

# Integrating Experts' knowledge in Machine Learning

Habilitation à diriger des recherches de l'Université Paris-Saclay

**Cristina Manfredotti**

25 juin 2024

**Jury :**

- Philippe Leray (reviewer)
- Andrea Passerini (reviewer)
- Nathalie Pernelle (reviewer)
- Thomas Guyet (examiner)
- Nicolas Maudet (examiner)
- Fatiha Saïs (examiner)
- Alexis Tsoukias (examiner)
- Antoine Cornuejols (Tuteur)



MIA  
PARIS-SACLAY  
EKINOCs



GROPARISTECH  
Institut des Sciences et Industries du Vivant et de l'Environnement

# Plan

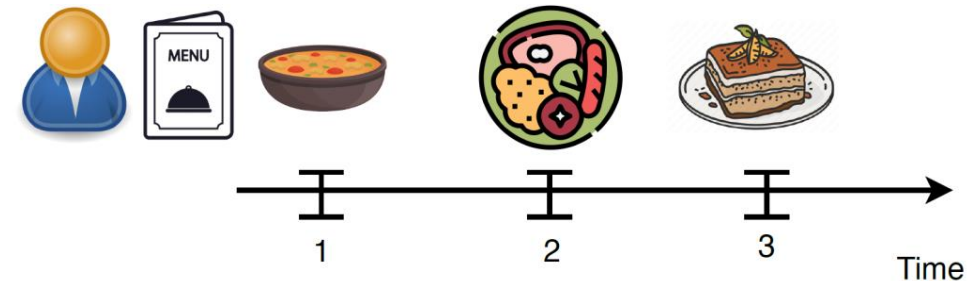
- Background : what I did before AgroParisTech

- Accomplished research

- **Experts' knowledge** and Probabilistic Relational Models (PRMs)
- **Experts' knowledge** for RecSys in the nutrition domain



- Drawbacks and Future Works



# My Background

2004 : Master (Math) U Mi-Bicocca, internship at l'EPFL, Swiss

IRM

2004-2006 : Research Assistant, U Mi-Bicocca, IT

Image segmentation and motion detection

2007-2009 : PhD (Info), U Mi-Bicocca  
Visiting period at University of Toronto

Tracking

Online activity recognition

2010 : PostDoc, U Regina, Canada

Learning

2011-2012 : PostDoc, U Copenhagen, Denmark

Non stationary models

2013-2014: PostDoc, LIP6 UPMC, France

From 2014 : MC(C), MIA Paris(-Saclay) AgroParisTech, France

EK ~ ontologies



# My Background

## Collaborations (2004-2014; before AgroParisTech)

- Milan : Enza Messina, Domenico Sorrenti, Francesco Archetti, Elisabetta Fersini, Luca Cattelani, Giorgio Consigli
- Toronto : David Fleet
- Regina : Sandra Zilles, Howard Hamilton
- Copenhagen : Kim Steenstrup Pedersen,
- Paris : Christophe Gonzales, Séverine Dubuisson

## Scientific production (2004-2014) :

2 journals, 9 conferences, 10 workshops

# Plan

- Background : how I got here and what I learnt from this exercise
- Accomplished research
  - **Experts' knowledge** and Probabilistic Relational Models (PRMs)
  - Experts' knowledge for RecSys in the nutrition domain
- Drawbacks and Future Works

# Experts' Knowledge and PRMs

- Collaborations : Juliette Dibie, Pierre-Henri Wuillemin, Cédric Baudrit, Mélanie Münch, Stéphane Dervaux, Thomas Allard, Solange Buchin, Elisabeth Guichard, Patrice Buche, Hélène Angellier-Coussy, Liliana Ibanescu, Fatiha Saïs
- PhD Thesis : Mélanie Münch
- Internships M2 : Mélanie Münch, Serife Akkoyunlu, Jiang You, Allan Kabbouh
- Projects : 1 ANR JCJC, 1 ANR, **1 APT, 1 these ABIES**
- Scientific production : 2 journals, 5 conferences, 3 workshops

# EK and PRMs : why ?

@ AgroParisTech :

- necessity of reasoning about transformation processes
  - already an ontology structuring this domain
- PRMs to reason on uncertainty in transformation processes
- Similarity between PRMs and Ontologies => mapping

# PRMs

A BN is the representation of a joint probability over a set of random variables that uses a DAG to encode probabilistic relations between variables

Combine advantages of relational data bases & **Bayesian networks**:

- natural domain modeling: objects, properties, relations;
- generalization over a variety of situations;
- compact, natural probability models.

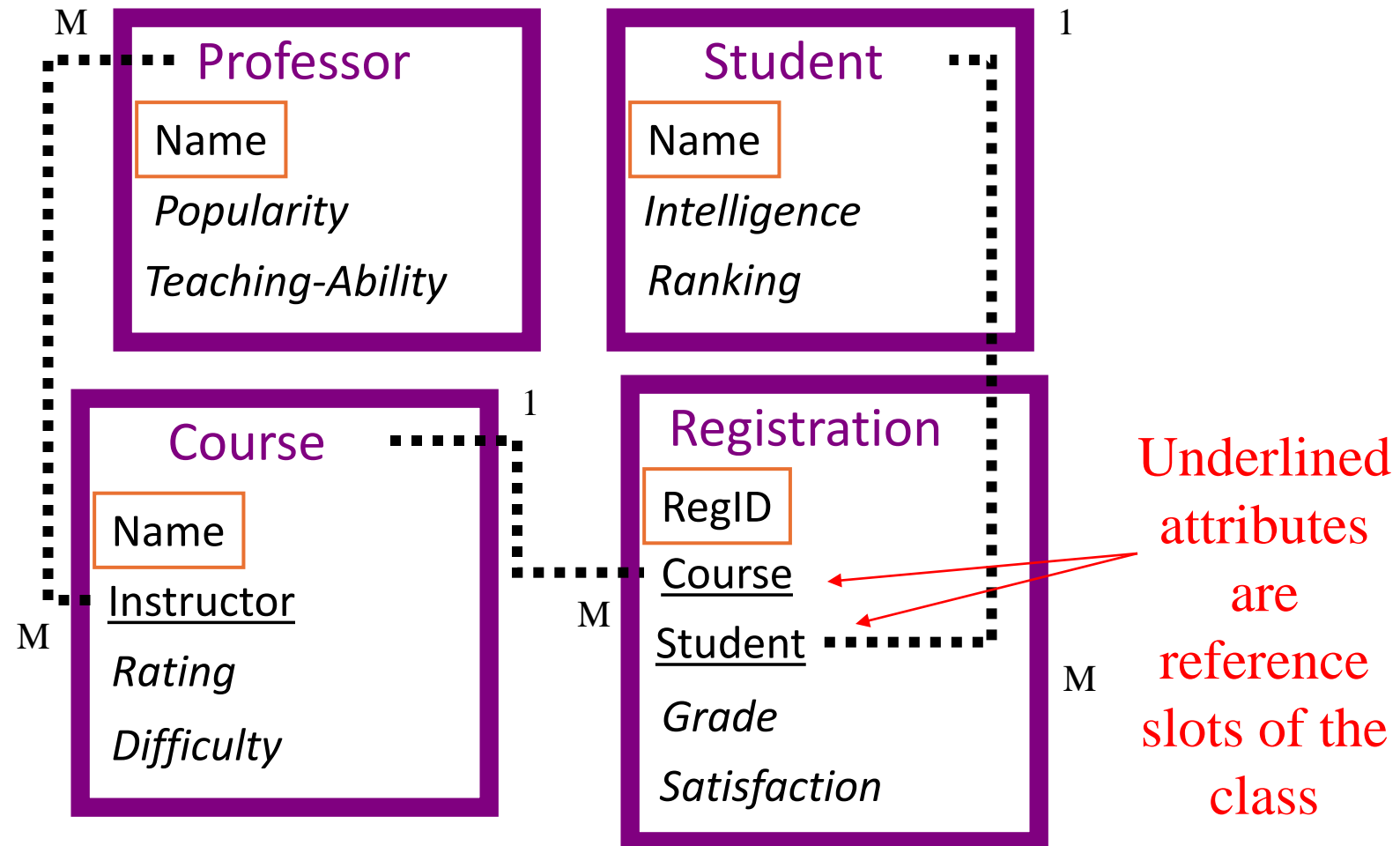
➤ **Relational Schema and Relational slots** (and slot chain)

PRM system => (big) BN



# PRM – Relational Schema [Getoor 01]

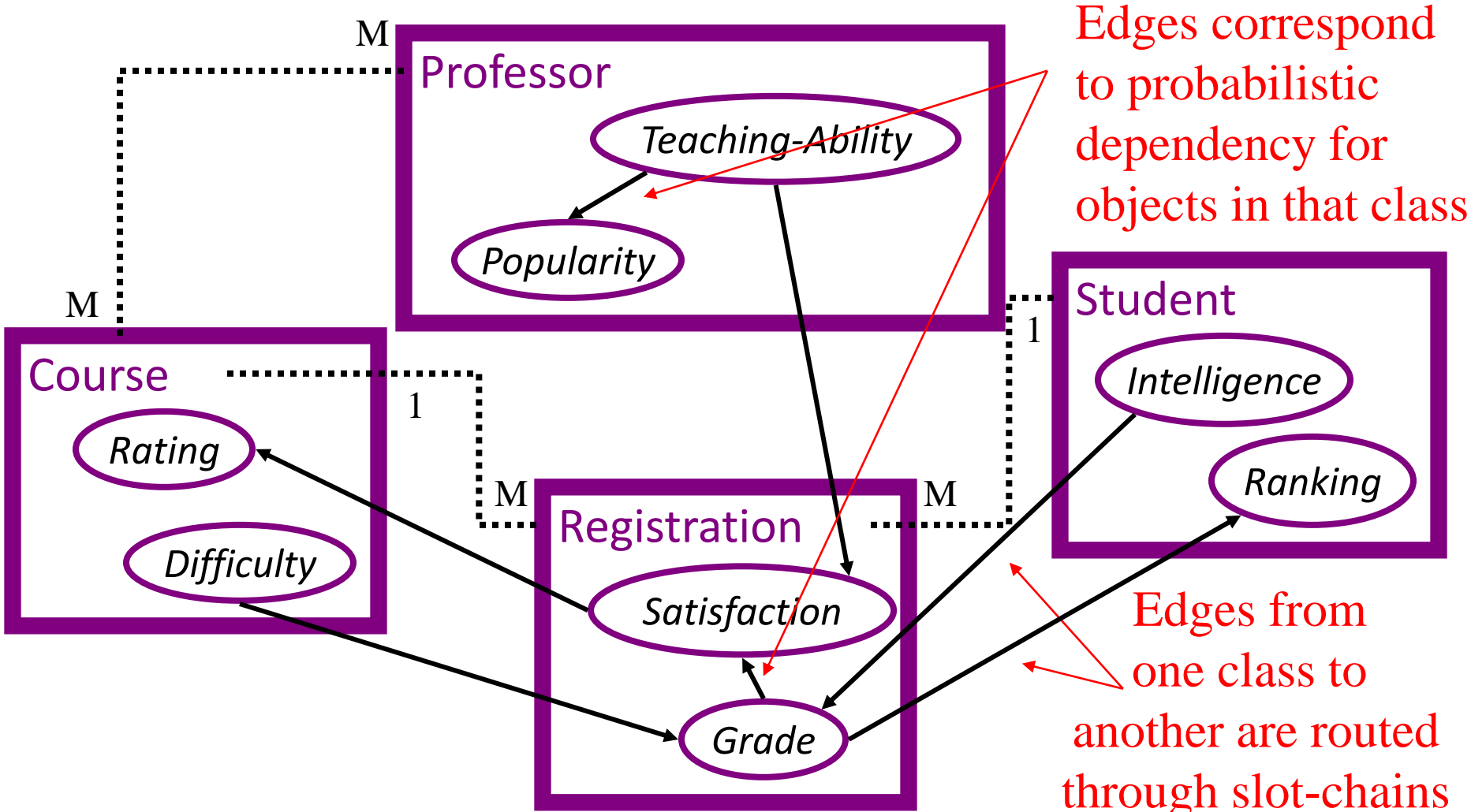
## University Domain Example



Underlined  
attributes  
are  
reference  
slots of the  
class

# PRM definition

## the University Domain



# PRMs

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Combine advantages of relational data bases & **Bayesian networks**:

- natural domain modeling: objects, properties, relations;
  - generalization over a variety of situations;
  - compact, natural probability models.
- 
- Relational Schema
  - Relational slots (and slot chain)

**PRM system => (big) BN**

# Ontologies

A KB = ontology + knowledge graph

Ontology = classes, properties, axioms

Knowledge graph = data organised following the ontology

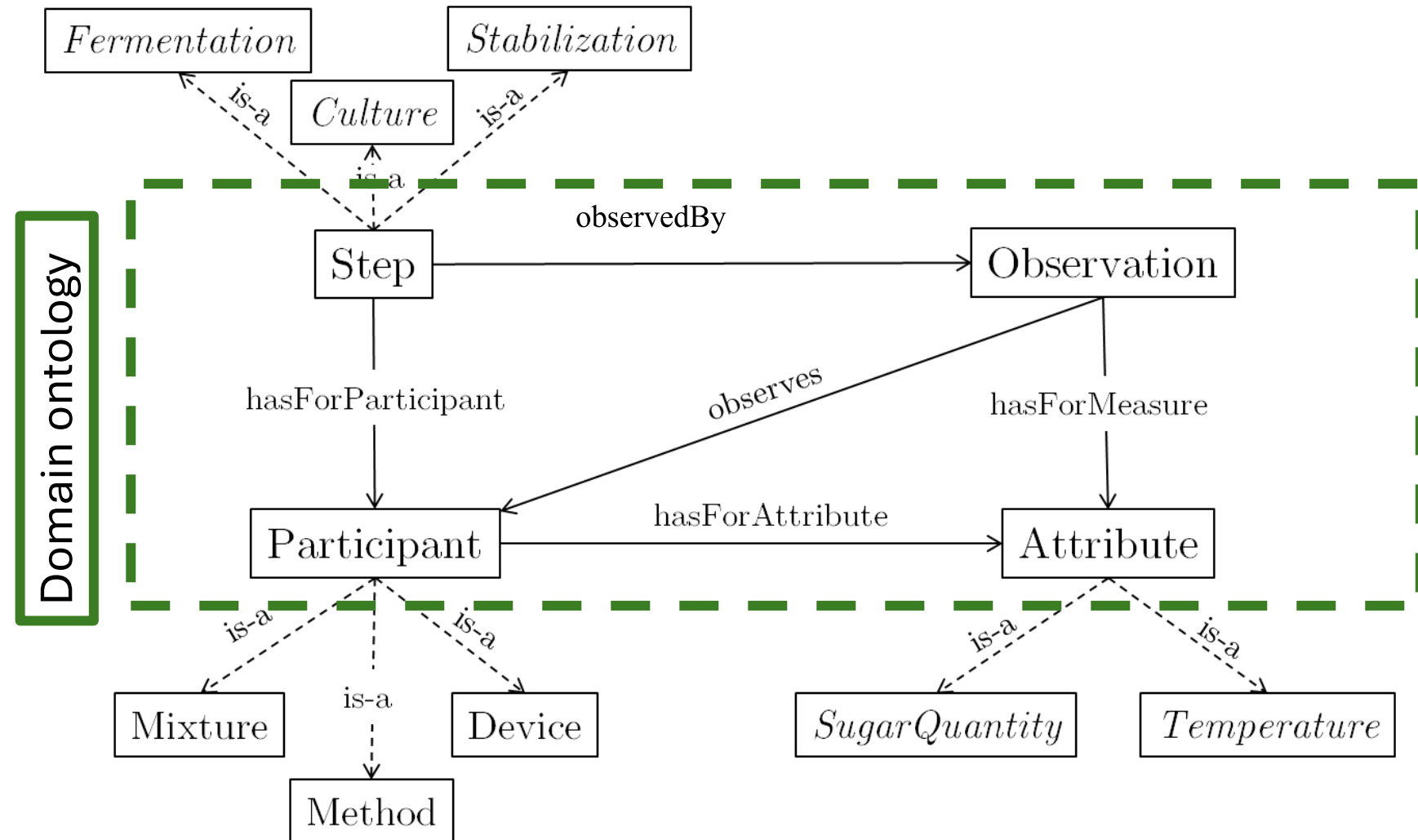
- Represent the knowledge on a domain with
  - classes,
  - relations (or properties) between these classes and
  - instances of these classes.
- Used as a common and standardized vocabulary for representing a domain.
- Data can be collected in a **knowledge base** that organises them according to the structure defined by an ontology.

# EK and PRMs : why ?

@ AgroParisTech :

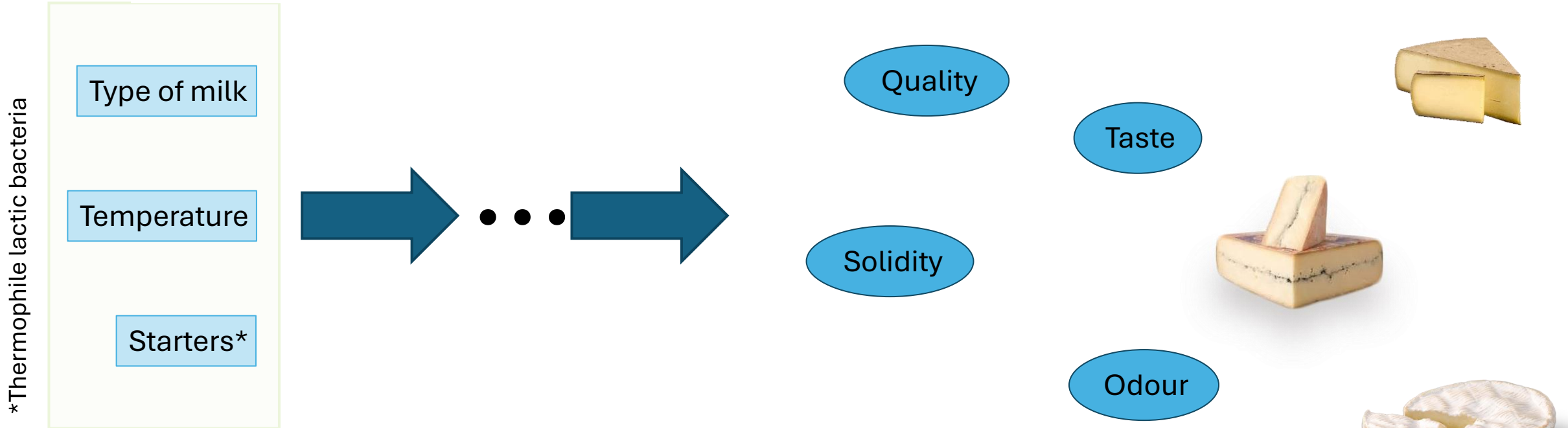
- necessity of reasoning about transformation processes
- already an ontology structuring this domain
  
- PRMs to reason on uncertainty in transformation processes
  
- **Similarity** between PRMs and Ontologies -> mapping

# The Process and Observation Ontology [Ibanescu16]



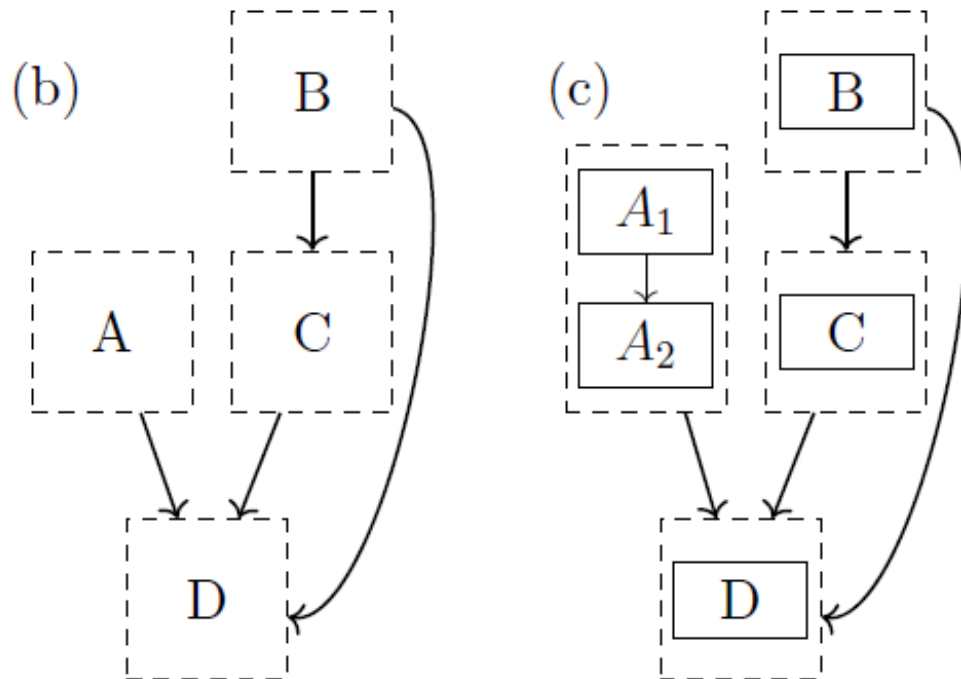
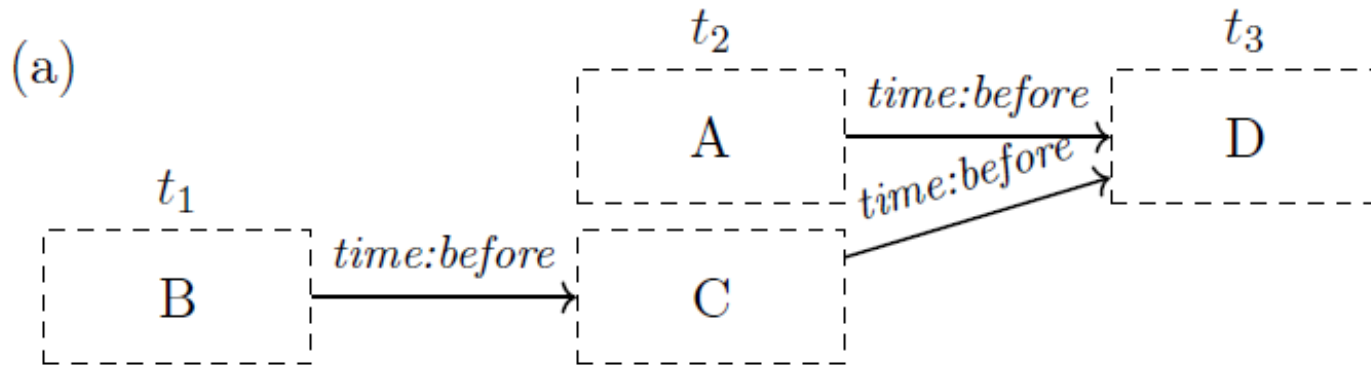
# Modeling Cheese fabrication Process

**QUESTION:** *Which attributes can define the final product? How?*



**TrueFood project** : to what extent the characteristics of some hard cooked cheese is affected by the use of various composition of different milks and by the use of different technological conditions.

# Mapping ontology and PRM : the stack model



Defined by **two constraints**:

- **temporal** (given by the ontology)
- **causal** (given by the expert)

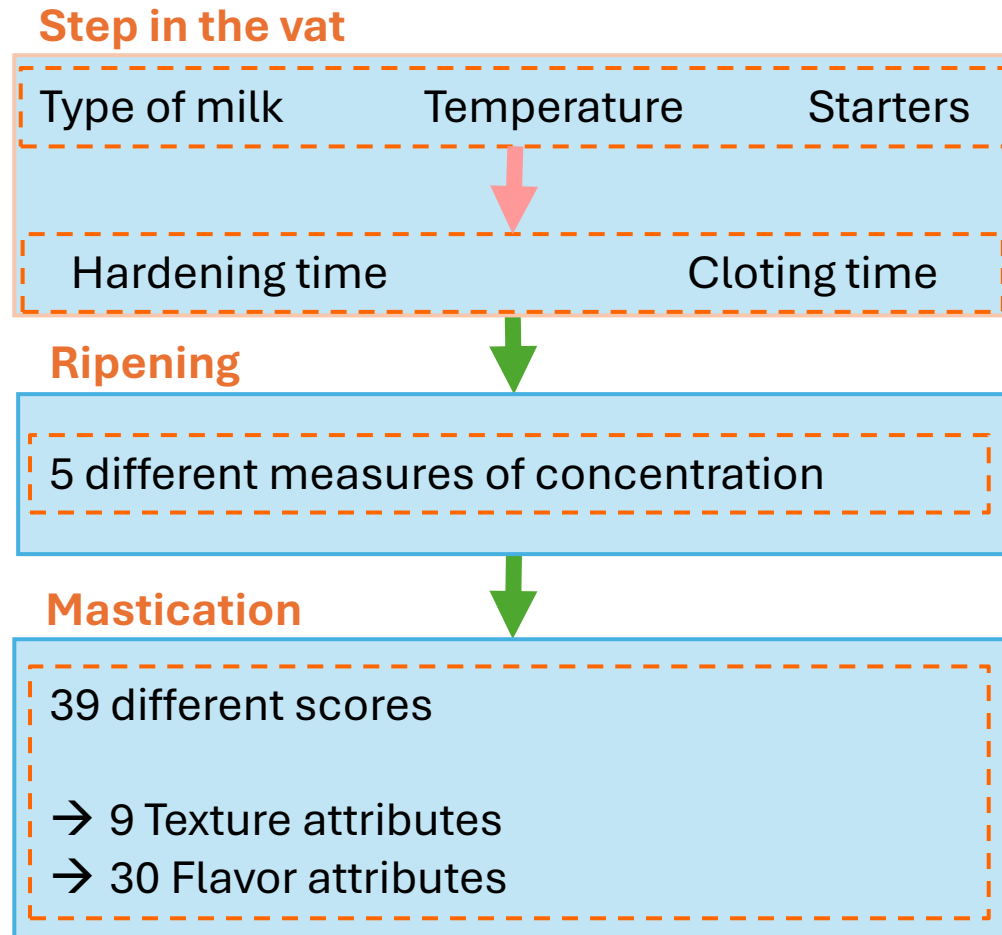
They define the ordering with which we learn

- M. Munch, J. Dibie, P-H. Wuillemin, C. Manfredotti. Towards Interactive Causal Relation Discovery Driven by an Ontology. FLAIRS Conference 2019: 504-508
- M. Munch, J. Dibie-Barthélemy, P-H. Wuillemin, C. Manfredotti. Interactive Causal Discovery in Knowledge Graphs. PROFILES/SEMEX@ISWC 2019: 78-93



# Cheese fabrication modeling

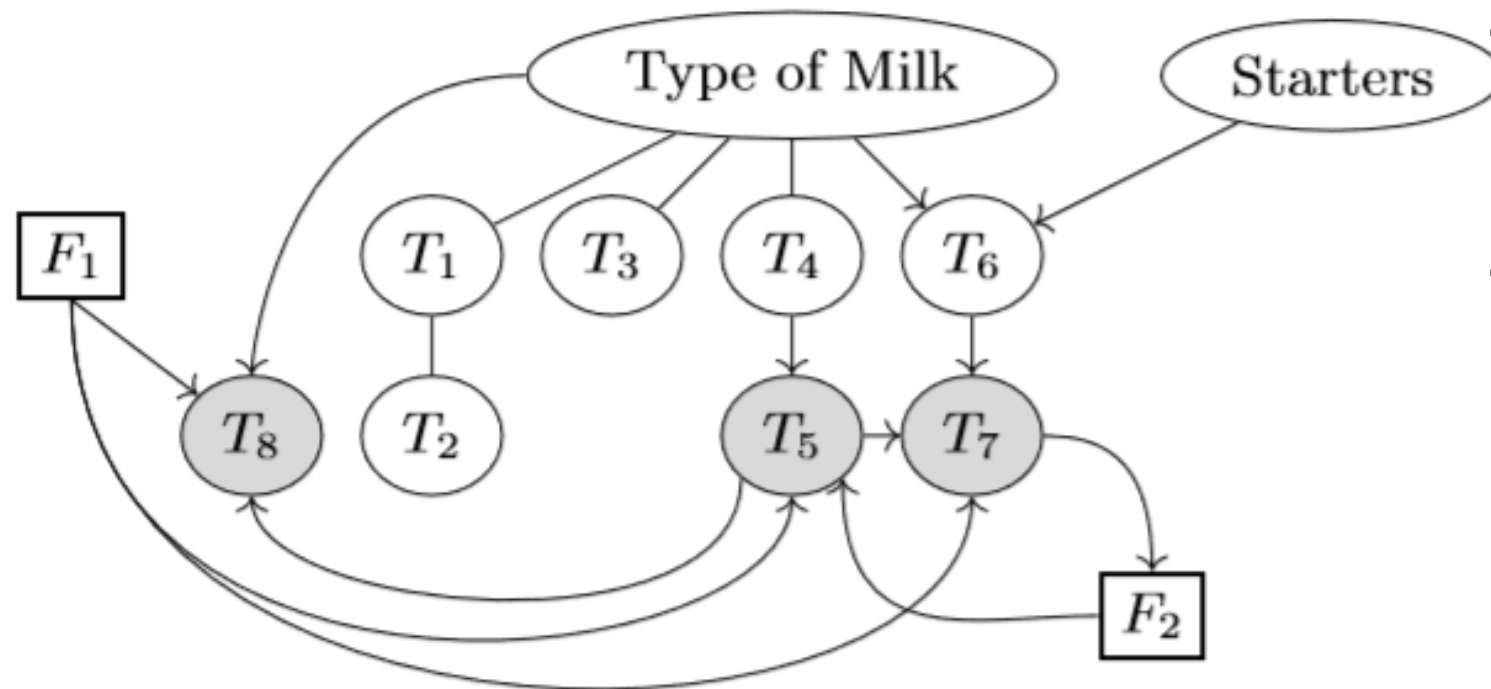
Construction of the **relational schema** with the expert



# Interpretation

**Excerpt** of the Essential Graph:

- T texture attributes
- F groups of flavor attributes

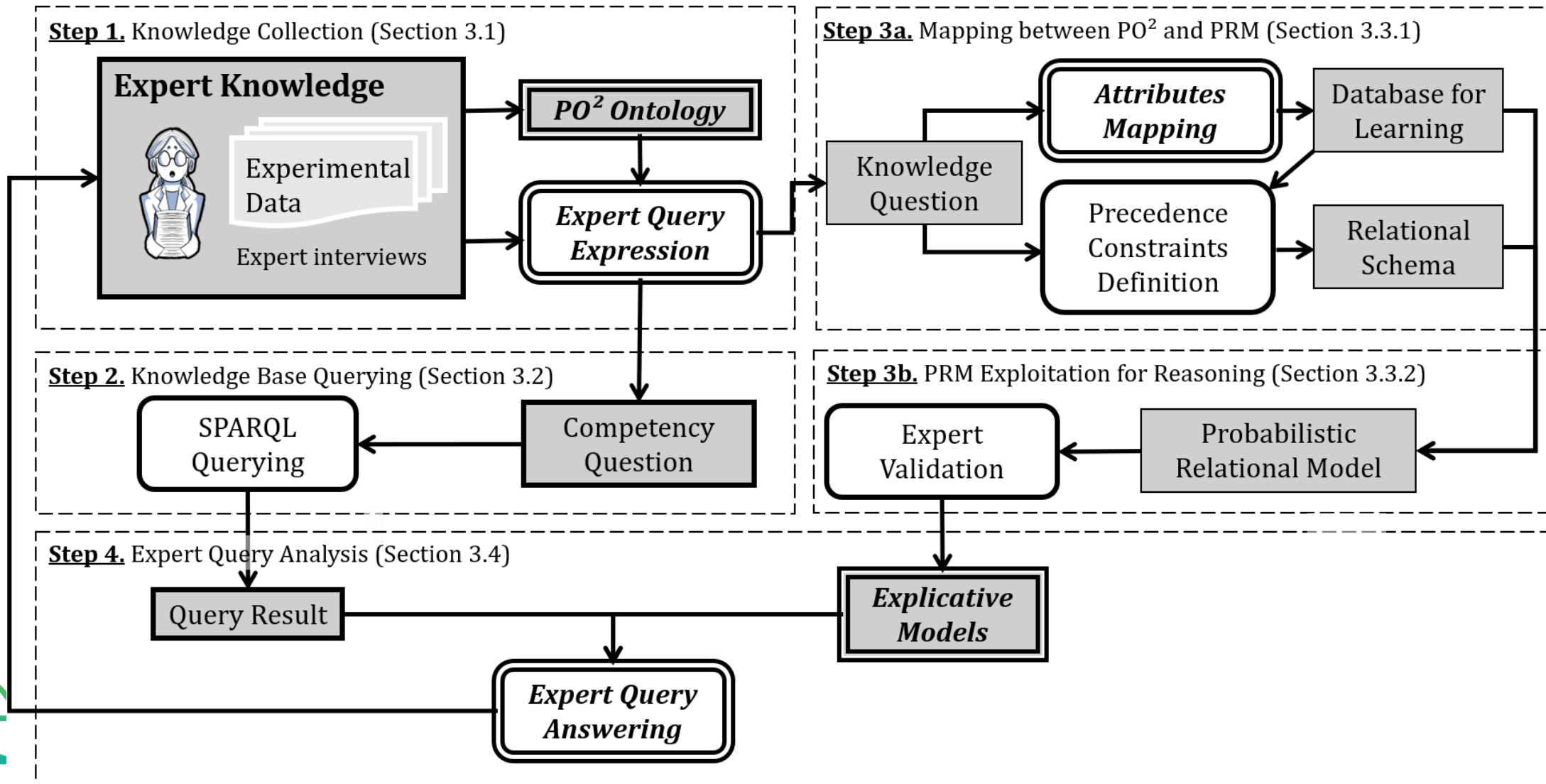


→ The type of milk mostly explain all **texture attributes**

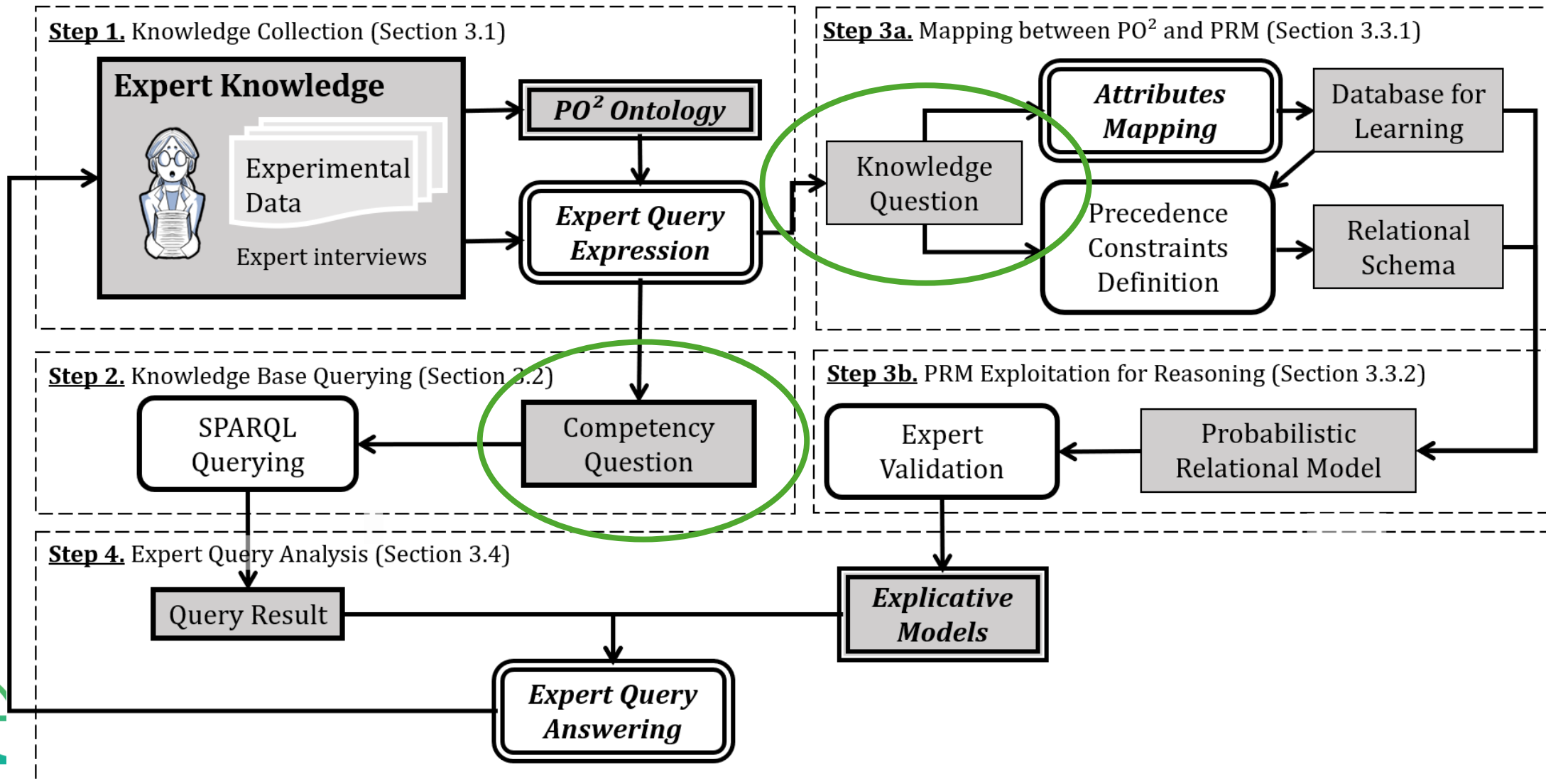
→ The **flavor attributes** are hardly explained by the control parameters

M.Munch, P-H. Wuillemin, J. Dibia, C. Manfredotti, T. Allard, S. Buchin, E. Guichard. Identifying Control Parameters in Cheese Fabrication Process Using Precedence Constraints. DS 2018: 421-434

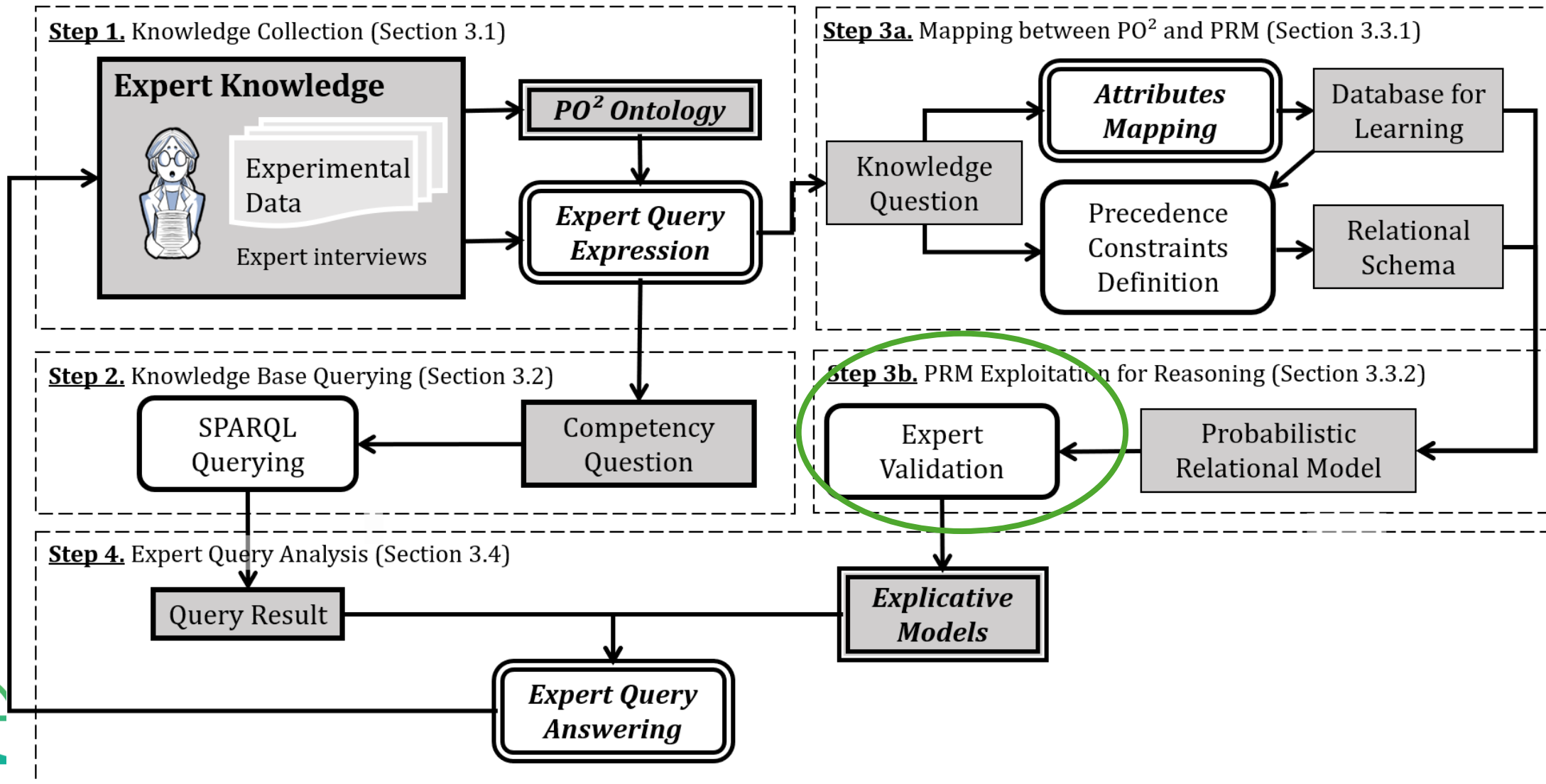
# Mapping ontology and PRM : POND



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# Mapping ontology and PRM : POND



# Food packaging biocomposite manufacturing

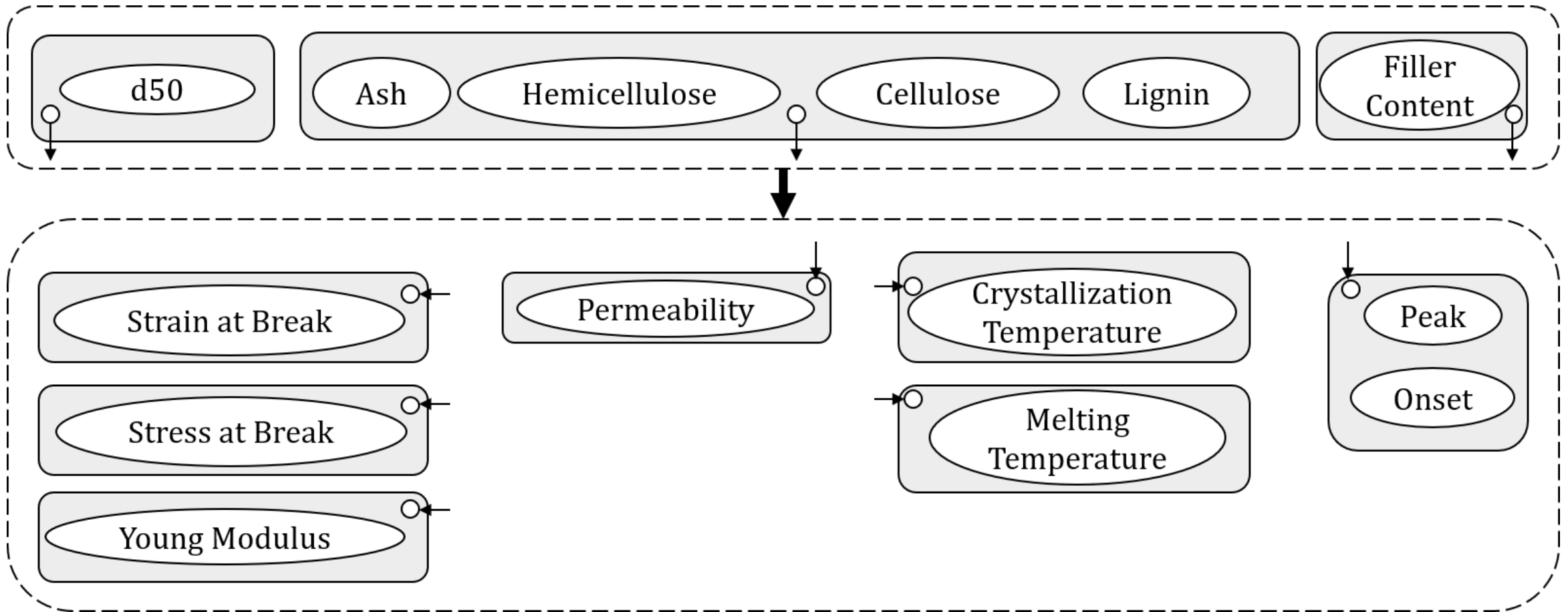
- PHBV : bacterial bio-polymer, biodegradable, expensive
- **Idea** : Mix it with lignocellulosic fillers (LF)

LF = Dry fractions of organic residues

- It reduces the overall cost
- But modulates the functional properties

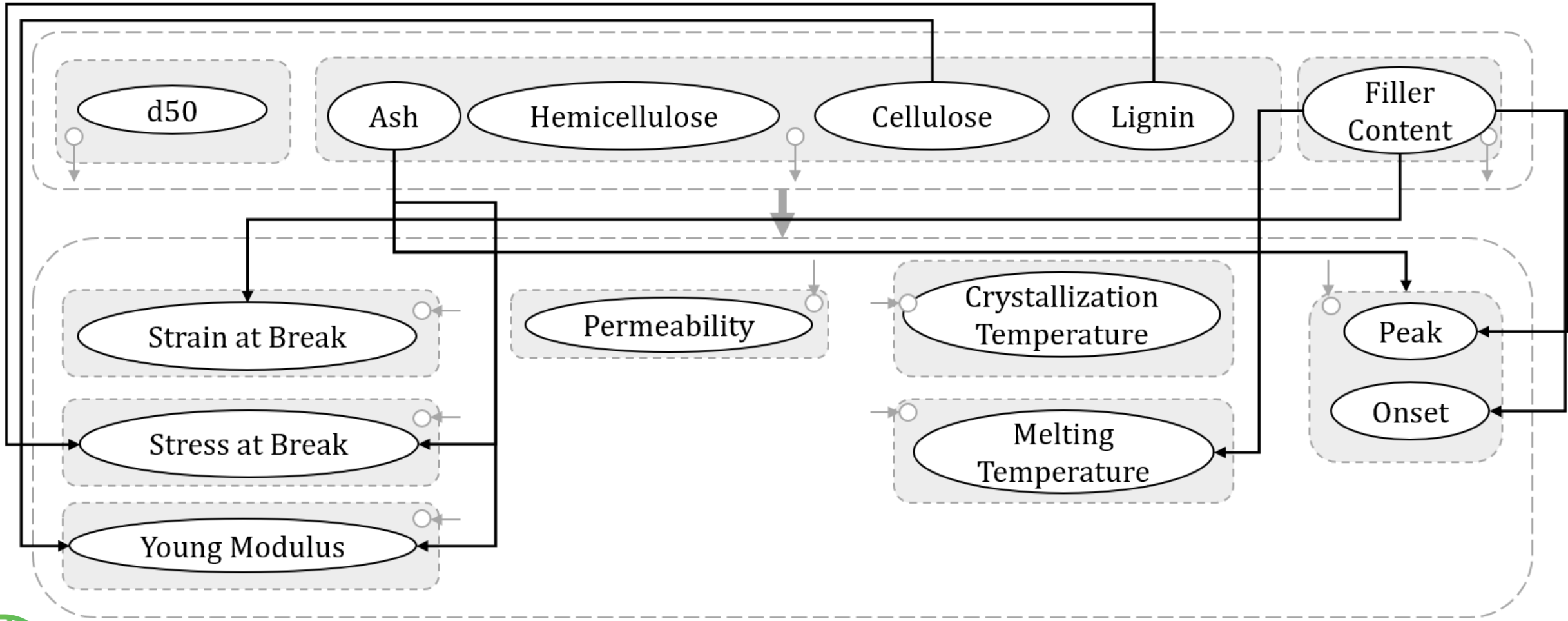
**Question** : find the right compromise between the maximum acceptable filler content (wrt overall product), filler size and resulting properties

# Mapping ontology and PRM : POND



**QUESTION:** *Which parameters explain the thermal degradation temperatures ?*

# Mapping ontology and PRM : POND





# Mapping ontology and PRM : POND

Filler Content	Peak Temperature		
	]0.72; 0.95]	]0.95; 1]	]1; 1.16]
]2; 4]	0.09	<b>0.82*</b>	0.09
]4; 11]	0.38	<b>0.52*</b>	0.1
]11; 21]	<b>0.91*</b>	0.09	0
]21; 50]	<b>0.6*</b>	0.2	0.2

Conditional Probability Table showing the influence of the Filler Content over the Peak Temperature distribution. \* shows the maximum likelihood.

# Mapping ontology and PRM: remarks

- Motivations :
  - Need to reason with uncertainty in transformation processes
  - Similarity between ontologies and PRMS
- The experts
  - give the ontology
  - structures the variables with his hypothesis
  - afterwards, critiques the model
- The approaches
  - Verify the expert's hypothesis
  - Suggest new experiments
  - Able to do prediction

# Mapping ontology and PRM: ideas for the future

- The expert's validation step could be investigated more
  - Exploring algorithms able to learn a network locally
  - Visualisation and human machine interaction
  - (automatic) Explanation, (also) to suggest new experiments
- The ontology could be used more
  - Answering competency questions to structure de domain giving more insights to the learning
- Transfer Learning, Data linking, Graph Matching

# Plan

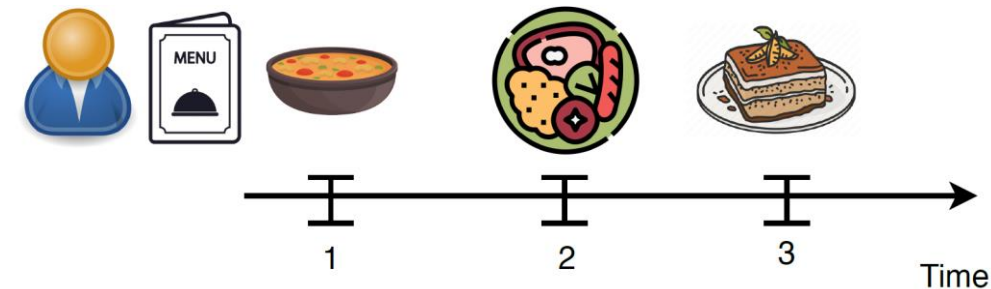
- Background : how I got here and what I learnt from this exercise
- Accomplished research
  - Experts' knowledge and PRMs
  - **Experts' knowledge** for RecSys in the nutrition domain
- Drawbacks and Future Works

# EK and RecSys in nutrition

- Collaborations : Antoine Cornuéjols, Nicolas Darcel, Fabien Delaere, Vincent Guigue, Fatiha Saïs, Stéphane Dervaux, Paolo Viappiani, Sabrina Teyssier
- PhD Thesis : Sema Akkoyunlu, Alexandre Combeau, Thomas Dheilily
- Stage M2 : Noémie Jacquet, Maeva Caillat, Yuhan Wang
- Projects : **1 Prj Danone**, 2 European Prj, **1 ANR**, 1 ANR, **1 DATAIA**
- Scientific production : 1 conferences, 4 workshops

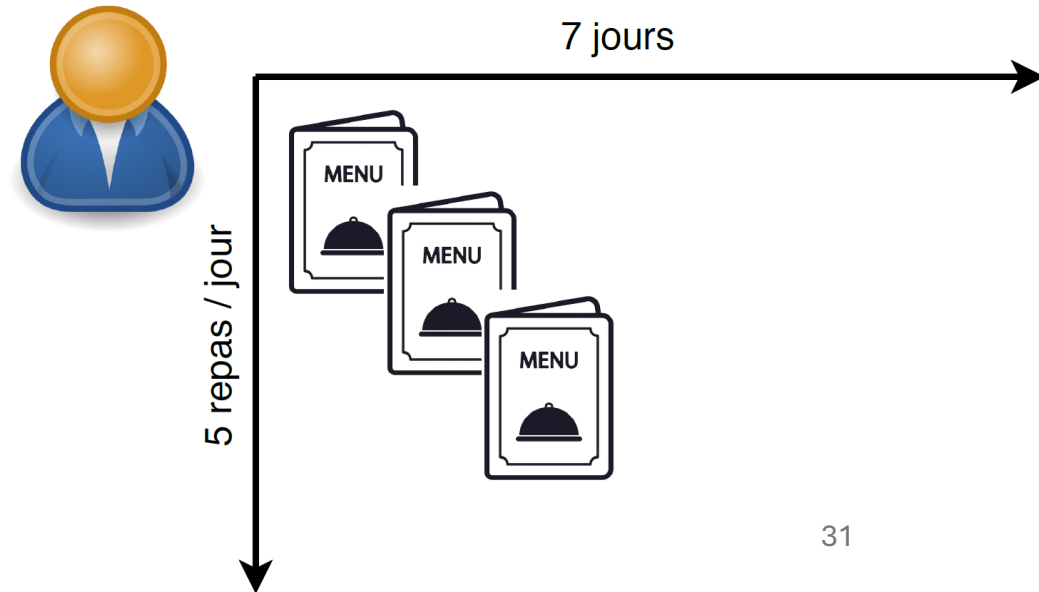
# RecSys in nutrition : importance & originality

- Unhealthy diet => diseases
- Ineffectiveness of healthy diet campaigns
- Need of long-term, health-aware recs
- Meal rec  $\neq$  dish rec  $\neq$  item rec
  - Dish and Meal structure
  - Sequentiality : coherent sequence of dishes
  - Food items frequency
  - Rules : control over nutritional quantity/quality
  - Context : sex, age, home/office, friends/family, ...



# RecSys in the nutrition domain : INCA2 dataset

- Quantity : 2624 adults individuals, **7 days, 5 meals**
- 280 food items organized in 44 **groups** and 110 sub-groups of food items
- **Context factors** : place, company, eater characteristics
- Structured, good quality, sequences of real consumptions over 7 days
- Consumptions are entered in order as they are consumed  
(+ transversal food items at the end)



- **Meal mean length : 7/8 items**

# INCA2 dataset : our choices

We did not consider consumed quantities of food items

- Consumption => implicit preference,
- Binary interaction matrix : food items/users

We separately modeled breakfast and lunch&dinner



- breakfast : repetitive, 11% new food items on the 7th day
- lunch&dinner : longer, 51% new food items on the 7th day  
(**almost cold start**)

- Sliding week

➤ no bias for the week-end



# INCA2 : our choices

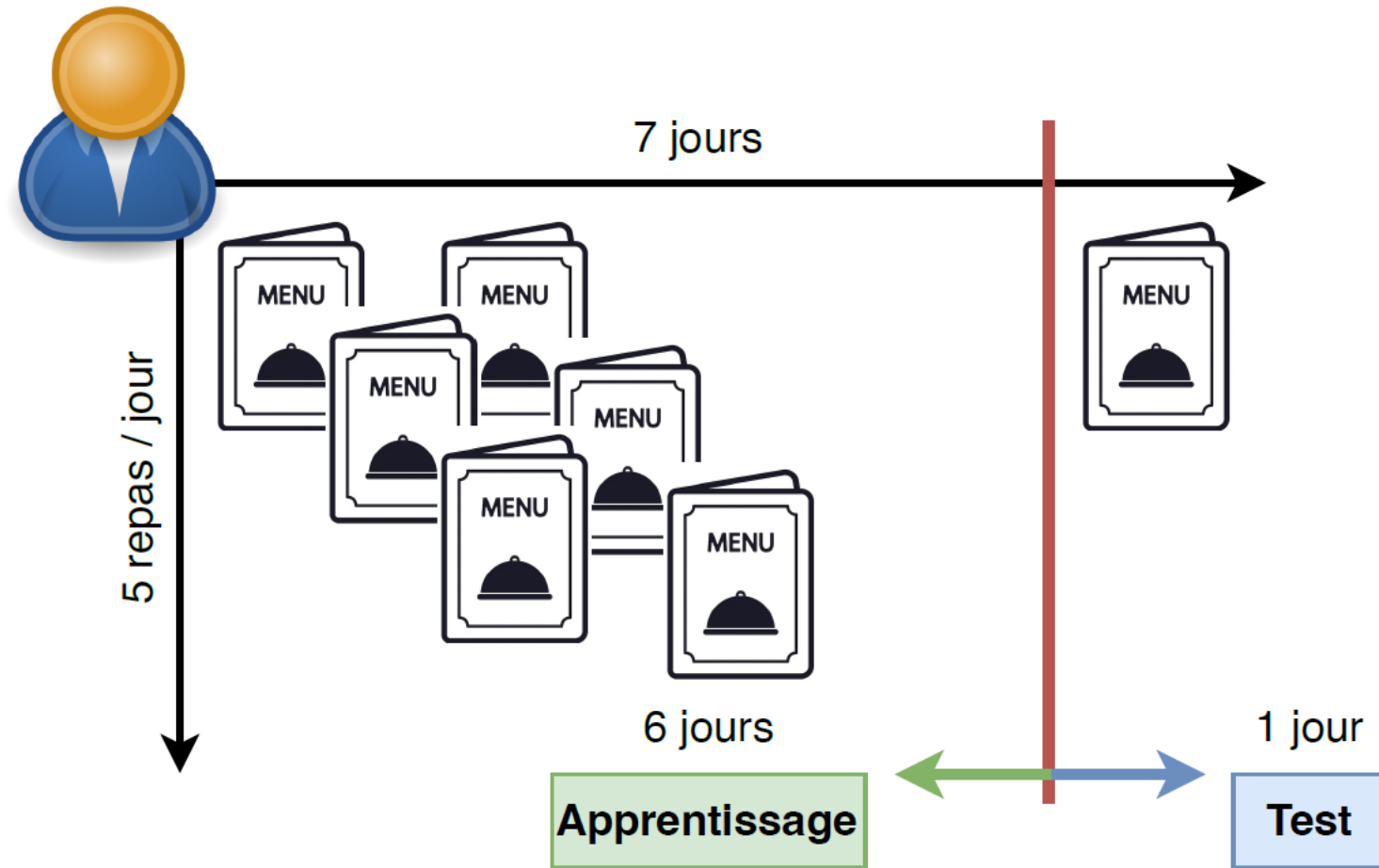
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- Binary interaction matrix: «food items»/«users»

We separately modeled breakfast

- breakfast : repetitive, 11%
- lunch&dinner : longer, 51% (quasi cold start)

- Sliding week
  - no bias for the week-end



# RecSys in the nutrition domain : substitutions

**Substitutability score** : takes into account associativity as well

meal graph  $G = (V, E)$  :

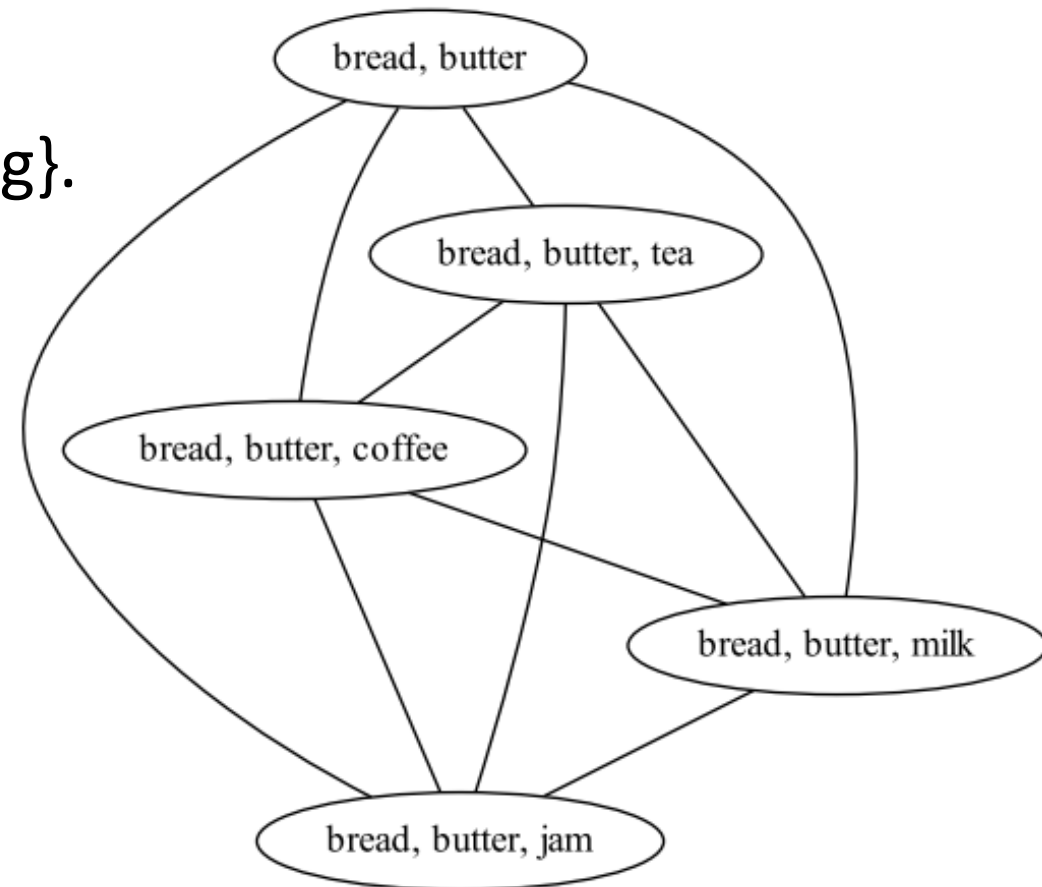
- Meal context {bread, butter}
- substitutable set {coffee, tea, milk, jam, nothing}.

*Discovering substitutable sets*

=

*mining maximal cliques in a graph*

$$f(x, y) = \frac{|C_x \cap C_y|}{|C_x \cup C_y| + |A_{x:y}| + |A_{y:x}|}$$



# The exersys\* project

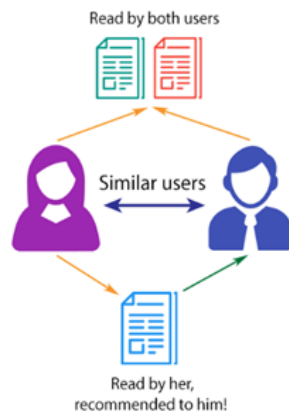
Develop a RecSys for meals recommendation combining

- User preferences *thanks to* « classic » recsys approaches
- Nutritional constraints *thanks to* knowledge graphs

1

## Axe 1:

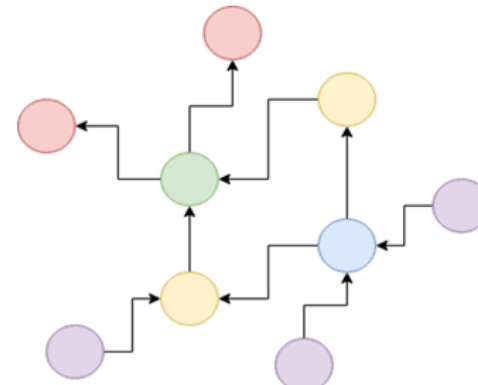
Recommandation basée sur les **préférences utilisateurs** par **apprentissage automatique**



2

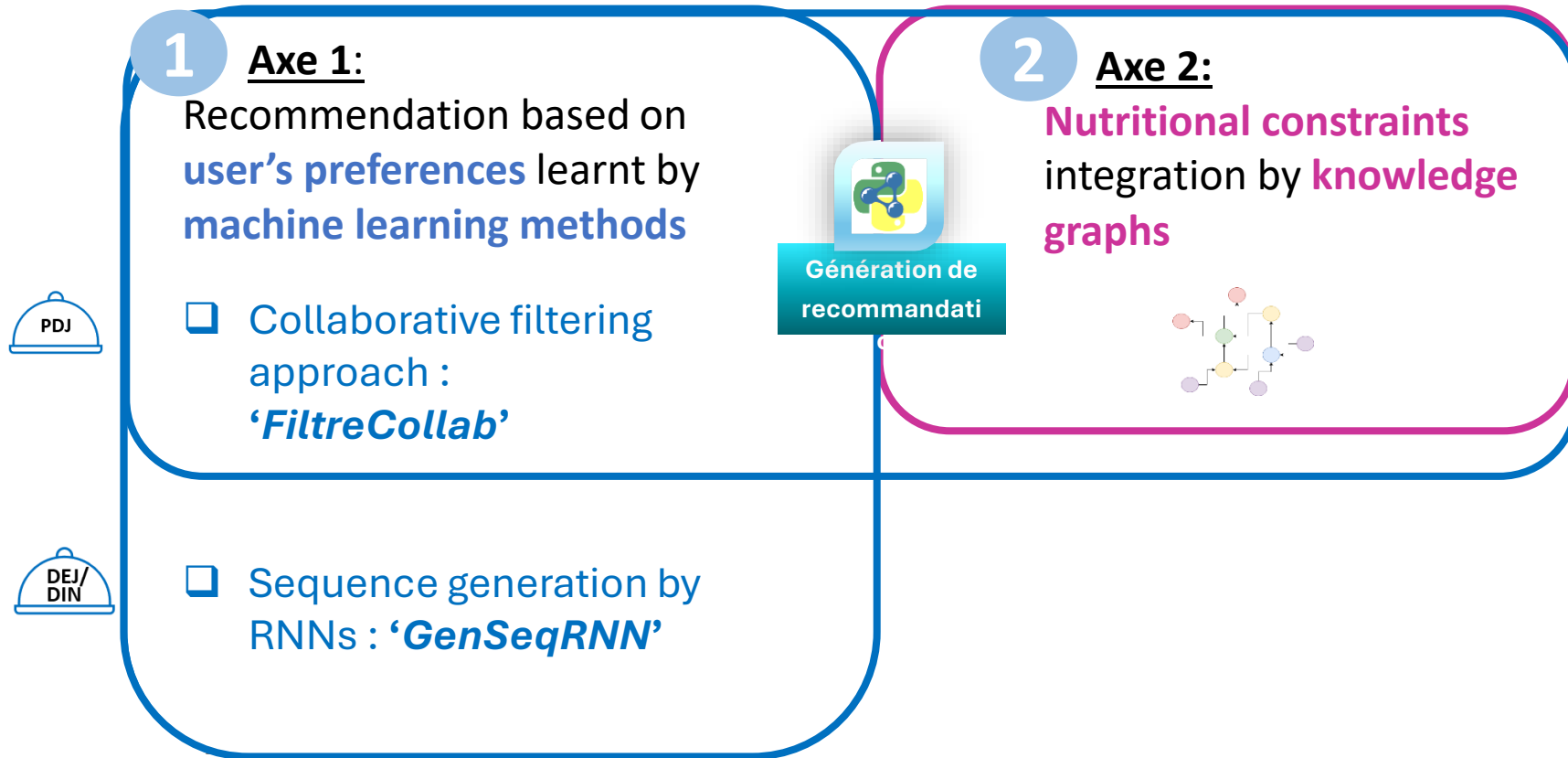
## Axe 2:

Intégration de **contraintes nutritionnelles** grâce aux **graphes de connaissance**



# The exersys project

Develop a RecSys for meals recommendation combining



# The exersys project : filtreCollab

Recommendation generation



1. Learn a representation space for food items

Word2Vec learnt on breakfast

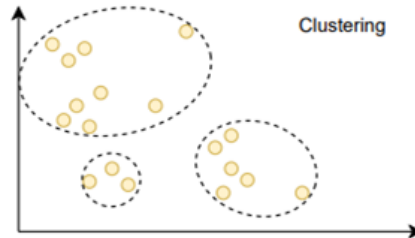


1 food item = 1 10 dimensions vector



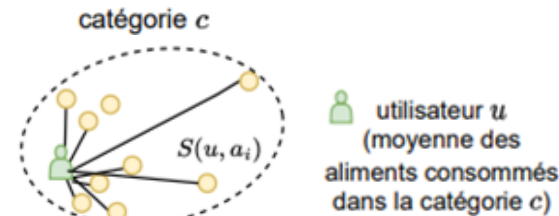
2. Categories of closed food items

K-means, k categories



3. Modeling and food items sampling by category

Food item recommendation : Sampling following a multinomia distribution

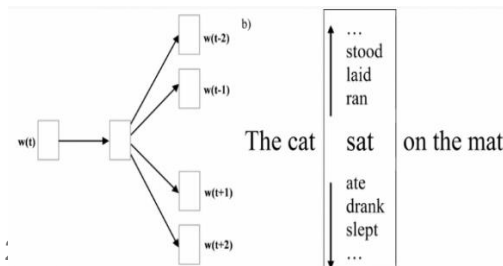


$S(u, a_i)$  similarité cosine entre  $u$  et  $a_i$

4. Meal recommendation

Meal recommendation :

- **Sampling**  
(1 food item per category already consumed and in  $\beta\%$  of cases otherwise)
- **Association/exclusion rules**



$$P(a_1 | c) = \frac{e^{\alpha \cdot S(u, a_1)}}{\sum_i e^{\alpha \cdot S(u, a_i)}}$$

$c$  catégorie consommée

# The exersys project : the knowledge graph

Multiple sources of data : INCA 2, CIQUAL 2020, Open Food Facts

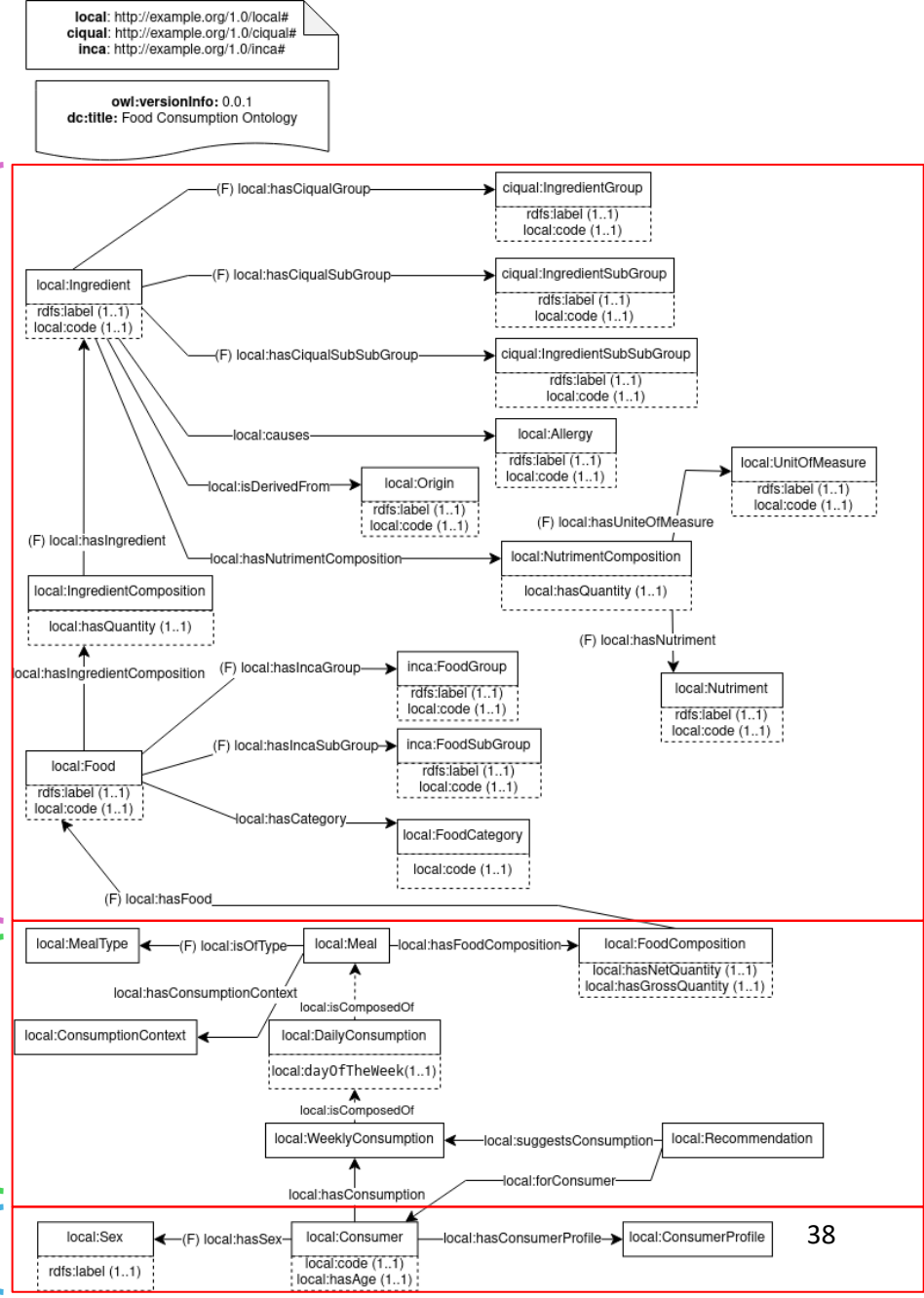
## Modeling

- consumer's profiles
- nutrition constraints
- Association rules
- Exclusion rules
- Cardinality rules

Food item part

Consummation part

Consumer part



# The exersys project : filtreCollab

Recommendation generation



1. Learn a representation space for food items

Word2Vec learnt on breakfast

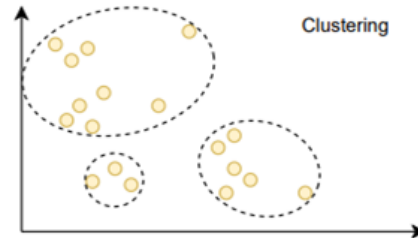


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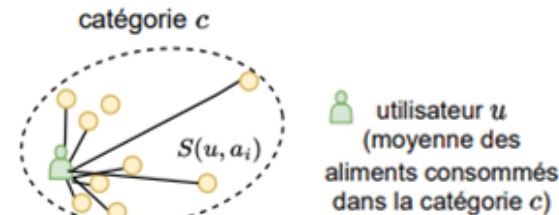
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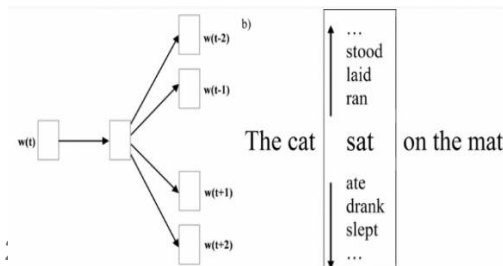


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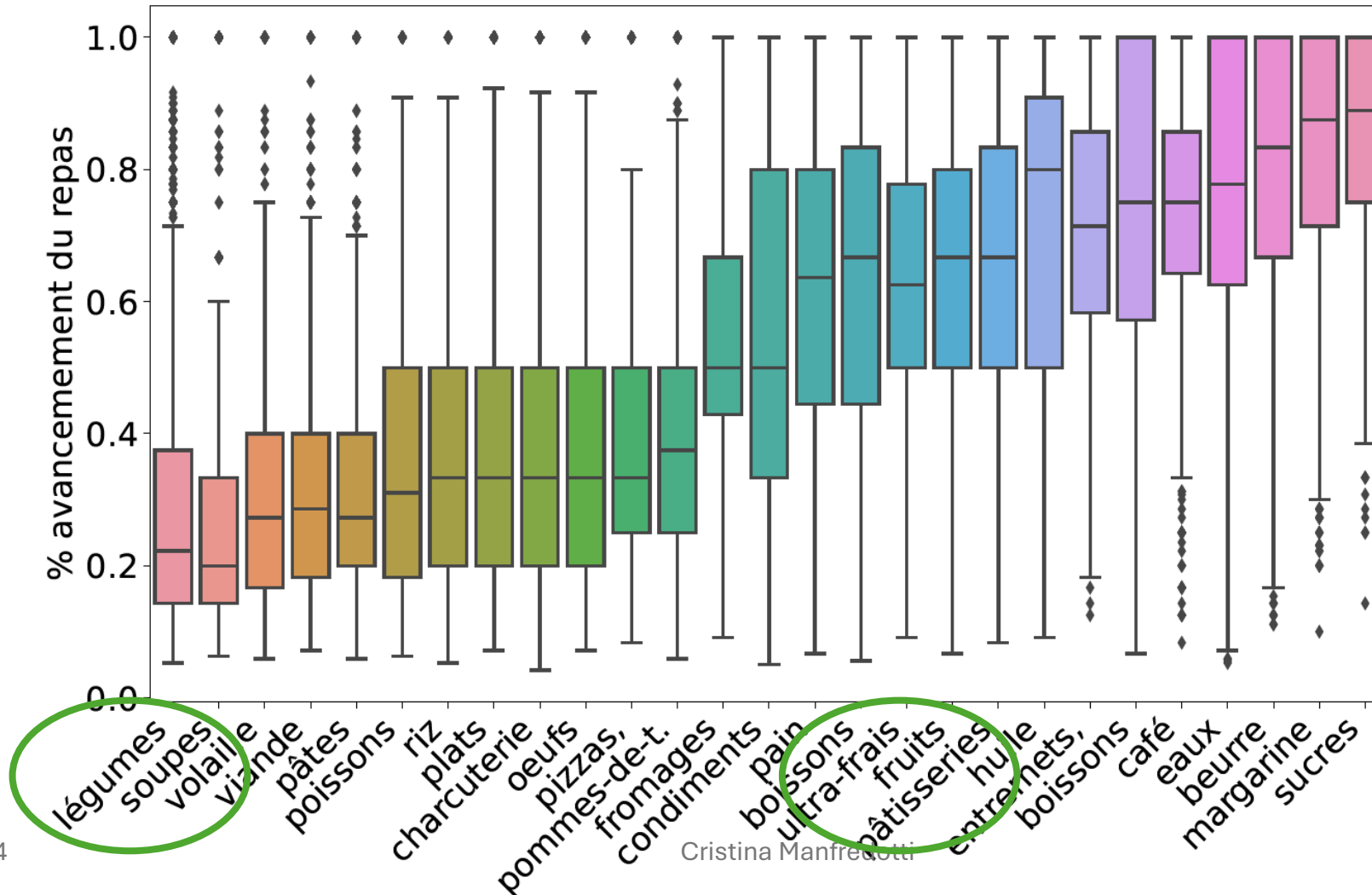


$$P(a_1 | c) = \frac{e^{\alpha \cdot S(u, a_1)}}{\sum_i e^{\alpha \cdot S(u, a_i)}}$$

$c$  catégorie consommée

# INCA2 : sequentiality

Food items temporal distribution during lunch and dinner.



Cristina Manfredotti



25/06/2024



# The exersys project : GenSeqRNN

## 1 Axe 1:

Recommendation based on **user's preferences** learnt by **machine learning methods**

❑ Collaborative filtering approach :  
*'FiltreCollab'*



❑ Sequence generation by RNNs : *'GenSeqRNN'*

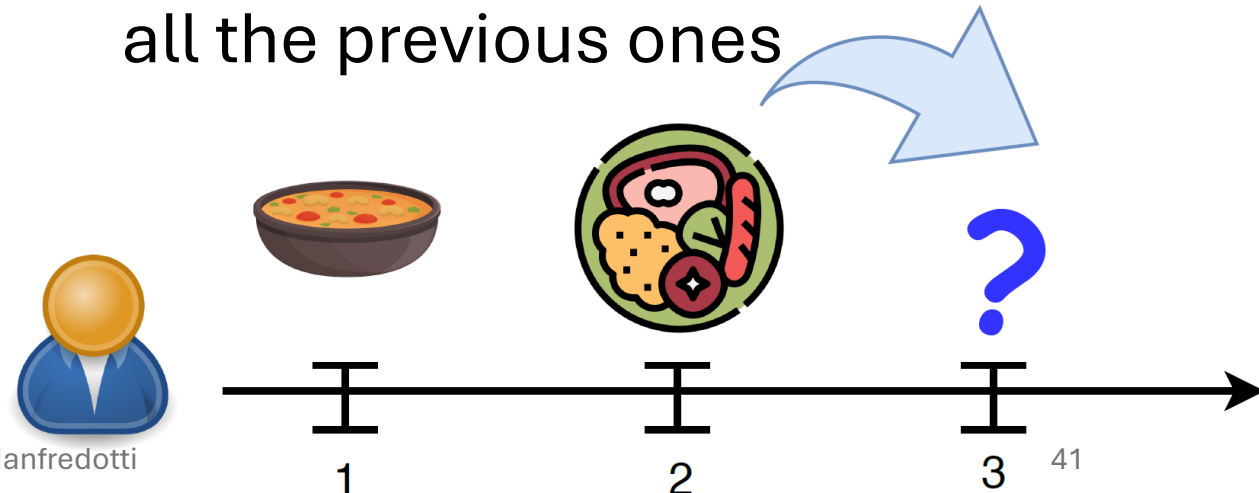


## Recurrent Neural Networks:

$$\mathbf{h}_t = g(W_1 \mathbf{a}_t + W_2 \mathbf{h}_{t-1})$$

$$\hat{\mathbf{p}} = \text{softmax}(W_3 \mathbf{h}_t)$$

- Next food item prediction wrt all the previous ones



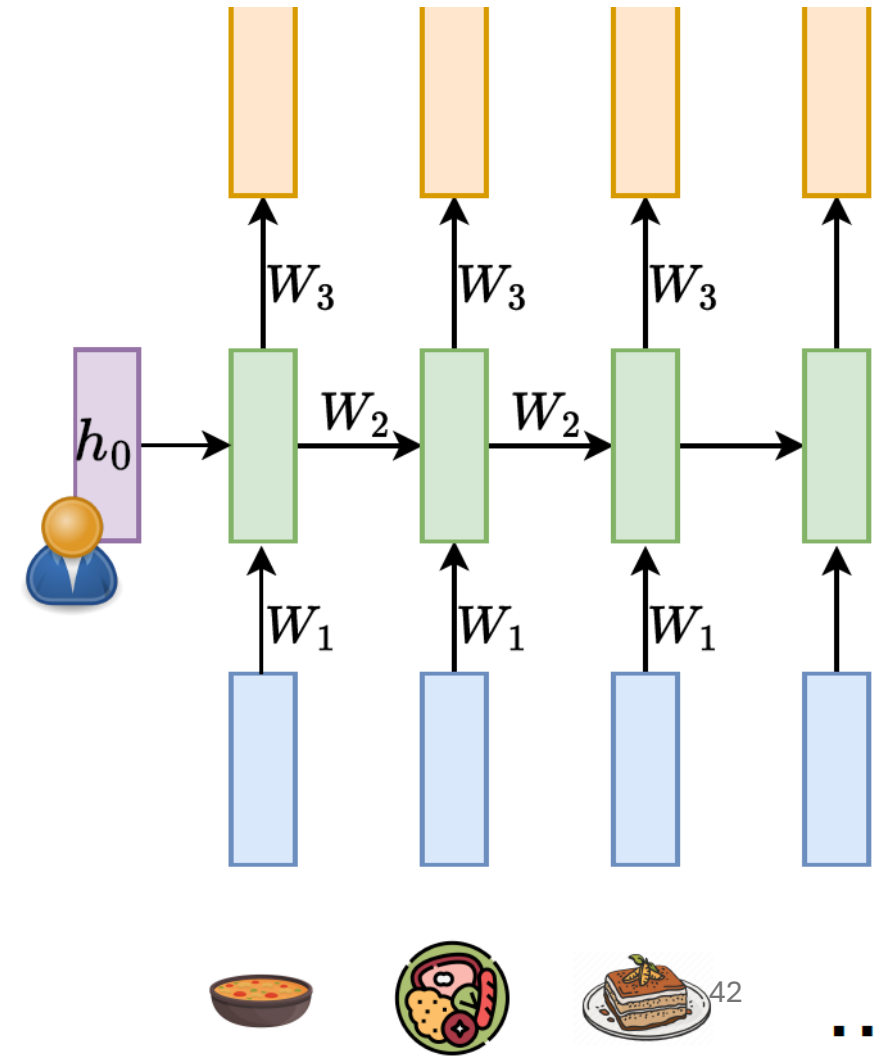
# Sequentiality modeling : RNN

Sequence prediction :

- Reconstructing a full sequence
- How to take into consideration the user ? The context ? First item prediction ?

User integration :

1. User = initial hidden state
  - First item prediction
2. User => concatenated with food items
  - Elegant architecture and less sensible to forgetting



# Test : exact prediction

Métriques	Tx	Tx-Top3	Tx-CAT	Tx	Tx-Top3	Tx-CAT
<b>Modèles</b>		DEJ+DIN			PT-DEJ	
Sans utilisateur	0.11	0.25	0.20	0.38	0.60	0.47
Util. = $h_0$	0.13	0.27	0.24	0.66	0.78	0.73
Concat. Util.+Alim.	0.16	0.30	0.24	0.71	0.83	0.77
Aléatoire	0.003	0.01	0.023	0.018	0.055	0.023

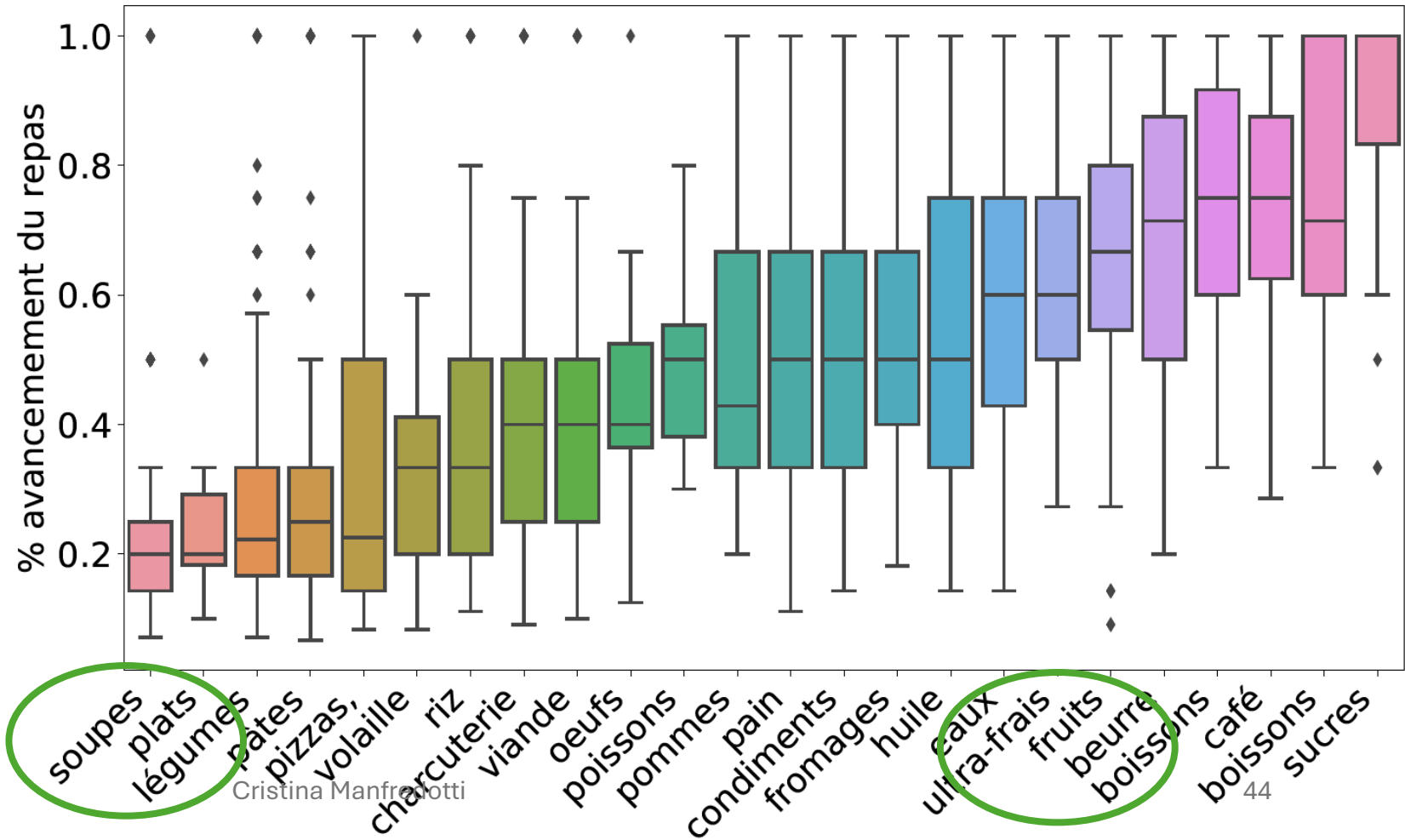
Tx : good prediction rate for the next food item,

Tx-Top3 : good prediction rate in top3.

Tx-Cat : good prediction rate for the INCA2 category.

# Test : sequentiality

Food items temporal distribution in the **RNN prediction in lunch and dinner.**



N. Jacquet, V. Guigue, C. Manfredotti, F. Saïs, S. Dervaux, P. Viappiani.  
Modélisation du caractère séquentiel des repas pour améliorer la performance d'un système de recommandation alimentaire. 24eme Conférence francophone sur l'Extraction et la Gestion des Connaissances (EGC 2024), Jan 2024, Dijon, France.

Cristina Manfredotti



25/06/2024

# The exersys project : ongoing work

- Currently :
  - considering more context elements (age, type of meal, etc.)
- Enrich the dataset
  - INCA2 + INCA3
  - with massive online food websites (Marmiton) ??
- Inject **EK** to the recommender system
  - guiding the prediction with rules and axioms deduced by the ontology
- Curriculum Learning for full sequence generation

# RecSys in the nutrition domain : future work

- Improve the explicability of the prediction
  - better system-human interaction
  - possible help from visualisation
- Probabilistic models to model dependencies between courses

# Plan

- Background : how I got here and what I learnt from this exercise
- Accomplished research
  - Experts' knowledge and PRMs
  - Experts' knowledge for RecSys
- **Drawbacks and Future Works**

# Experts' knowledge : common points

- How **EK** can **improve** the learning of a probabilistic model for inference and prediction and the recommendation of an item in a RecSys for nutrition
- We dealt with applications where **data are scarce**, **EK** helps in enriching them :
  - They specify them
  - They constraints them
- **EK** help in **explicability** and add **rules** ( $\Rightarrow$  causality)



# Experts' knowledge : future works

- Relying more on the knowledge graphs
  - Exersys => *planned*
  - PRMs => *to investigate*
- Data linking
  - INCA2 + INCA3
  - Transfer learning
- Expert inclusion and visualisation
- Using the mapping for RecSys



## Journal papers:

- J. Vandeputte, P. Herold, M. Kuslii, P. Viappiani, L. Muller, C. Martin, O. Davidenko, F. Delaere, C. Manfredotti, A. Cornuéjols, N. Darcel. Principles and Validations of an Artificial Intelligence-Based Recommender System Suggesting Acceptable Food Changes. *Journal of Nutrition*, 153, 2 (2023).
- M. Münch, P. Buche, C. Manfredotti, P-H. Wuillemin, H. Angellier-Coussy. Formalizing Contextual Expert Knowledge for Causal Discovery in linked Knowledge Graphs about Transformation Processes: Application to processing of bio-composites for food packaging *International Journal of Metadata, Semantics and Ontologies IJMSO-349696*
- M. Münch, P. Buche, S. Dervaux, J. Dibie, L. Ibanescu, C. Manfredotti, P-H. Wuillemin, H. Angellier-Coussy. Combining ontology and probabilistic models for the design of bio-based product transformation processes. *Expert Systems for Applications* 203: 117406 (2022)
- L. Cattelani, C. Manfredotti, E. Messina. A Particle Filtering Approach for Tracking an Unknown Number of Objects with Dynamic Relations. *Journal of Mathematical Modeling and Algorithms in OR* 13(1): 3-21 (2014)
- E. Fersini, E. Messina, F. Archetti, C. Manfredotti. Combining Gene Expression Profiles and Drug Activity Patterns Analysis: A Relational Clustering Approach. *Journal of Mathematical Modeling and Algorithms*, 9(3): 275-289 (2010)

## Conference papers:

- N. Jacquet, V. Guigue, C. Manfredotti, F. Saïs, S. Dervaux, P. Viappiani. Modélisation du caractère séquentiel des repas pour améliorer la performance d'un système de recommandation alimentaire. 24eme Conférence francophone sur l'Extraction et la Gestion des Connaissances (EGC 2024), Jan 2024, Dijon, France.
- M. Munch, P. Buche, C. Manfredotti, P-H. Wuillemin, H. Angellier-Coussy. A process reverse engineering approach using Process and Observation Ontology and Probabilistic Relational Models: application to processing of bio-composites for food packaging. 15th International Conference on Metadata and Semantics Research 2021.
- C. Manfredotti, P. Viappiani. A Bayesian Interpretation of the Monty Hall Problem with Epistemic Uncertainty. MDAI 2021: 93-105
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# Mapping ontology and PRM: remarks

- Motivations :
  - Need to reason with uncertainty in transformation processes
  - Similarity between ontologies and PRMS
- The experts
  - give the ontology
  - structures the variables with his hypothesis
  - afterwards, critiques the model
- The approaches
  - Verify the expert's hypothesis
  - Suggest new experiments
  - Able to do prediction

# Mapping ontology and PRM: ideas for the future

- The expert's validation step could be investigated more
  - Exploring algorithms able to learn a network locally
  - Visualisation and human machine interaction
  - (automatic) Explanation, (also) to suggest new experiments
- The ontology could be used more
  - Answering competency questions to structure de domain giving more insights to the learning
- Transfer Learning, Data linking, Graph Matching



# The exersys project : ongoing work

- Currently :
  - considering more context elements (age, type of meal, etc.)
- Enrich the dataset
  - INCA2 + INCA3
  - with massive online food websites (Marmiton) ??
- Inject **EK** to the recommender system
  - guiding the prediction with rules and axioms deduced by the ontology
- Curriculum Learning for full sequence generation

# RecSys in the nutrition domain : future work

- Improve the explicability of the prediction
  - better system-human interaction
  - possible help from visualisation
- Probabilistic models to model dependencies between courses