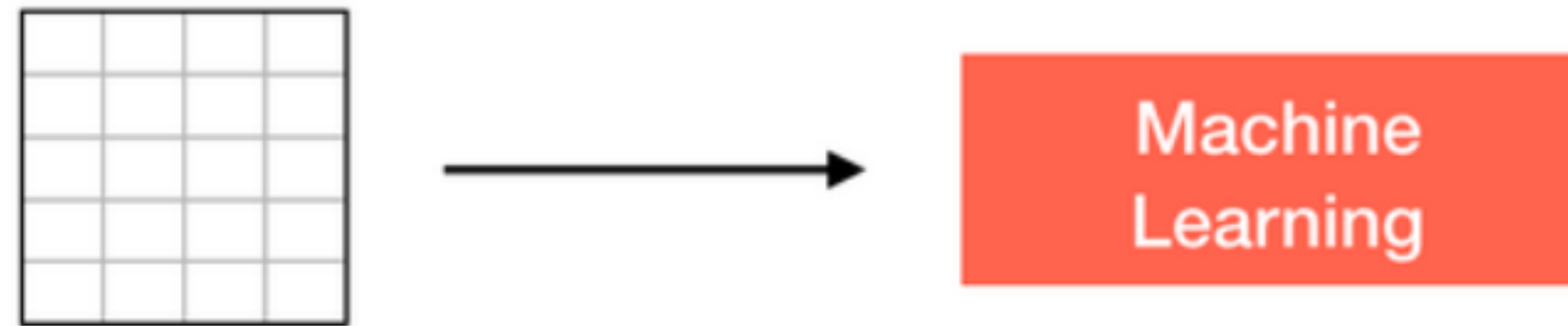
For **tabular** data :



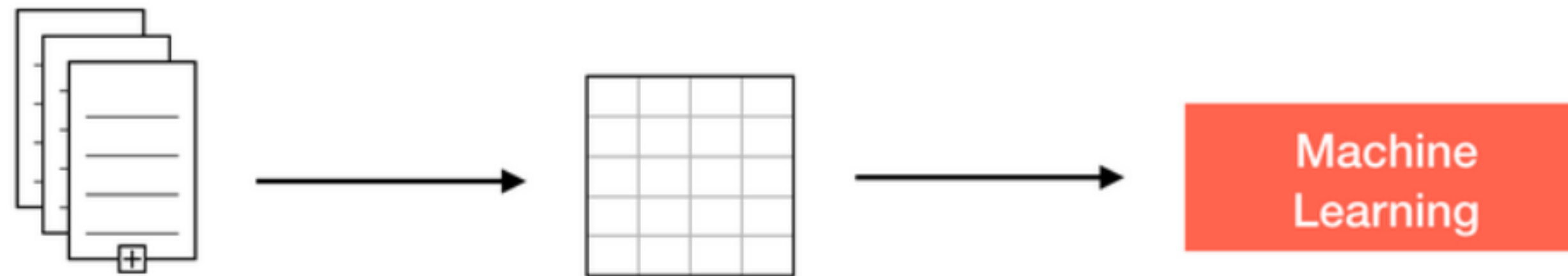
2. Introduction to NLP

Processing : Textual data into tabular data

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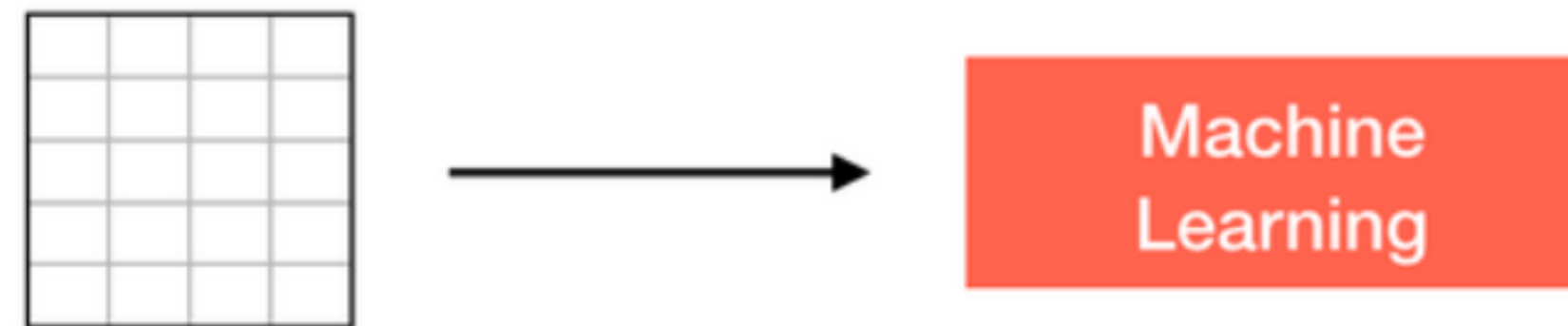
For **textual** data :



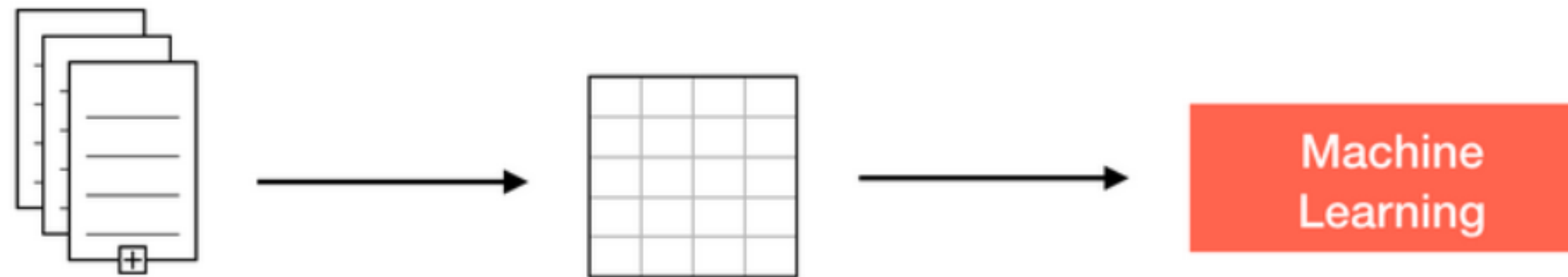
2. Introduction to NLP

Processing : Textual data into tabular data

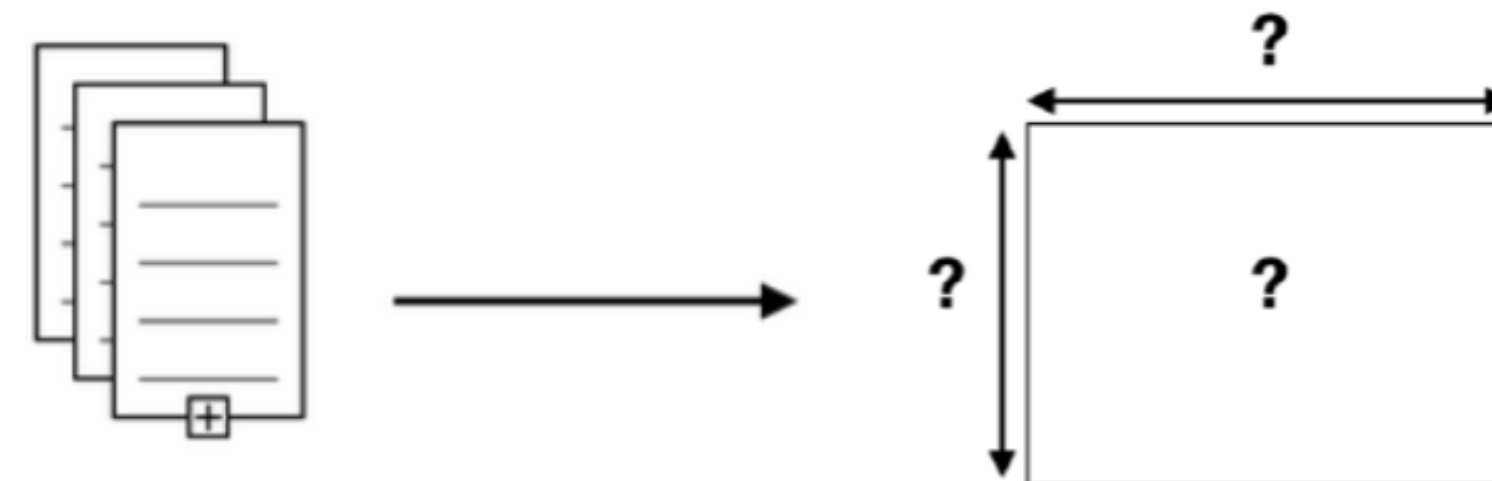
For **tabular** data :



For **textual** data :



Problems :

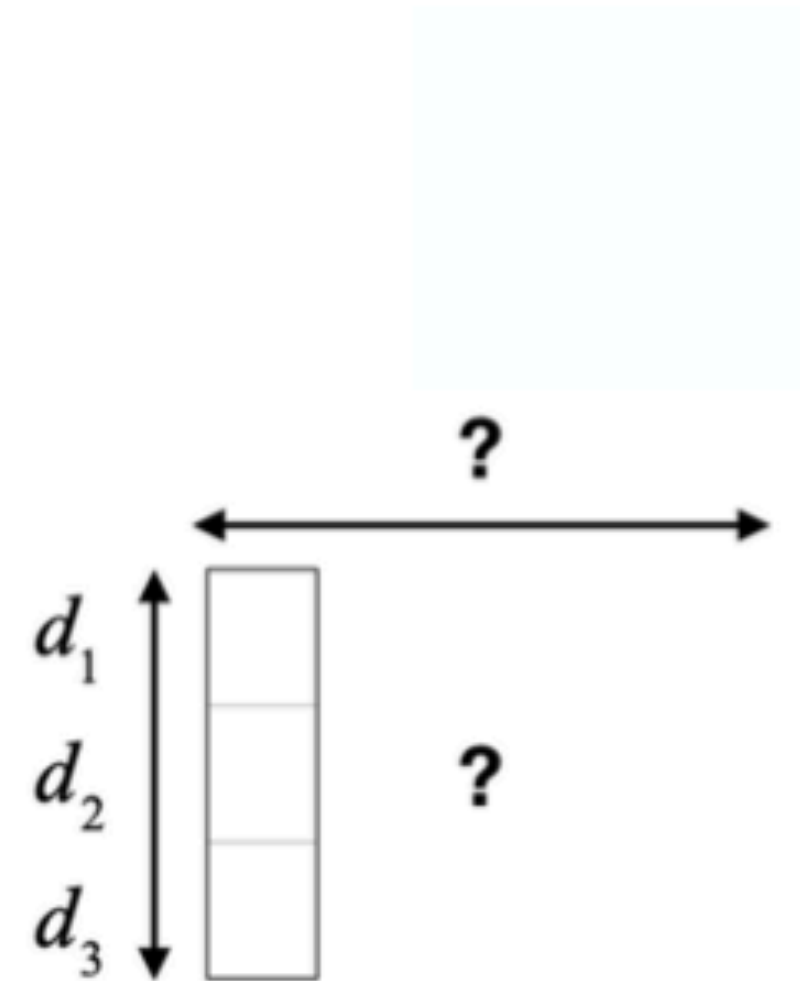


2. Introduction to NLP

Processing : Textual data into tabular data

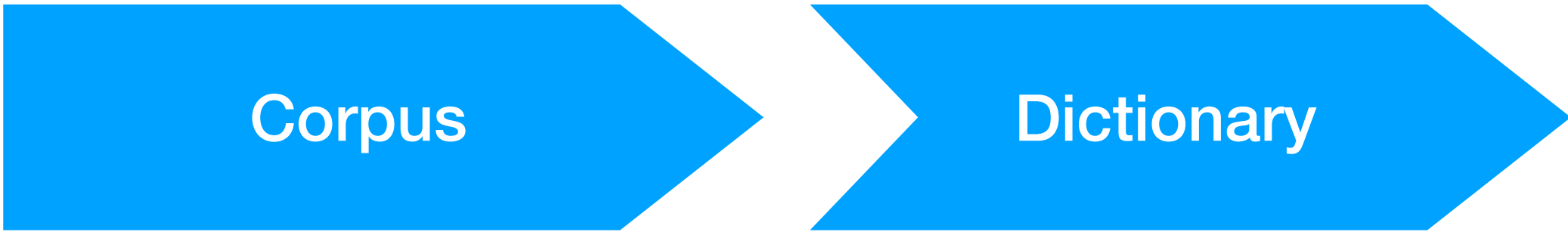
Corpus

d_1	trouver bonne assurance
d_2	contrat satisfaisant
d_3	changement contrat assurance



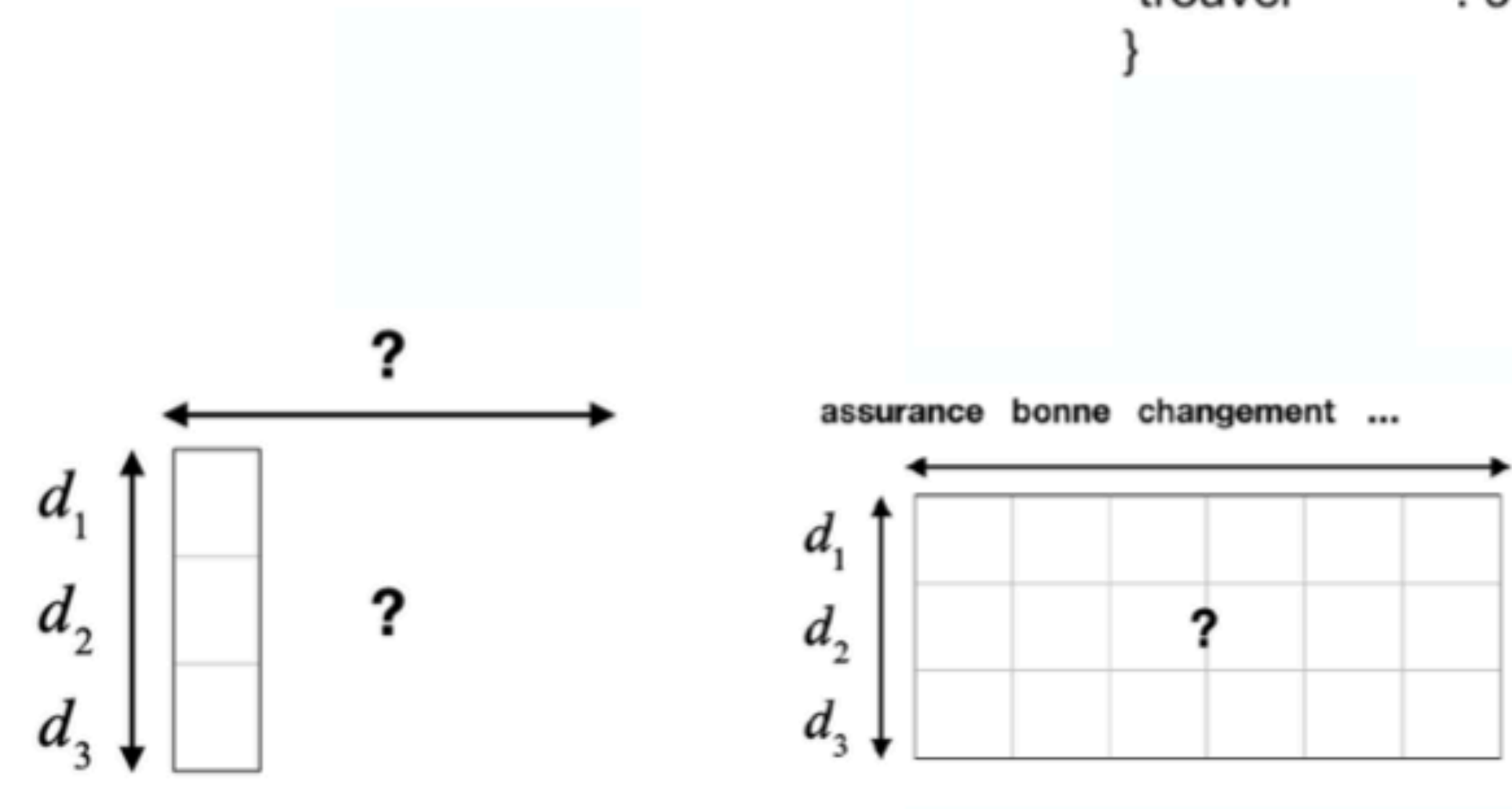
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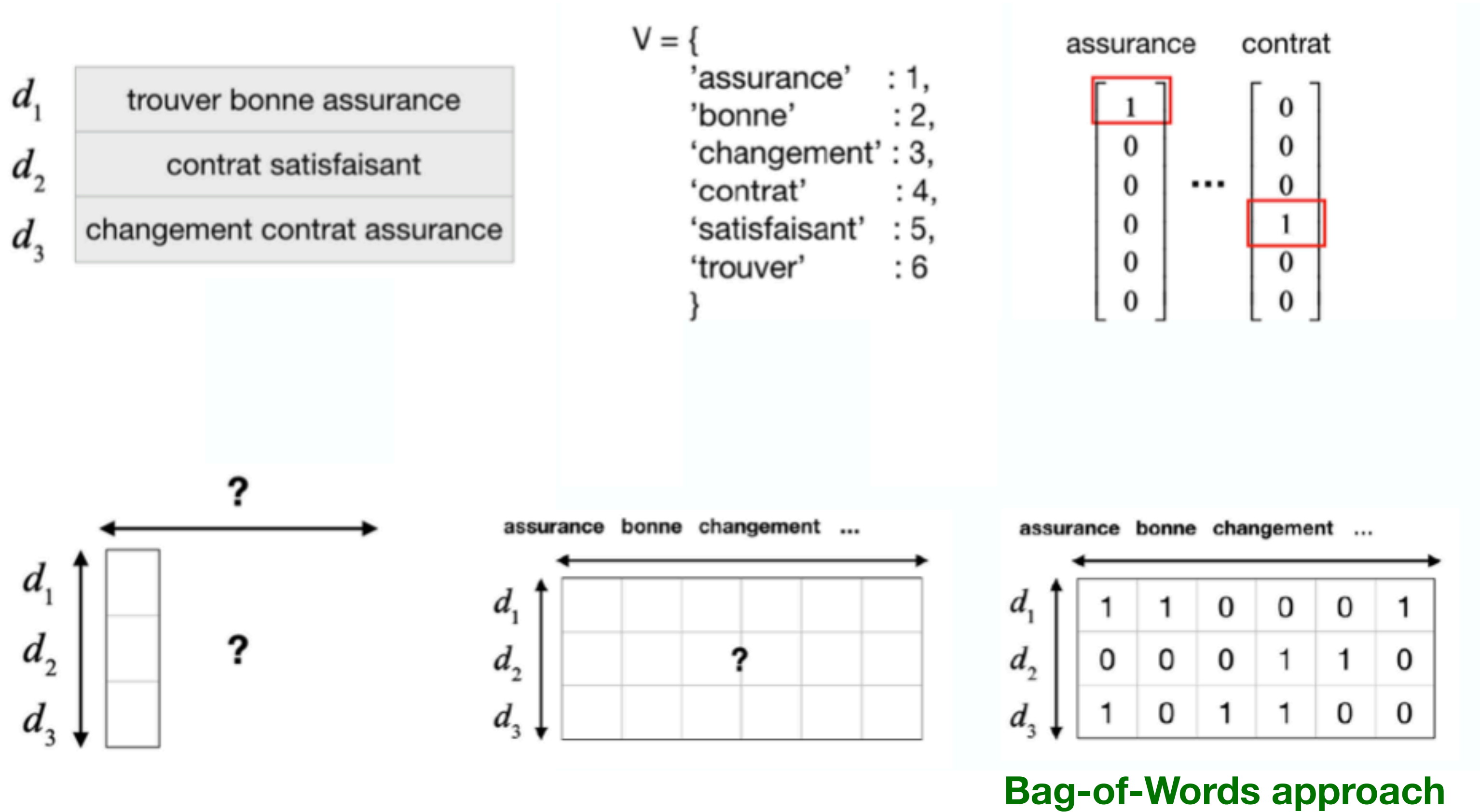
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d_3	changement contrat assurance

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



2. Introduction to NLP

Processing : Textual data into tabular data



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	...

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

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

Bag-of-Words (BoW) approach

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

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)

TF-IDF approach

- Based on the product of two values :

- **Term frequency (TF) :**

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

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

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

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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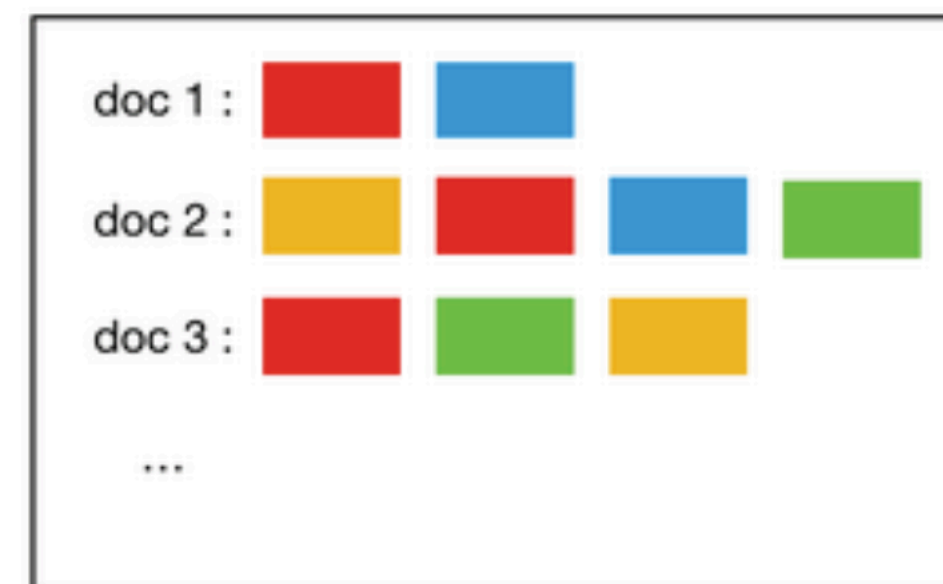
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Textual data



topic modeling

topics in documents



words in topics



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Textual data



topic modeling

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words in topics



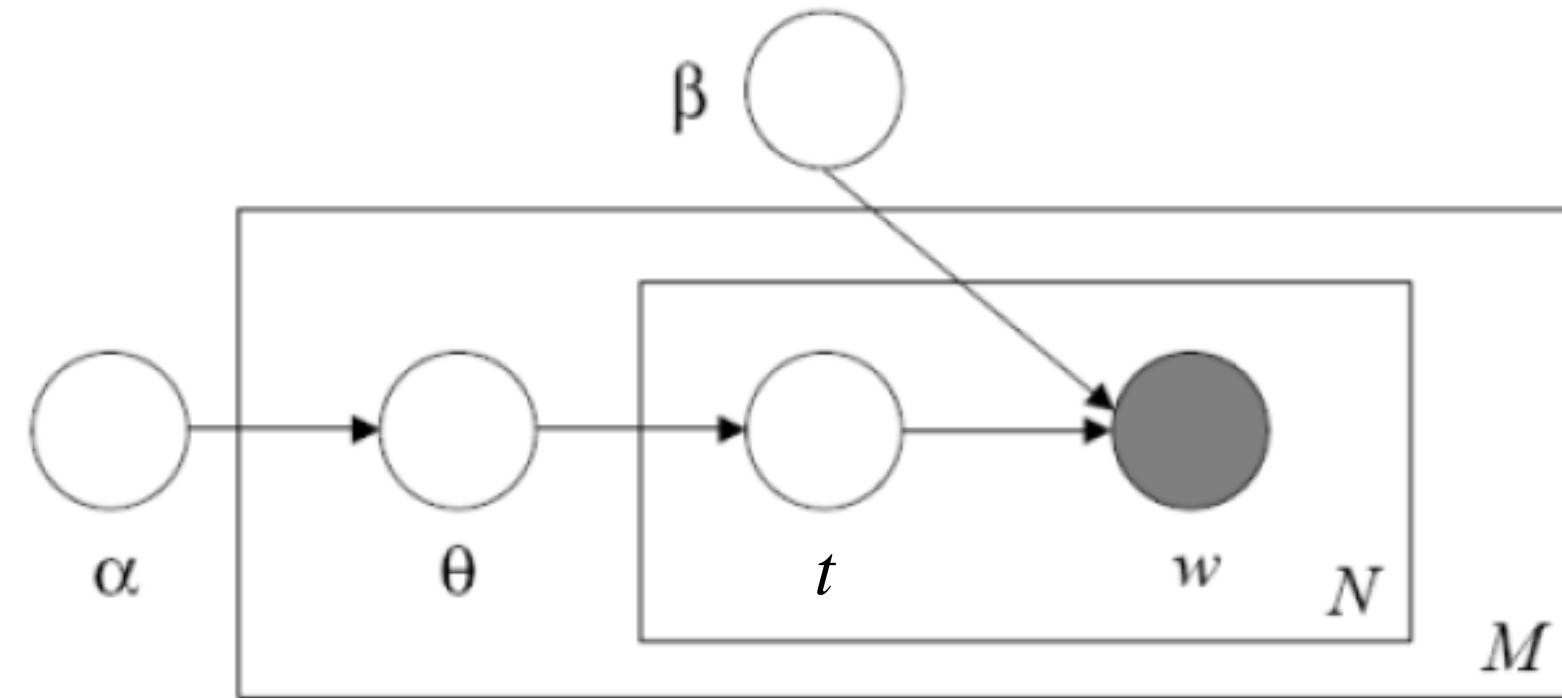
Idea :

- 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



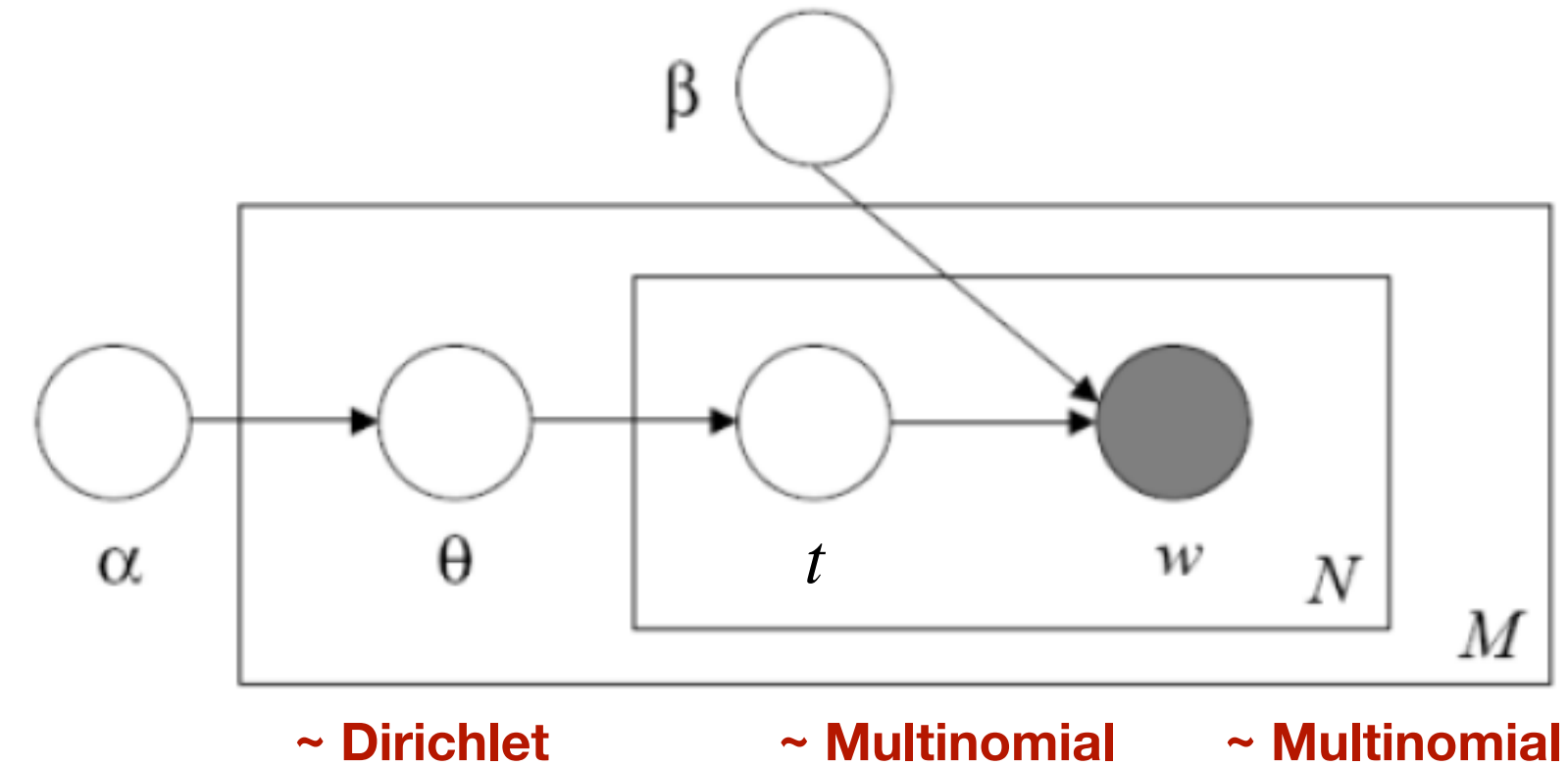
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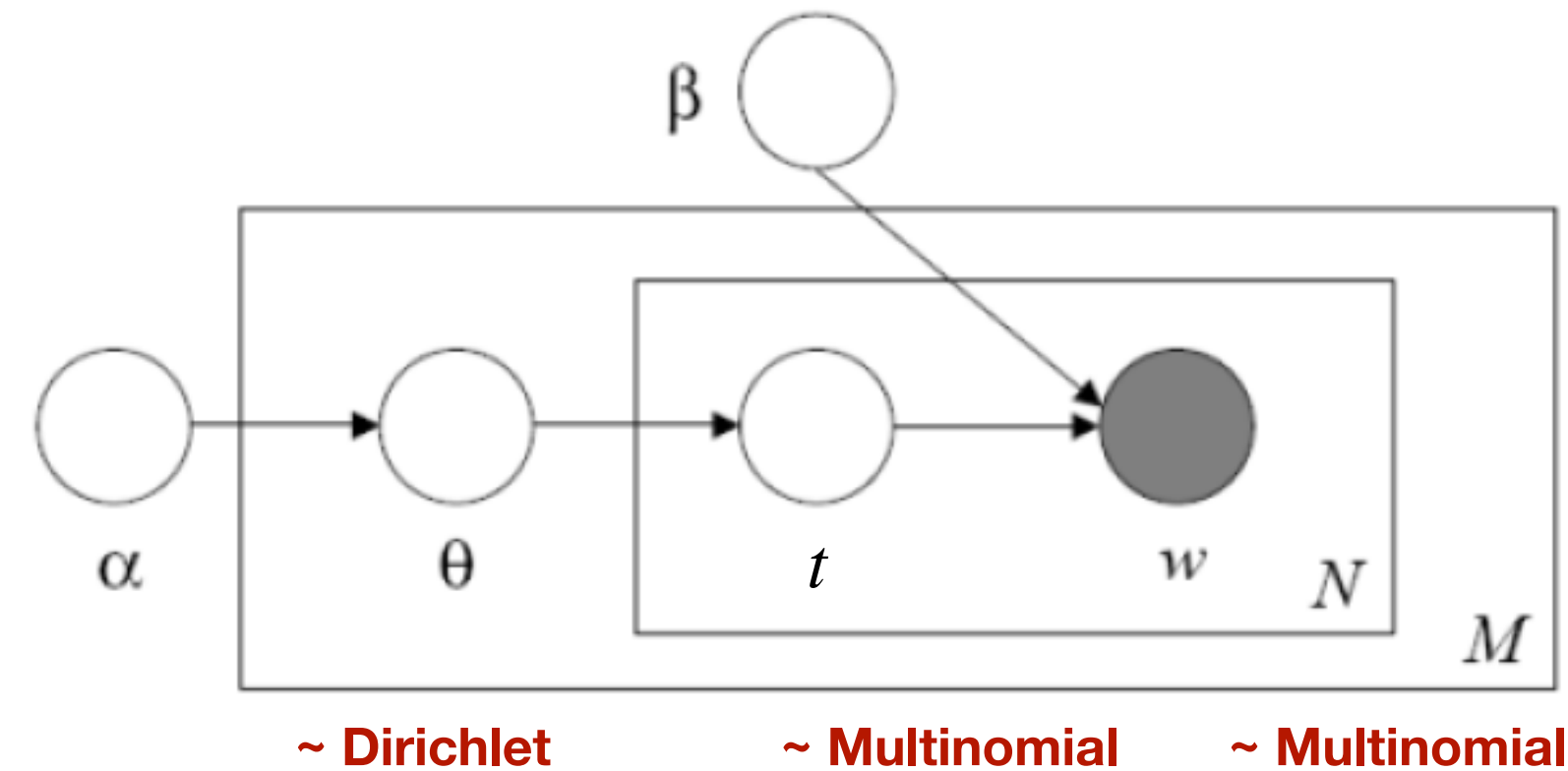
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~ Dirichlet ~ Multinomial ~ Multinomial

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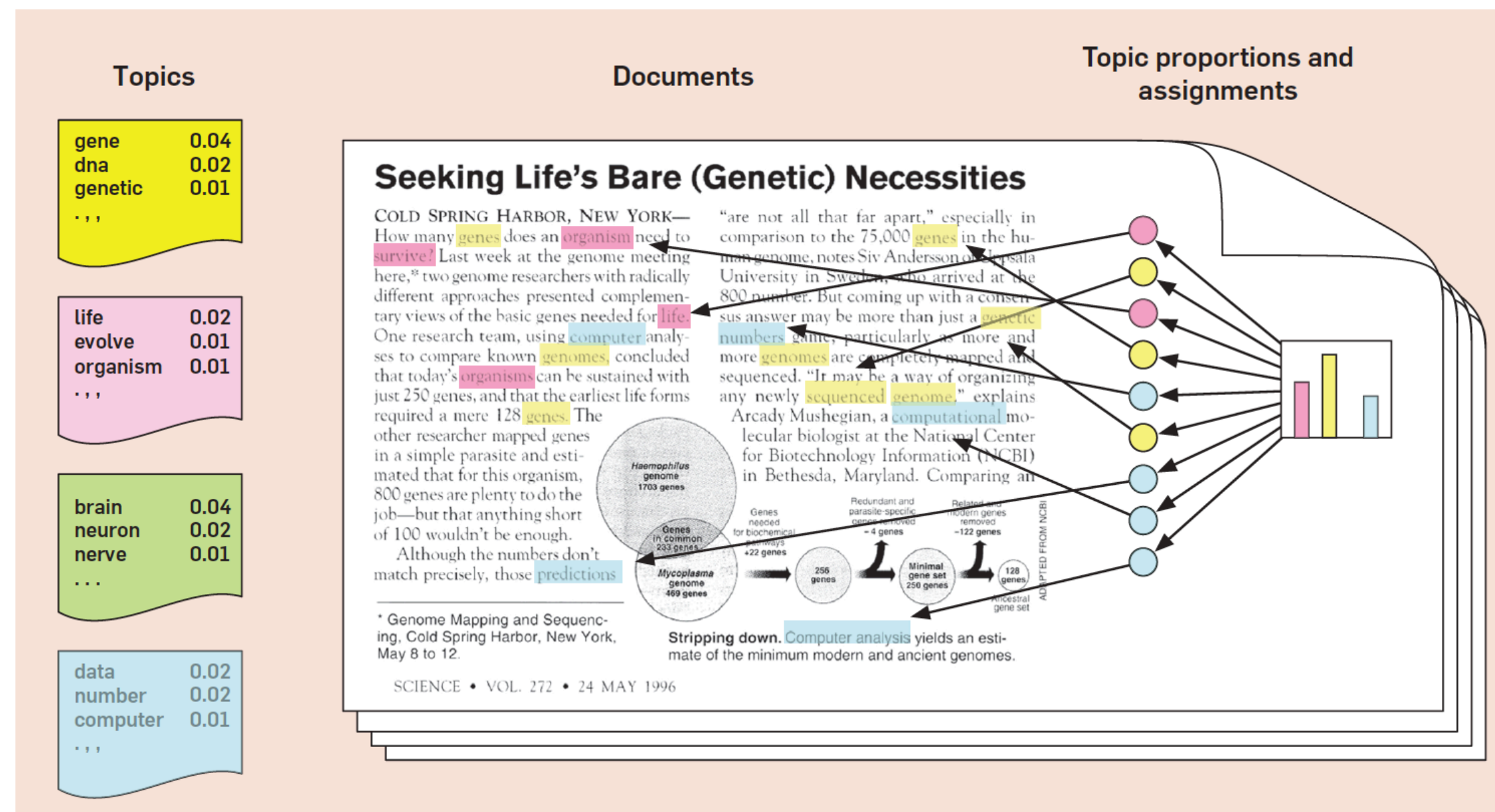


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~ Dirichlet ~ Multinomial ~ Multinomial

Example :



Assumption on the generation of texts :

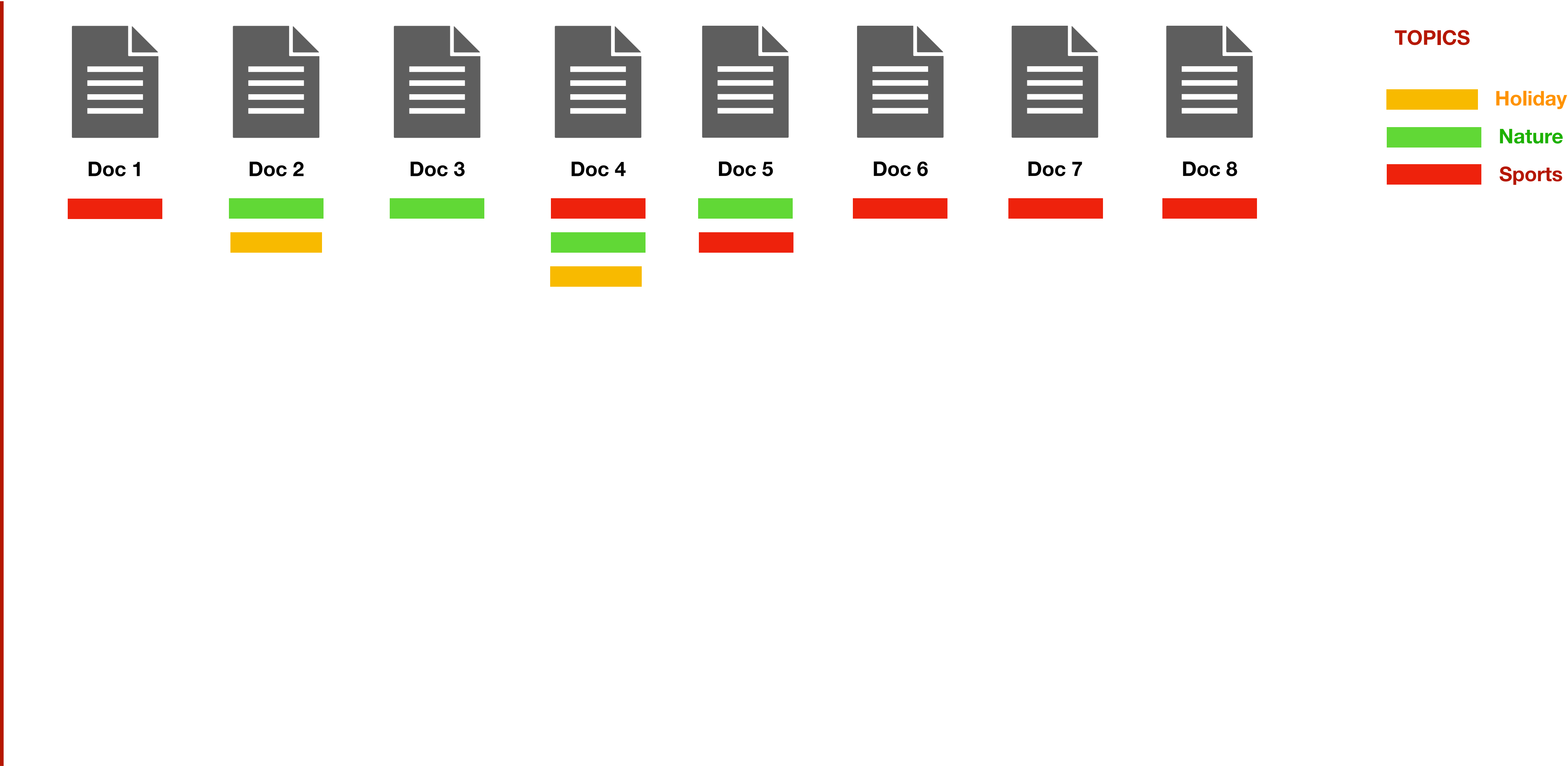
For each of M documents d ,

- 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

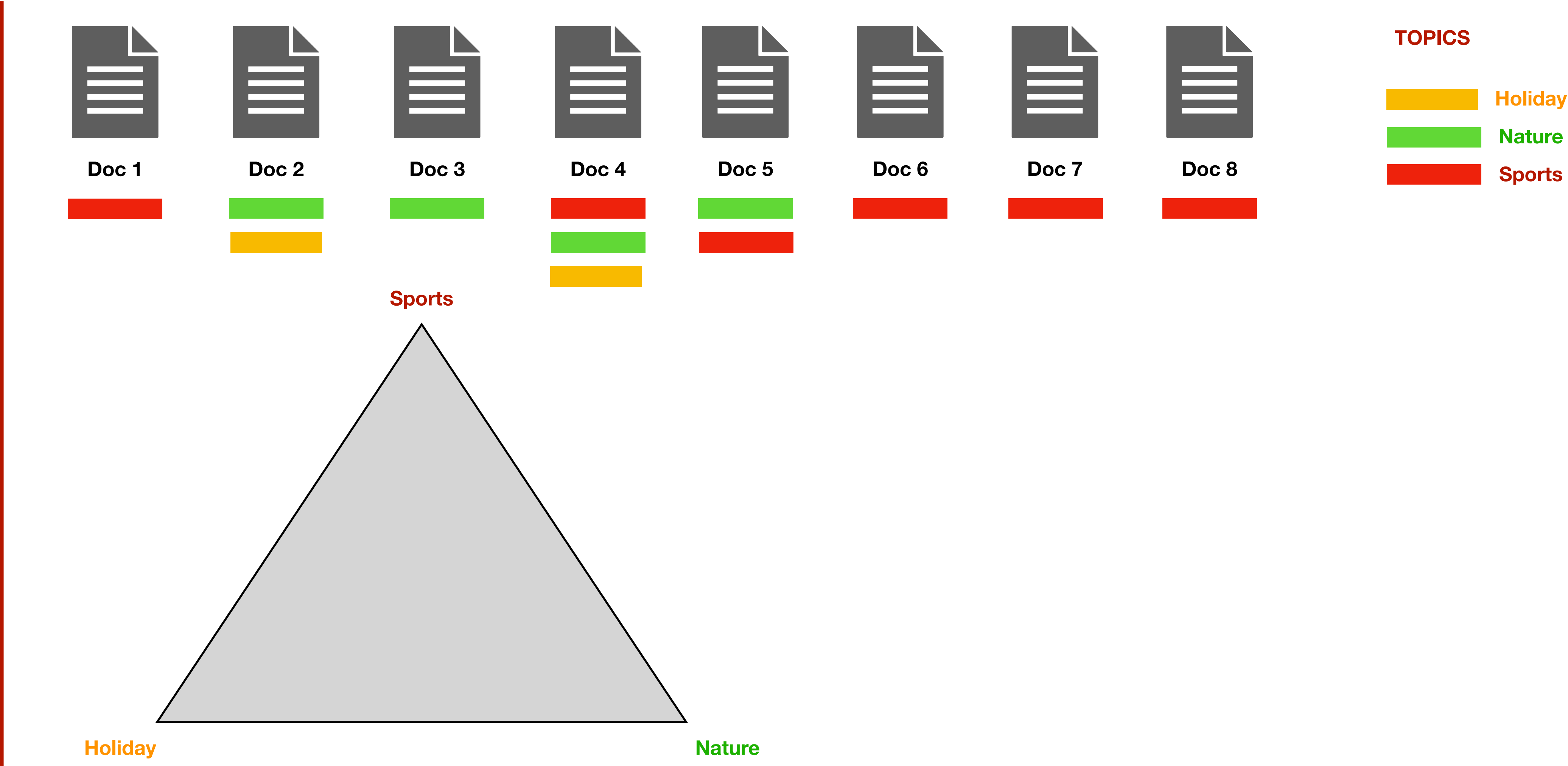
Dirichlet distribution (dimension 3) :



3. Latent Dirichlet Allocation

LDA : Dirichlet distribution

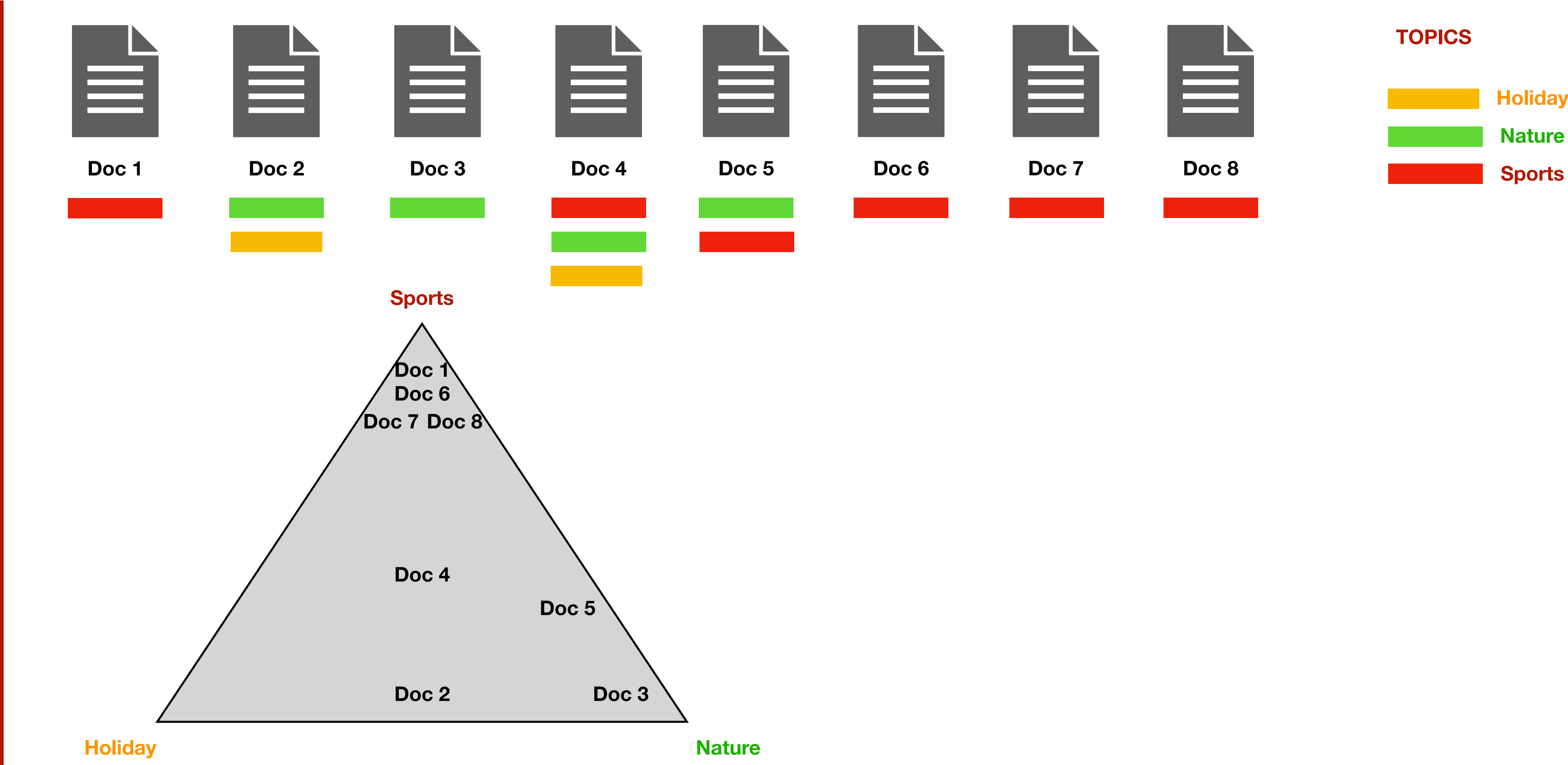
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3. Latent Dirichlet Allocation

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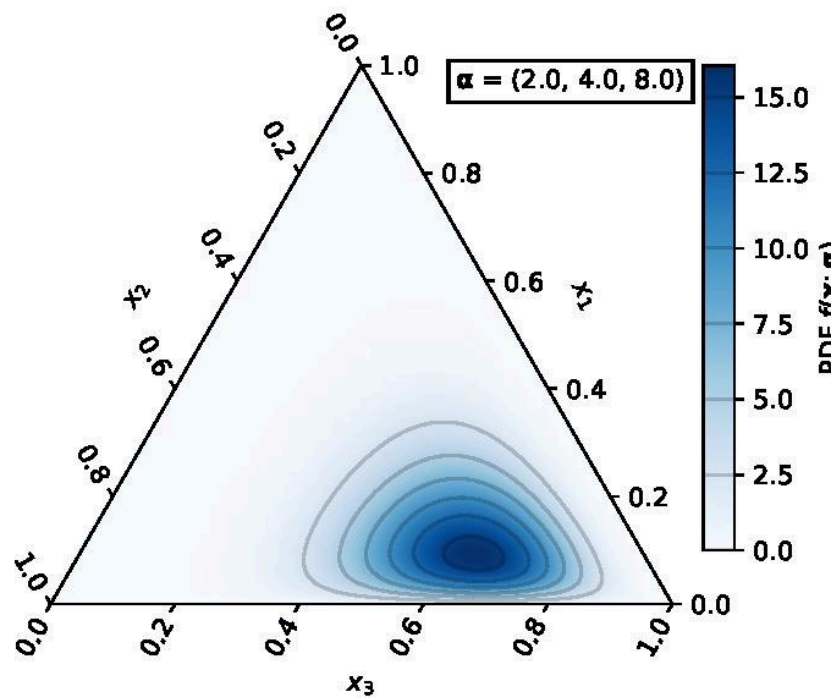
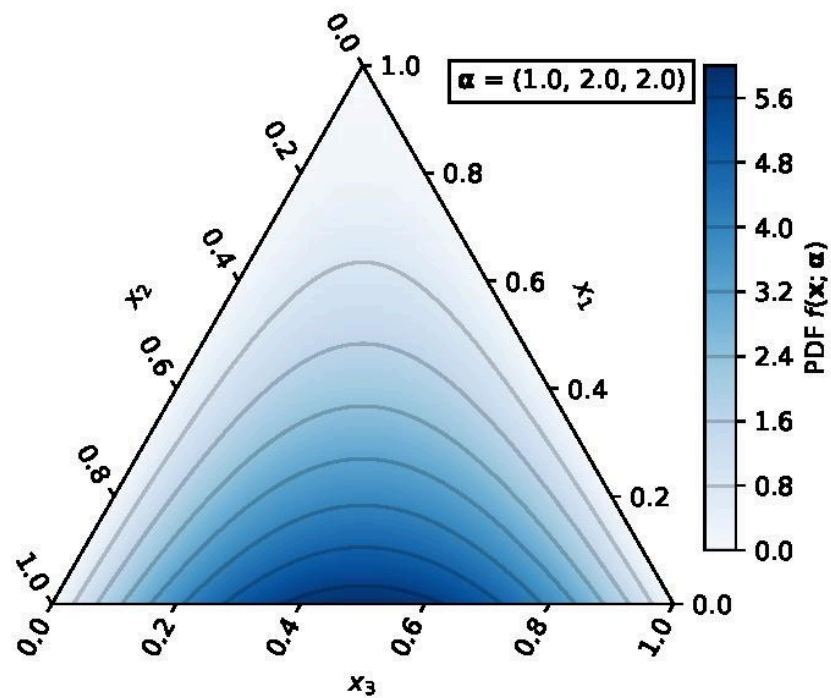
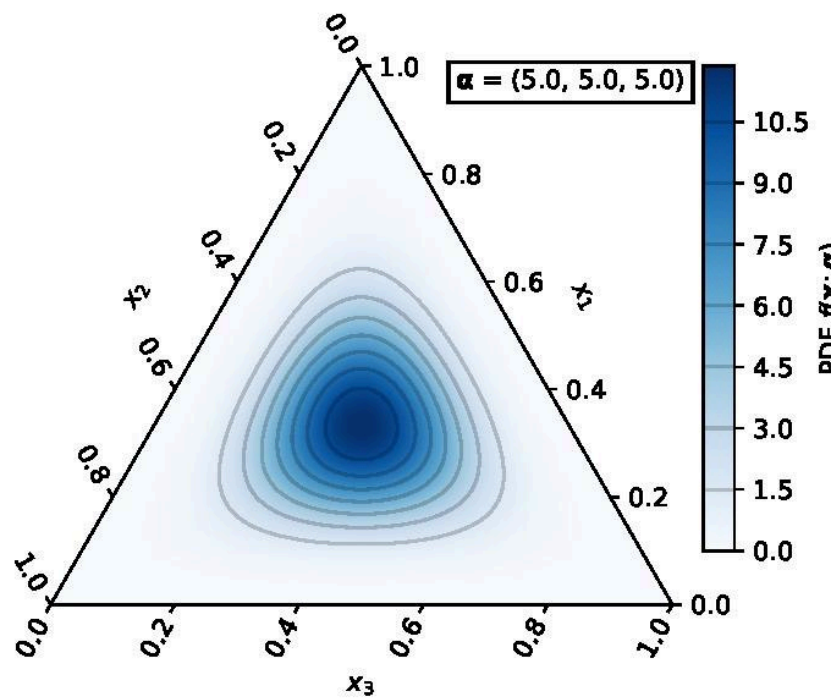
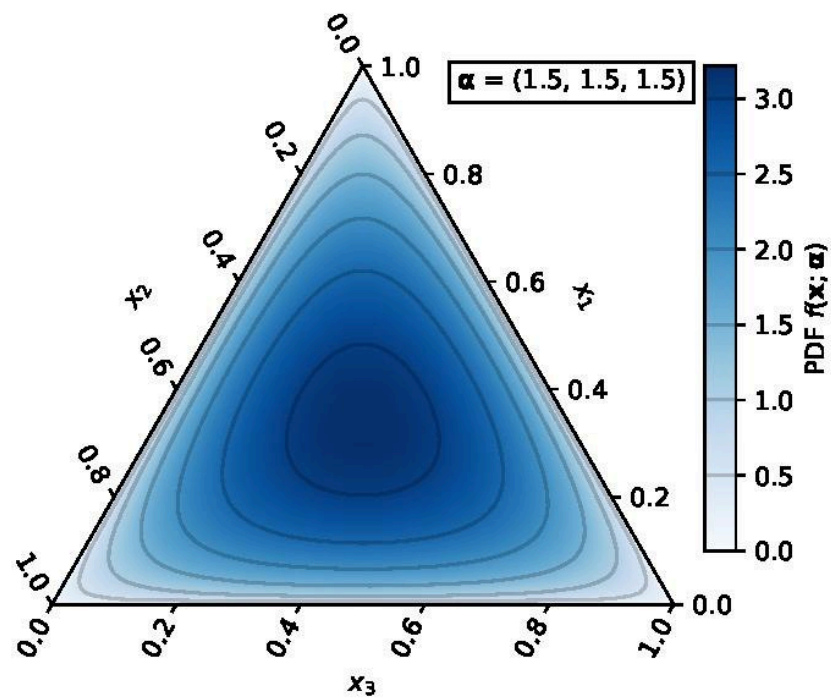
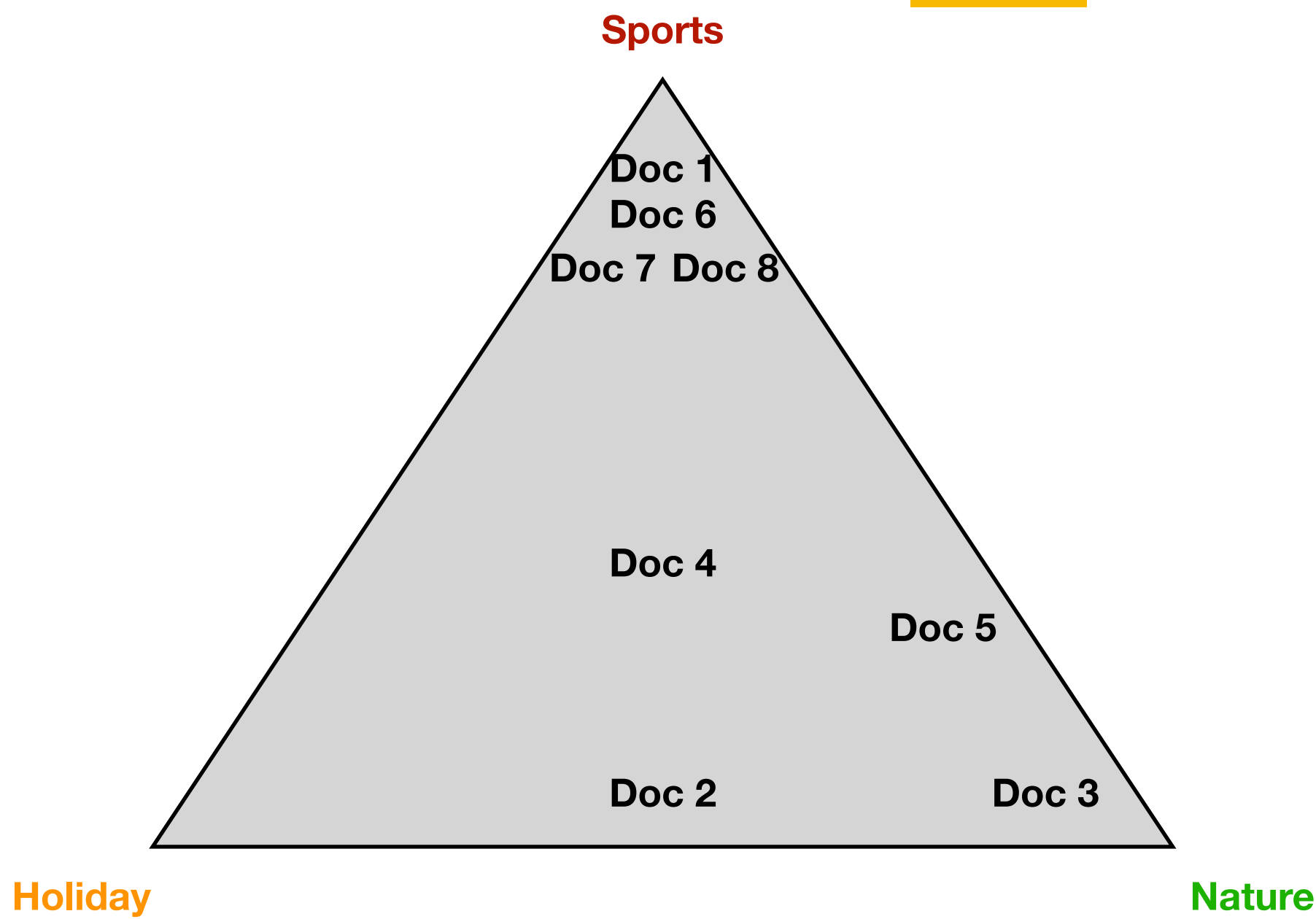
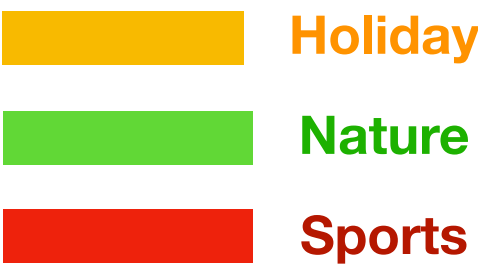
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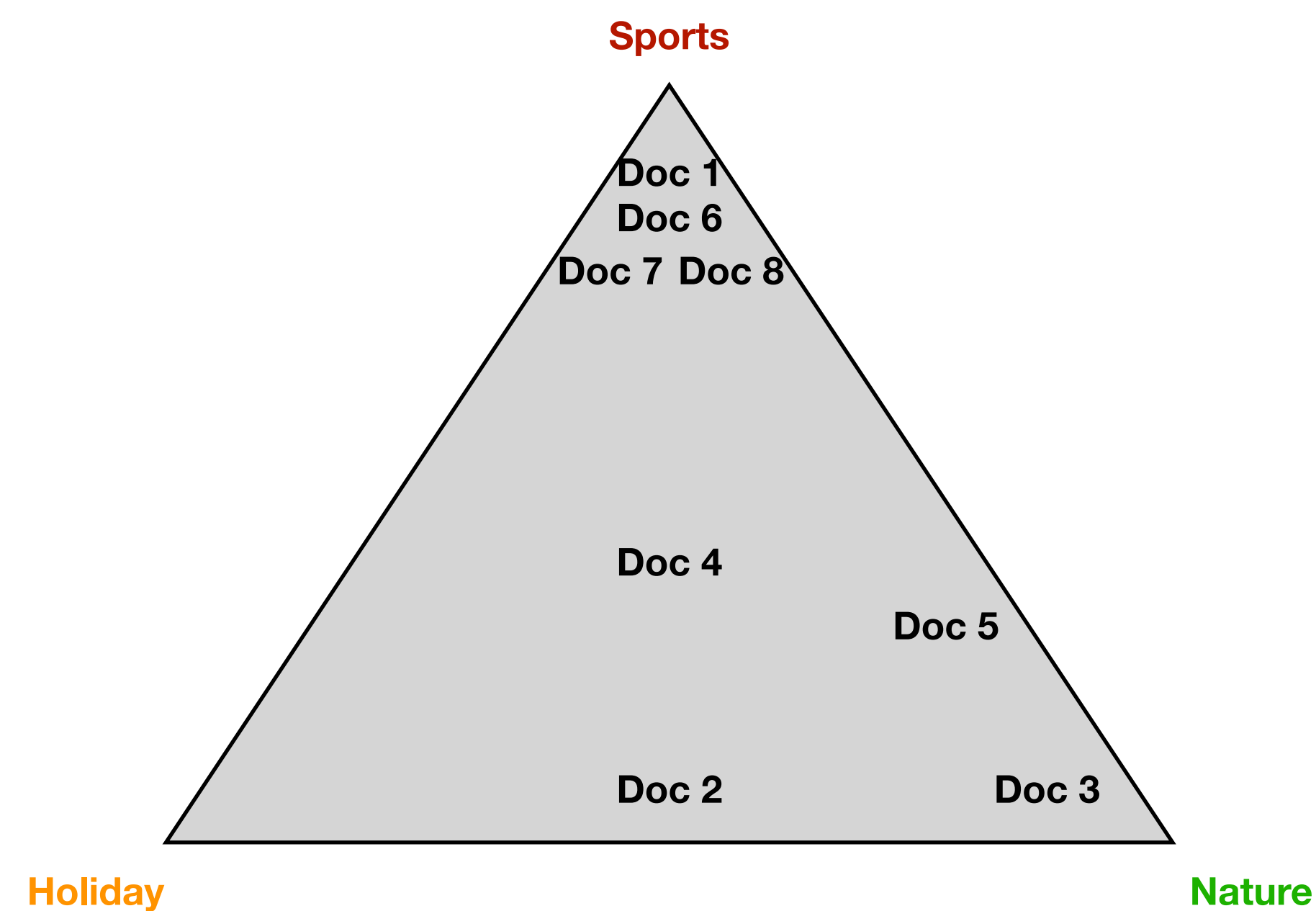


TOPICS



3. Latent Dirichlet Allocation

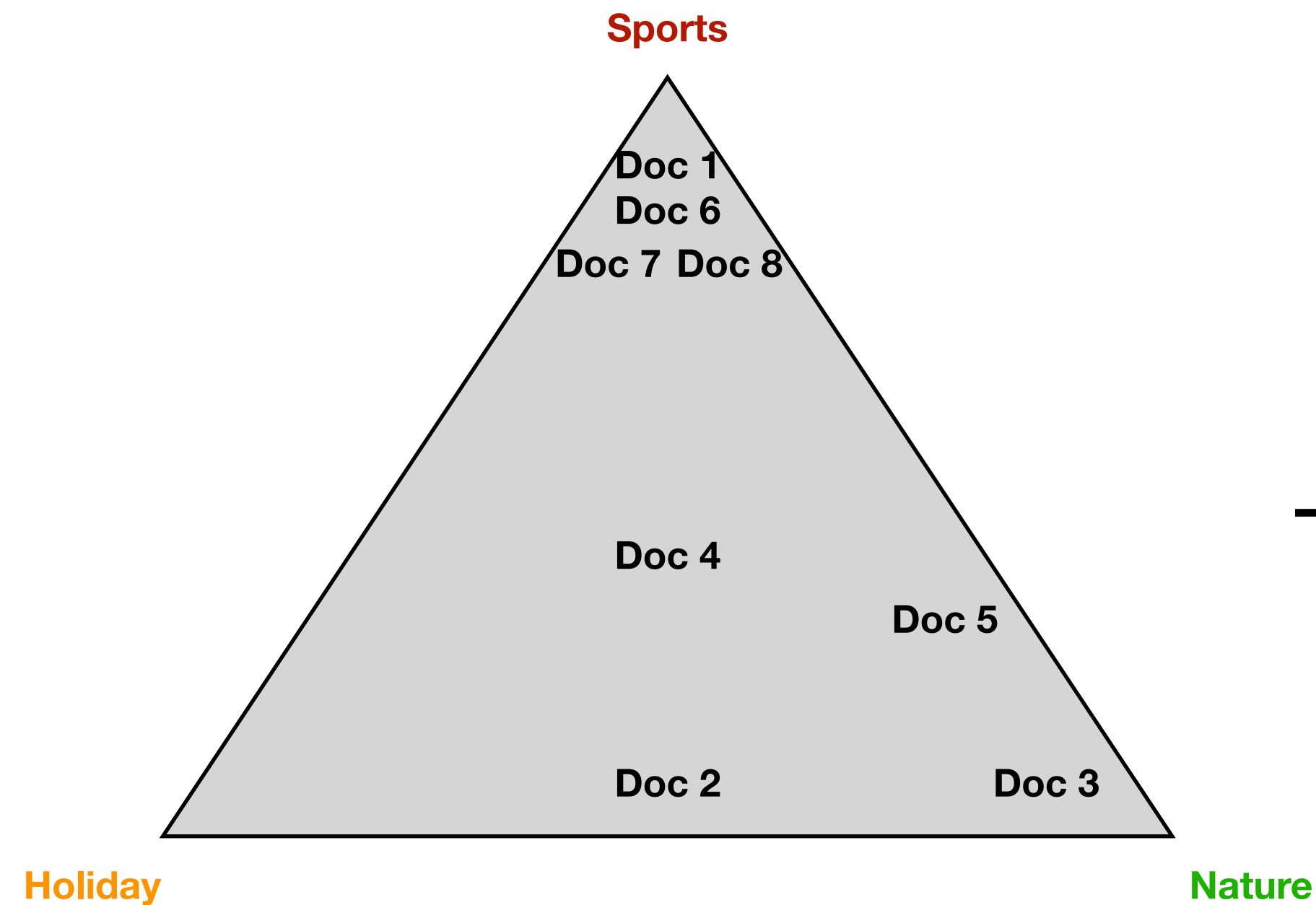
LDA : Multinomial distribution



Dirichlet distribution
« distribution of distribution »

3. Latent Dirichlet Allocation

LDA : Multinomial distribution

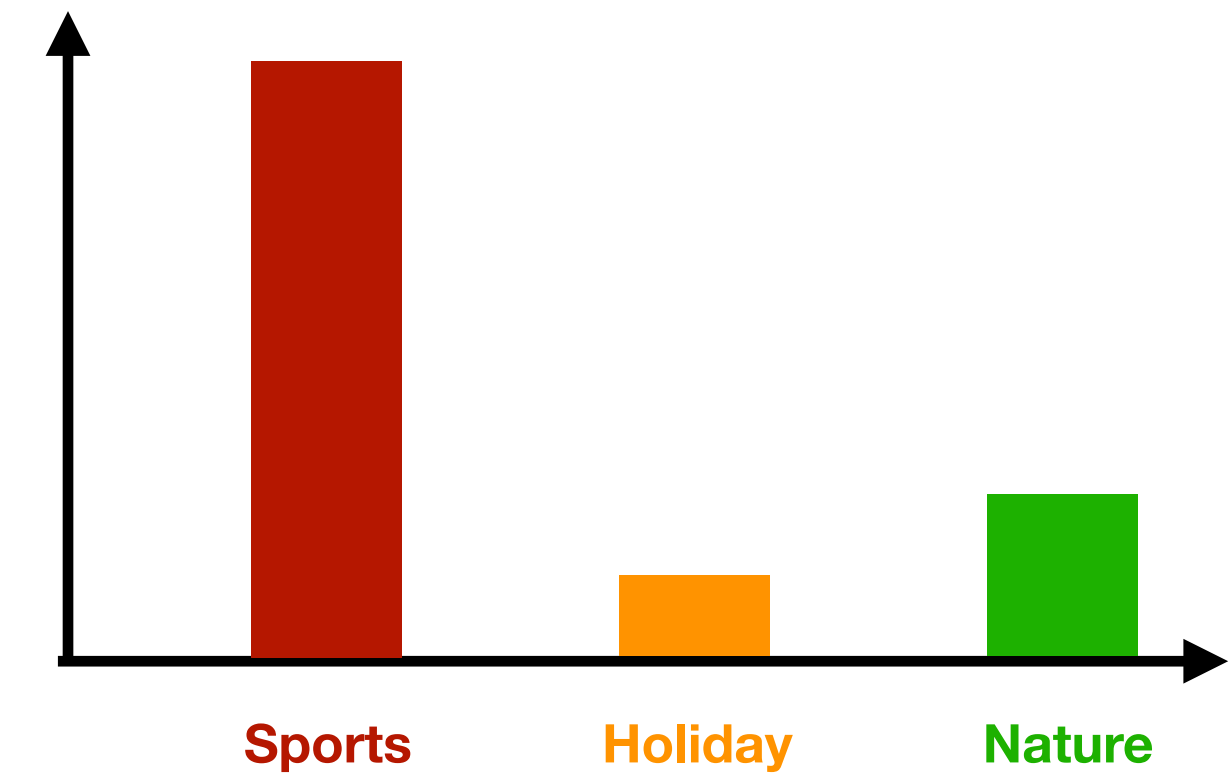


Dirichlet distribution
« distribution of distribution »

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

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

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

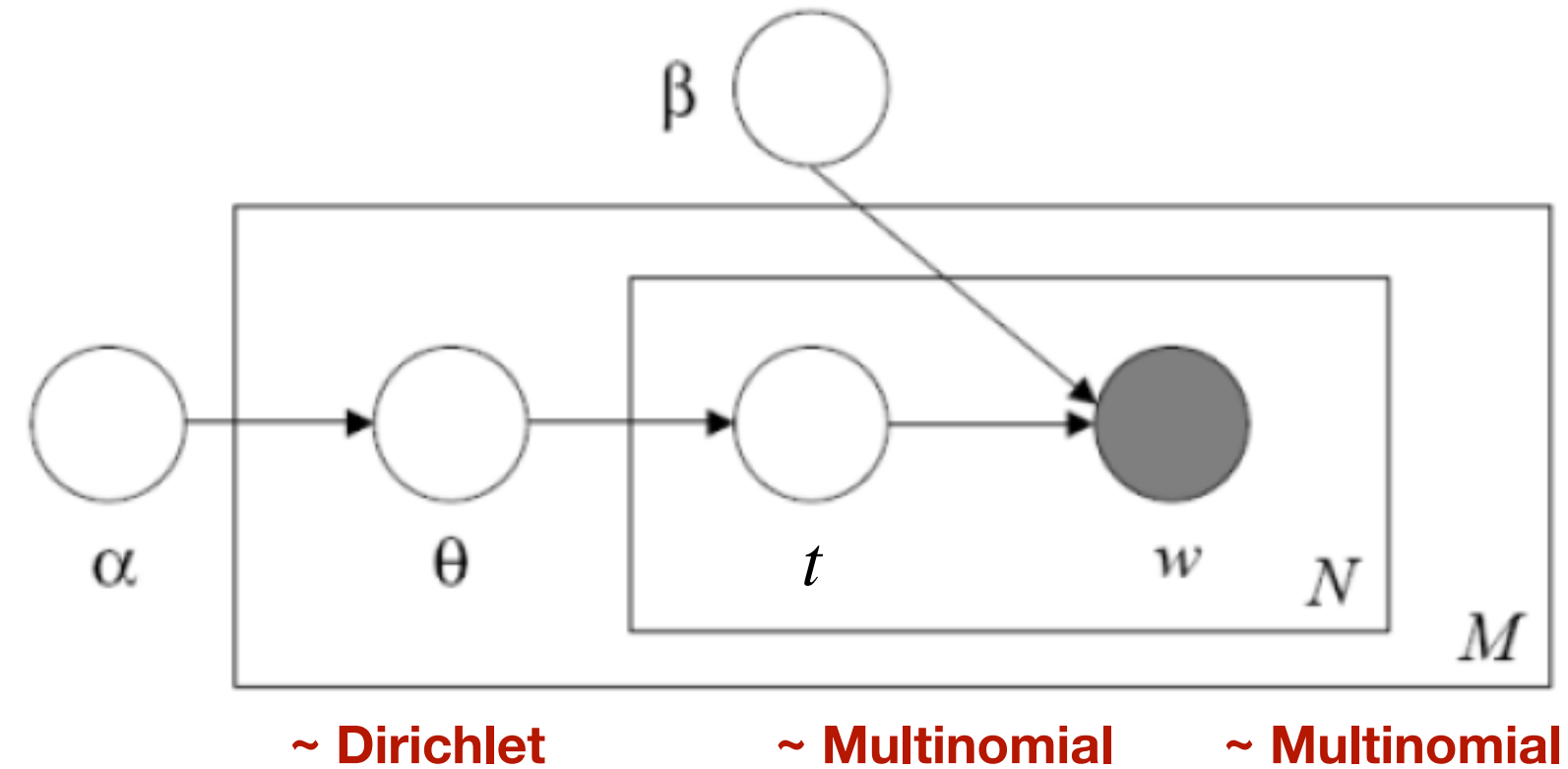


Multinomial distribution

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



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

$$= \prod_{d \in [M]} \text{Dir}(\theta_d \mid \alpha) \cdot \prod_{n \in [N]} \text{Multi}(t_{d,n} \mid \theta_d) \cdot \text{Multi}(w_{d,n} \mid t_{d,n})$$

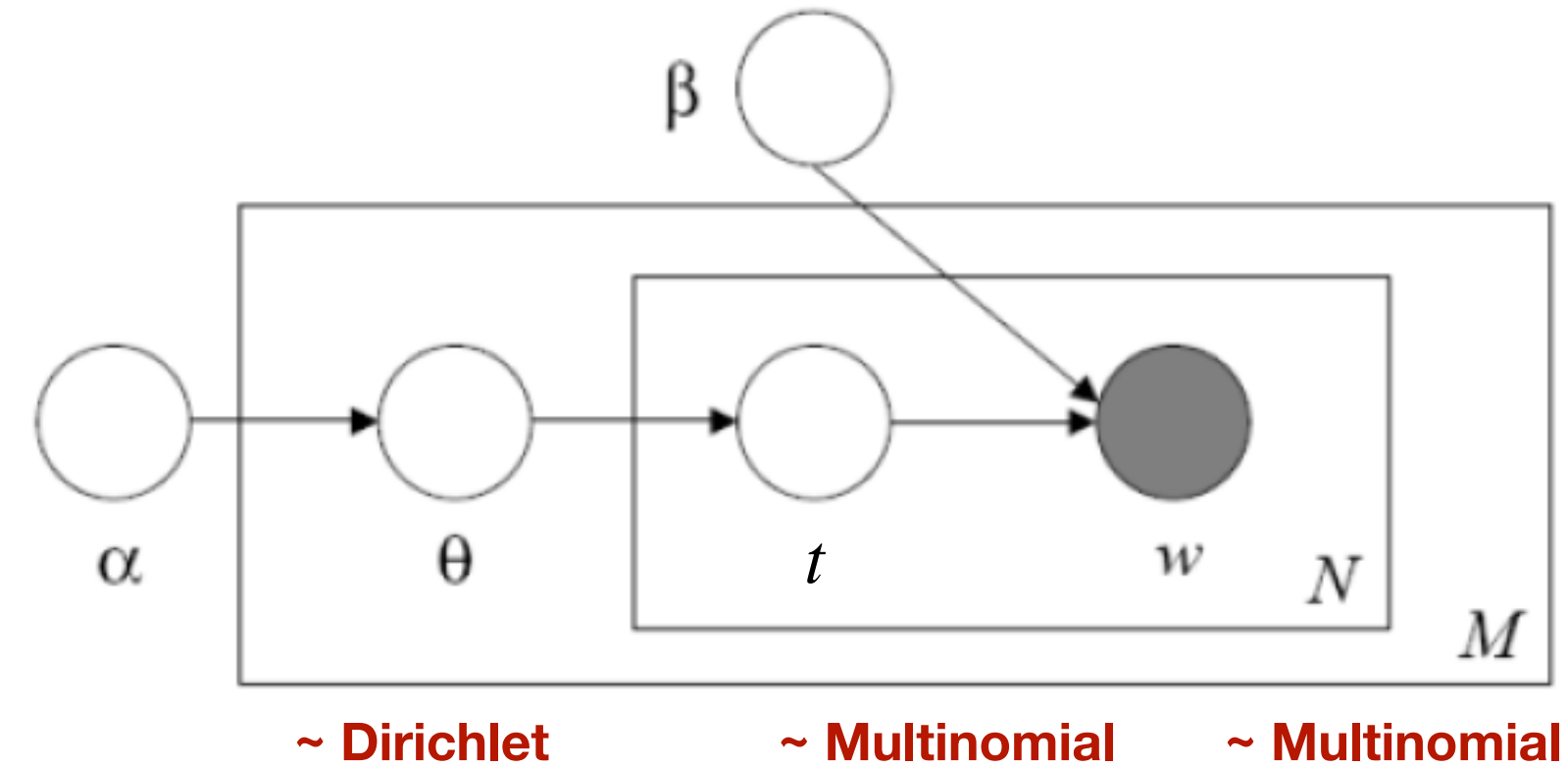
$$\propto \prod_{d \in [M]} \prod_{k \in [K]} \theta_{d,k}^{\alpha_k - 1} \cdot \prod_{n \in [N]} 1_{k=t_{d,n}} \cdot \theta_{d,t_{d,n}} \cdot \beta_{t_{d,n}, w_{d,n}}$$

E step :

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E step :

Objective :

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

Optimal solution :

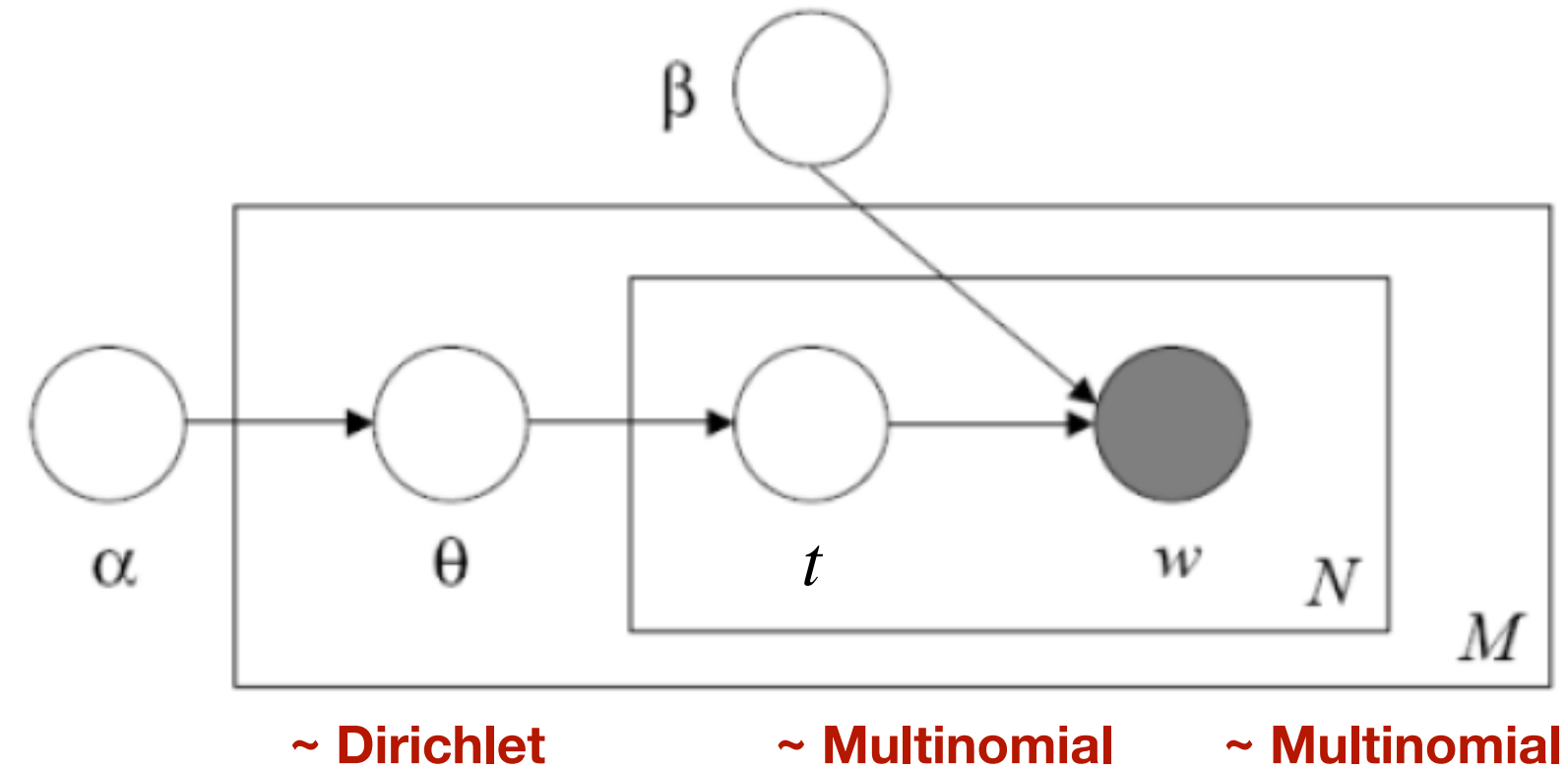
$$\log \hat{P}(\theta) = \mathbb{E}_{Q(t)} [\log P(\theta, t, w)] + \text{const}$$

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

for θ ,

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

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

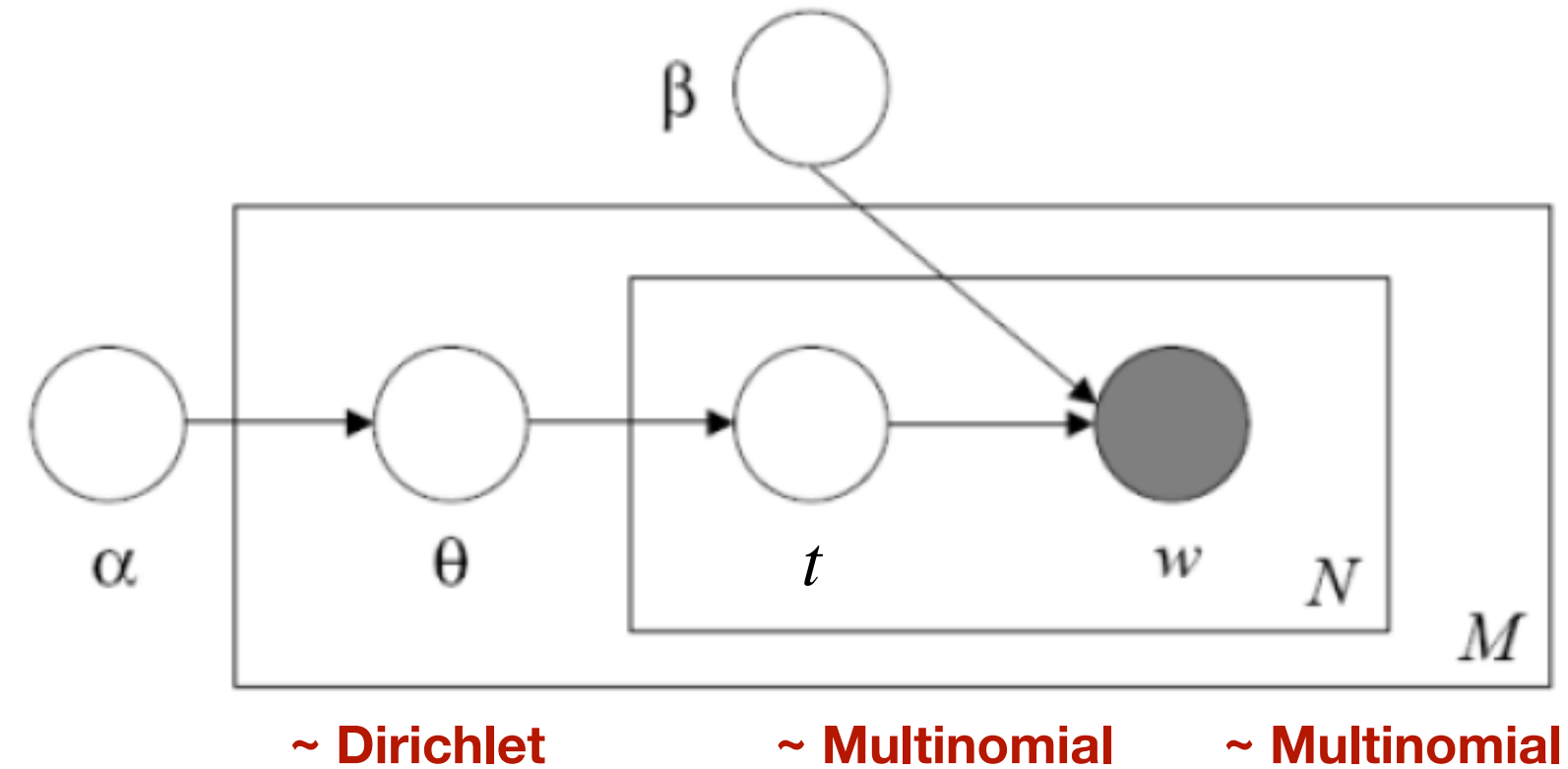
$$= \sum_{d \in [M]} \sum_{k \in [K]} \left[(d_k - 1) + \sum_{n \in [N]} \underbrace{\mathbb{E}_{Q(t_{d,n})} [1_{t_{d,n}=k}]}_{\gamma_{d,n}(k)} \right] \times \log \theta_{d,k} + \text{const}$$

$$\hat{P}(\theta) \propto \prod_{d \in [M]} \prod_{k \in [K]} \theta_{d,k}^{d_k + \sum_n \gamma_{d,n}(k) - 1} \Rightarrow \hat{P}(\theta_d) \propto \text{Dir}(\theta_d | d + \sum_n \gamma_{d,n}(k))$$

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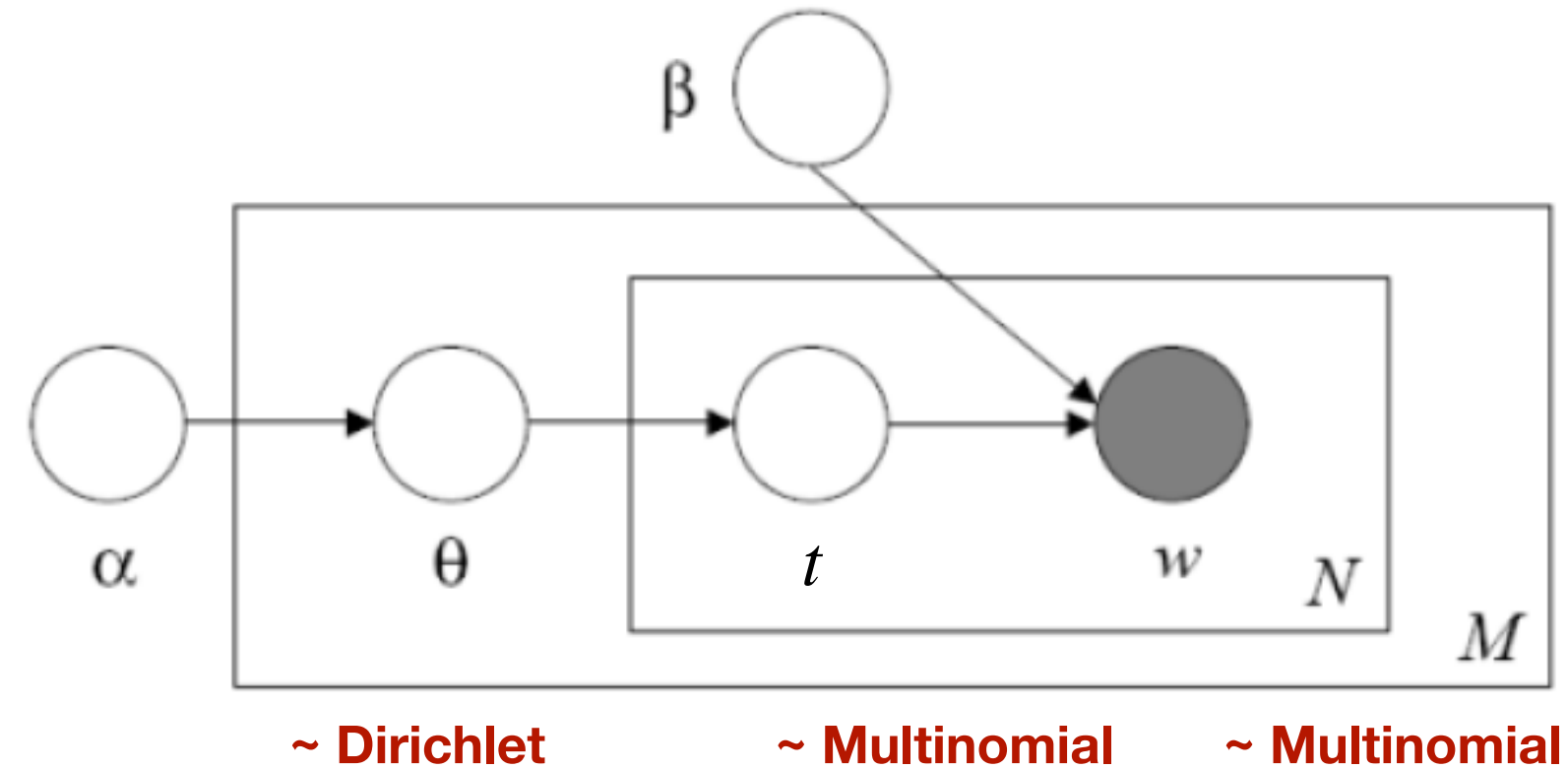
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$$\hat{P}(t) = \prod_d \prod_n \hat{P}(t_{d,n}) \Rightarrow \hat{P}(t_{d,n}=k) = \frac{\beta_{k, w_{d,n}} e^{\mathbb{E}_{Q(\theta)} [\log \theta_{d,k}]}}{\sum_k \beta_{k, w_{d,n}} e^{\mathbb{E}_{Q(\theta)} [\log \theta_{d,k}]}}$$

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M step :

Objective :

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

$$\parallel$$

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

with the following constraint :

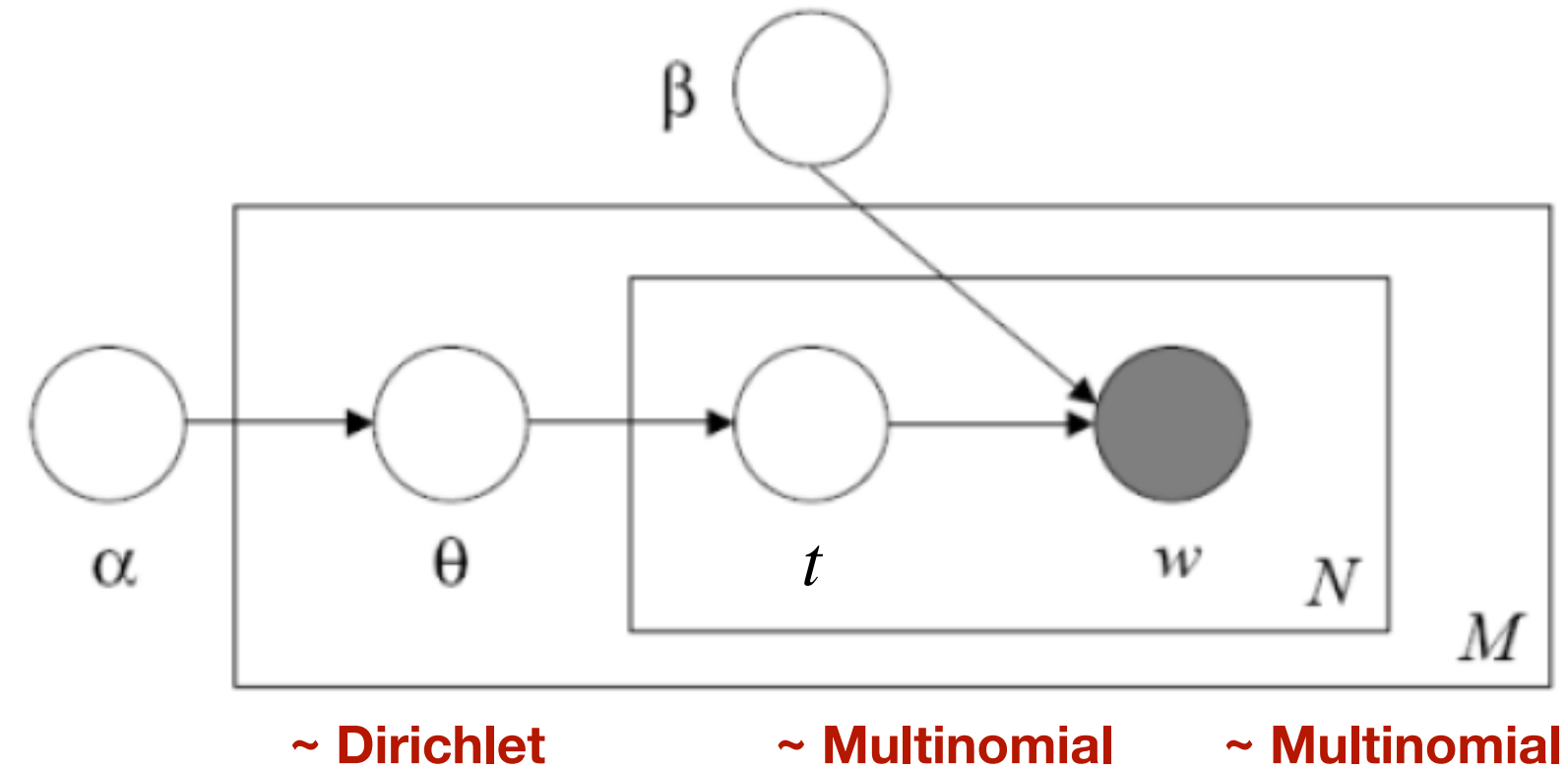
$$\begin{cases} \beta_{k,w} \geq 0 \\ \sum_w \beta_{k,w} = 1 \text{ for all } k \in [K] \end{cases}$$

Let's compute the Lagrange

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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.

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

$$\frac{\partial L}{\partial \beta_{k,w}}(x, \lambda) = 0 \Leftrightarrow$$

left as exercise

$$\beta_{k,w} = \frac{\sum_{d,n,k} \gamma_{d,n}(k) 1_{\{w_{d,n}=w\}}}{\sum_{w',d,n,k} \gamma_{d,n}(k) 1_{\{w_{d,n}=w'\}}}$$

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)

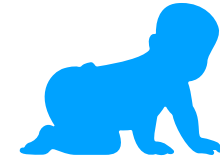
TODO : Part2, +0.5 point

TODO



Road map

Bayesian statistics (03/05/21)



1

Bayesian perspective :

$$P(\theta|X) = \frac{P(X, \theta)}{P(X)} = \frac{\overset{\text{Likelihood}}{P(X|\theta)} \cdot \overset{\text{Prior distribution}}{P(\theta)}}{\underset{\text{Evidence}}{P(X)}}$$

Posterior distribution

θ parameters

X observations

Exemple :
Naive Bayes classifier,
Linear regression,

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

Conjugate distribution

Pros :

- exact posterior

Cons :

- conjugate prior maybe inadequate

Latent variable models (17/05/21)



2

Hidden variable models :

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

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

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