

IA & Energie

Human in the loop : Interactivity & visualization

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Plan

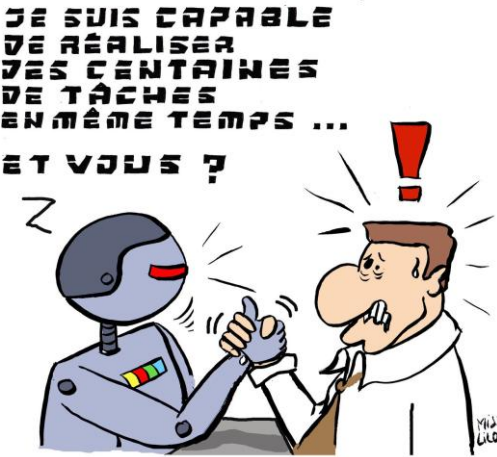
1. Introduction
2. Problematics
3. Approaches :
 1. Visual analytics
 2. Visual data mining
 3. Interactive machine learning
4. Application to French power grid :
 1. Grammatical evolutionary algorithm
 2. Reinforcement learning
 3. Interactive machine learning algorithms
5. Conclusion and perspectives

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Introduction

AI in the news

MATCH IA VS HUMAIN ...

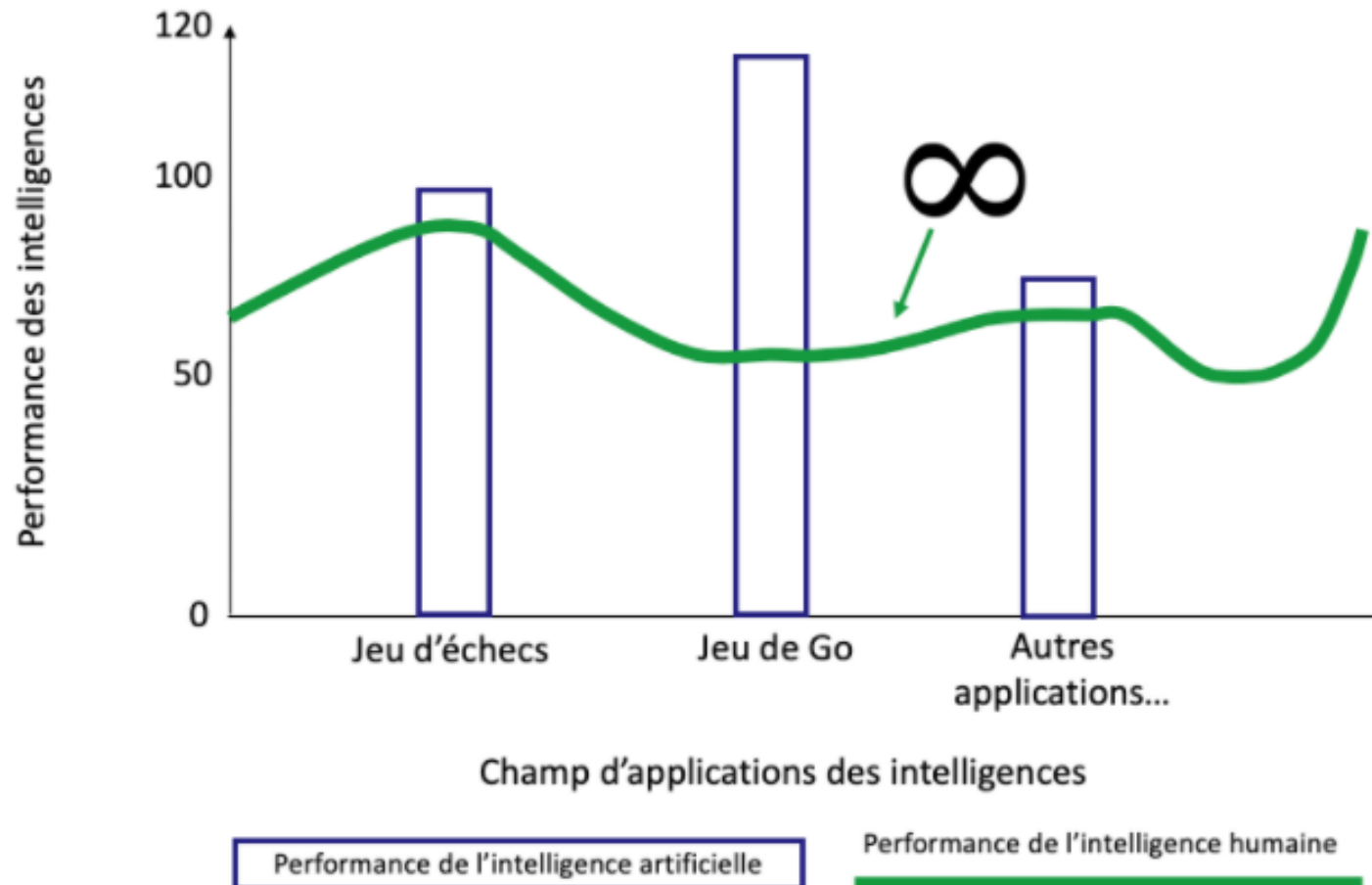


Ouverture du restaurant Robot à Bangalore, le 17 août 2019. Manjunath Kiran / AFP

Artificial Intelligence

L'intelligence artificielle et l'intelligence humaine sont différentes

L'intelligence humaine est capable d'appréhender un nombre infini d'enjeux tandis que l'intelligence artificielle n'est capable que de traiter que des sujets pour lesquels elle fut programmée



Artificial Intelligence

Artificial Intelligence (AI) :

- thanks to the cross-referencing of an increasing amount of data (big data)
 - a rapidly expanding field of research
 - applications that concern all human activities,
-
- **Medical:** assisted interventions, remote monitoring of patients, personalized treatment,...
 - **Environnement:** prevent the risk of forest fires, analyze the migratory flow of storks, geese,...
 - **Energy:** consumption prediction, predicting or explaining network failures

Multiple approaches & techniques :

- ontology construction,
- automatic language processing - NLP,
- data mining,
- machine learning.

Artificial Intelligence

Definitions

What is Data Mining?

Data mining is considered the process of extracting useful information from large amounts of data. It is used to discover new, accurate and relevant patterns in the data.

What is machine learning?

It is the design, study, and development of algorithms that allow machines to learn from data.

It is a tool that makes machines a little smarter.

It Automates a large part of the manual data mining tasks, mainly featuring, at the expense of model interpretability.

2

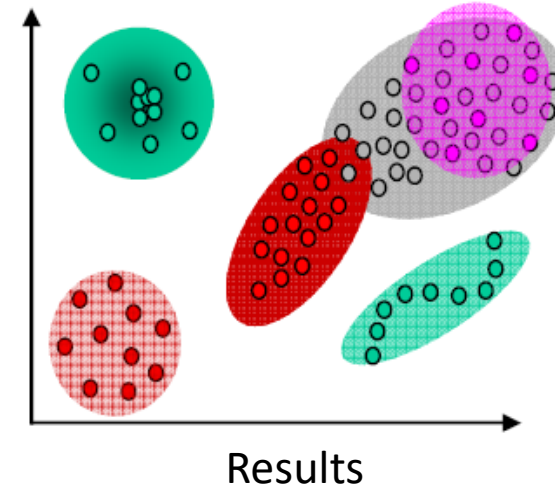
Why human-in-the-loop approaches ?

Data Mining

Observations

Attributs		
	V_1	V_2
I_1	2	3.4
I_2	1	-0.7
I_3	0.33	4
...	...	...

Data



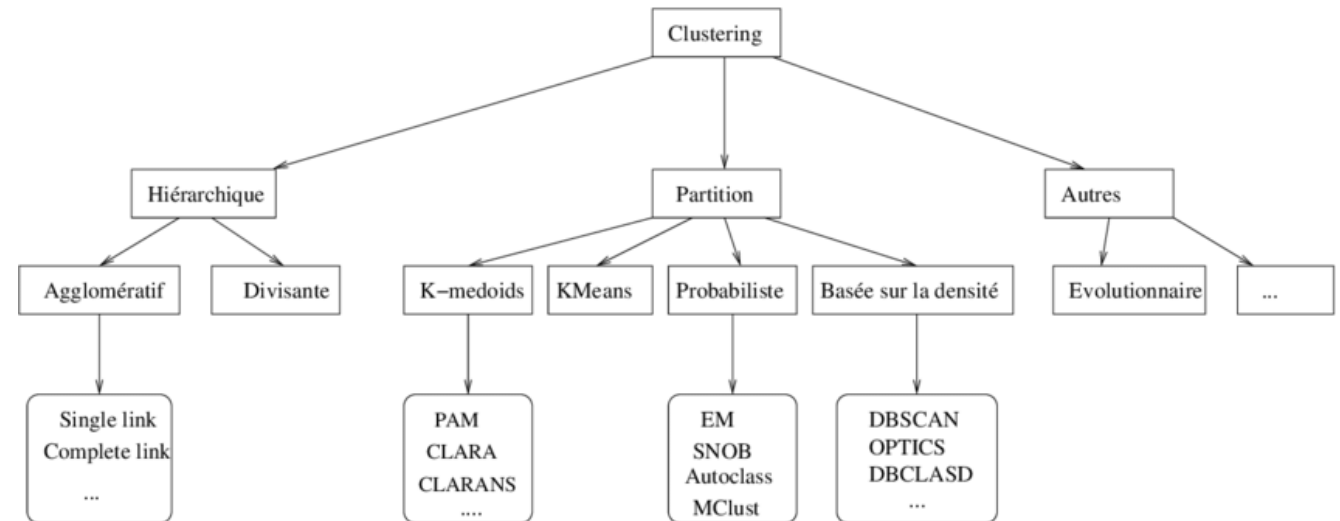
Clustering

Goal:

Homogeneous sets of individuals sharing same characteristics

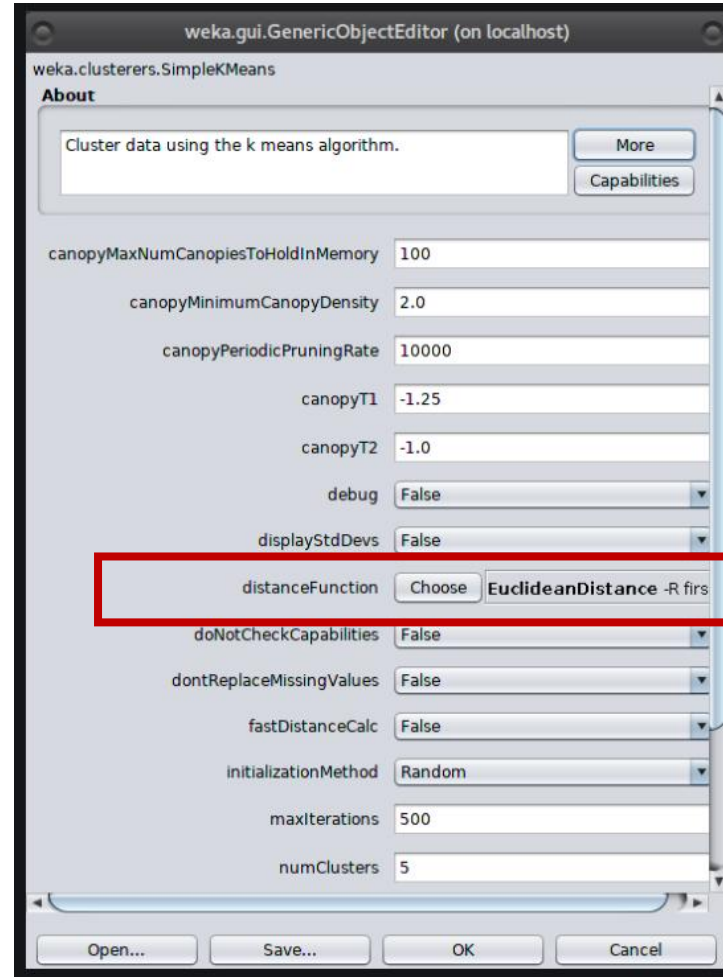
Classical process:

- 1- the user sets the number of clusters
- 2- a partitioning is generated
- 3- evaluation:
 - by the user himself,
 - by homogeneity criteria,
- 4- validation:
 - results can be challenged



Clustering

Cluster algorithm	Complexity	Capability of tackling high dimensional data
K-means	$O(NKd)$ (time) $O(N + K)$ (space)	No
Fuzzy c-means	Near $O(N)$	No
Hierarchical clustering*	$O(N^2)$ (time) $O(N^2)$ (space)	No
CLARA	$O(K(40+K)^2 + K(N-K))$ (time)	No
CLARANS	Quadratic in total performance	No
BIRCH	$O(N)$ (time)	No
DBSCAN	$O(N \log N)$ (time)	No
CURE	$O(N_{sample}^2 \log N_{sample})$ (time) $O(N_{sample})$ (space)	Yes
WaveCluster	$O(N)$ (time)	No
DENCLUE	$O(N \log N)$ (time)	Yes
FC	$O(N)$ (time)	Yes
CLIQUE	Linear with the number of objects, Quadratic with the number of dimensions	Yes
OptiGrid	Between $O(Nd)$ and $O(Nd \log N)$	Yes
ORCLUS	$O(K_0^3 + K_0Nd + K_0^2d^3)$ (time) $O(K_0d^2)$ (space)	Yes



Measures	Forms
Minkowski distance	$D_{ij} = \left(\sum_{l=1}^d x_{il} - x_{jl} ^{1/n} \right)^n$
Euclidean distance	$D_{ij} = \left(\sum_{l=1}^d x_{il} - x_{jl} ^{1/2} \right)^2$
City-block distance	$D_{ij} = \sum_{l=1}^d x_{il} - x_{jl} $
Sup distance	$D_{ij} = \max_{1 \leq l \leq d} x_{il} - x_{jl} $
Mahalanobis distance	$D_{ij} = (\mathbf{x}_i - \mathbf{x}_j)^T \mathbf{S}^{-1} (\mathbf{x}_i - \mathbf{x}_j)$, where $\mathbf{S}$ is the within-group covariance matrix.
Pearson correlation	$D_{ij} = (1 - r_{ij}) / 2$, where $r_{ij} = \frac{\sum_{l=1}^d (x_{il} - \bar{x}_i)(x_{jl} - \bar{x}_j)}{\sqrt{\sum_{l=1}^d (x_{il} - \bar{x}_i)^2 \sum_{l=1}^d (x_{jl} - \bar{x}_j)^2}}$
Point symmetry distance	$D_{ir} = \min_{\substack{j=1, \dots, N \\ \text{and } j \neq i}} \frac{\ (\mathbf{x}_i - \mathbf{x}_r) + (\mathbf{x}_j - \mathbf{x}_r)\ }{\ (\mathbf{x}_i - \mathbf{x}_r)\ + \ (\mathbf{x}_j - \mathbf{x}_r)\ }$
Cosine similarity	$S_{ij} = \cos \alpha = \frac{\mathbf{x}_i^T \mathbf{x}_j}{\ \mathbf{x}_i\ \ \mathbf{x}_j\ }$

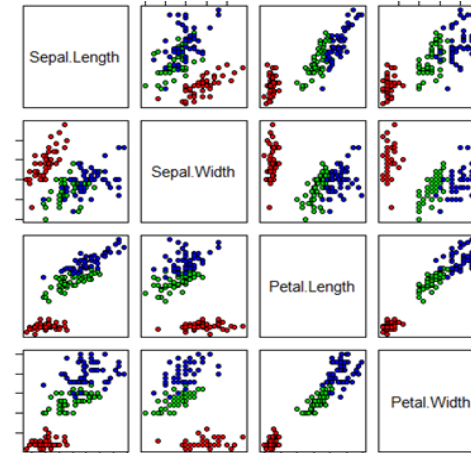
Clustering

Evaluation: different point of views

<i>Index</i>	<i>Rule</i>
Ball_Hall	<i>max diff</i>
Banfeld_Raftery	<i>min</i>
C_index	<i>min</i>
Calinski_Harabasz	<i>max</i>
Davies_Bouldin	<i>min</i>
Det_Ratio	<i>min diff</i>
Dunn	<i>max</i>
GDI	<i>max</i>
Gamma	<i>max</i>
G_plus	<i>min</i>
Ksq_DetW	<i>max diff</i>
Log_Det_Ratio	<i>min diff</i>
Log_SS_Ratio	<i>min diff</i>
McClain_Rao	<i>min</i>
PBM	<i>max</i>
Point_biserial	<i>max</i>
Ratkowsky_Lance	<i>max</i>
Ray_Turi	<i>min</i>
Scott_Symons	<i>min</i>
SD	<i>min</i>
S_Dbw	<i>min</i>
Silhouette	<i>max</i>
Tau	<i>max</i>
Trace_W	<i>max diff</i>
Trace_WiB	<i>max diff</i>
Wemmert_Gancarski	<i>max</i>
Xie_Beni	<i>min</i>

Iris Fischer (150 obs., 4 var., 3 classes)

The Czekanowski-Dice index
 The Folkes-Mallows index .
 The Hubert $\hat{\Gamma}$ index
 The Jaccard index
 The Kulczynski index
 The McNemar index
 The Phi index
 The Rand index
 The Rogers-Tanimoto index
 The Russel-Rao index
 The Sokal-Sneath indices .



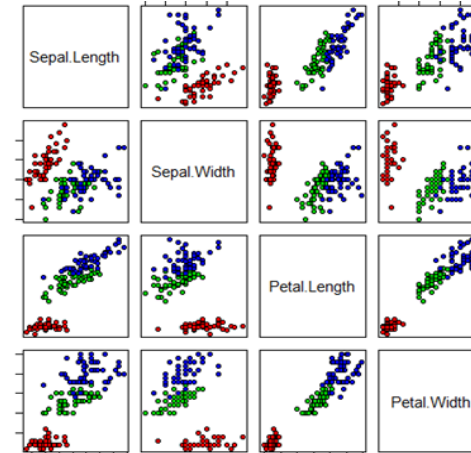
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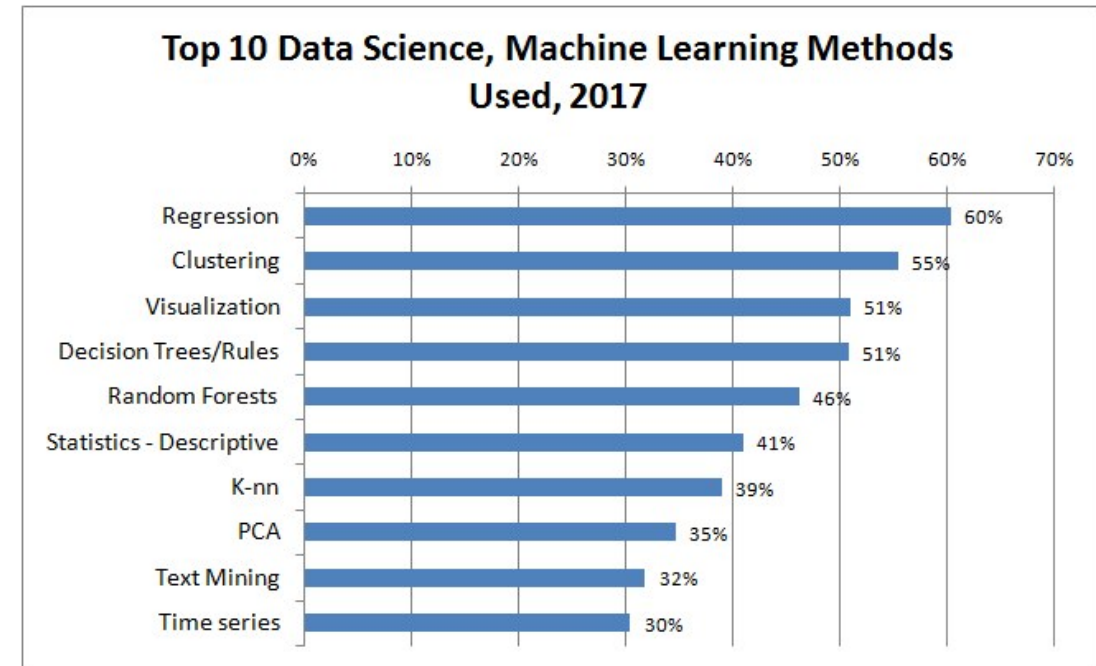
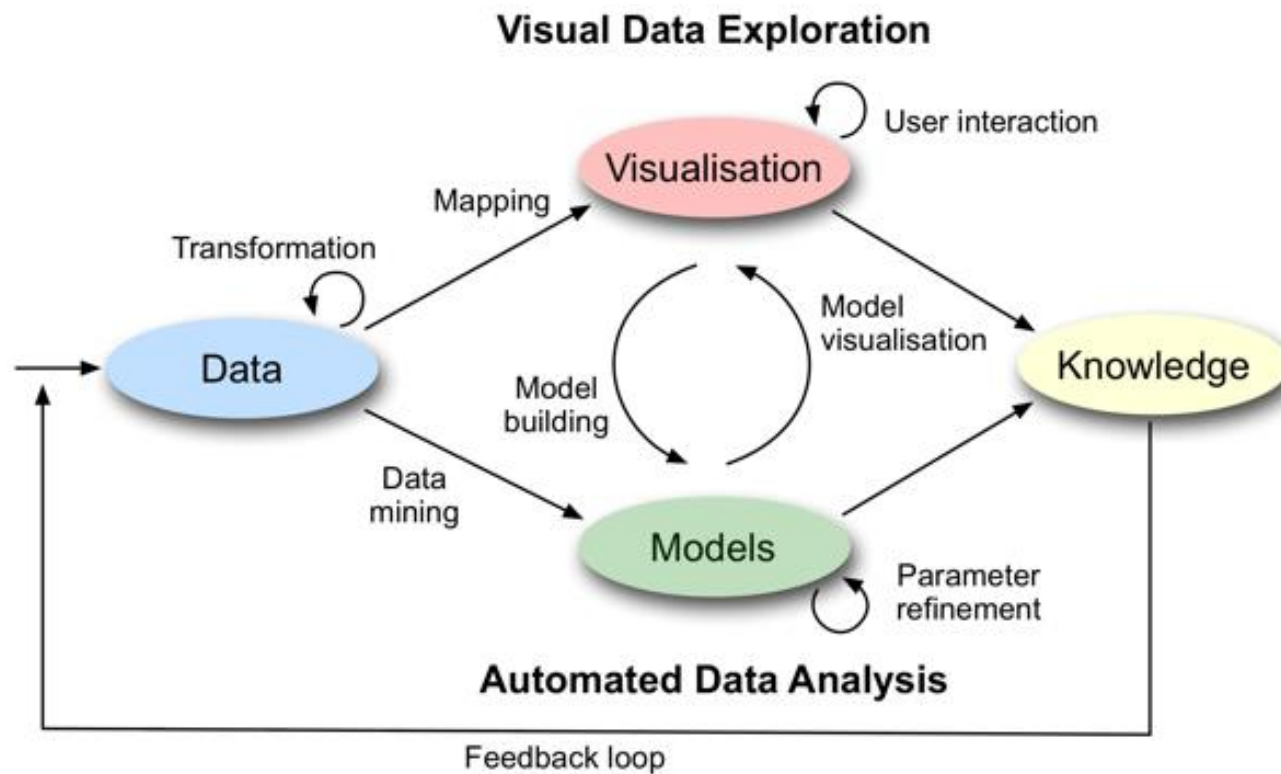
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Visual Data Mining

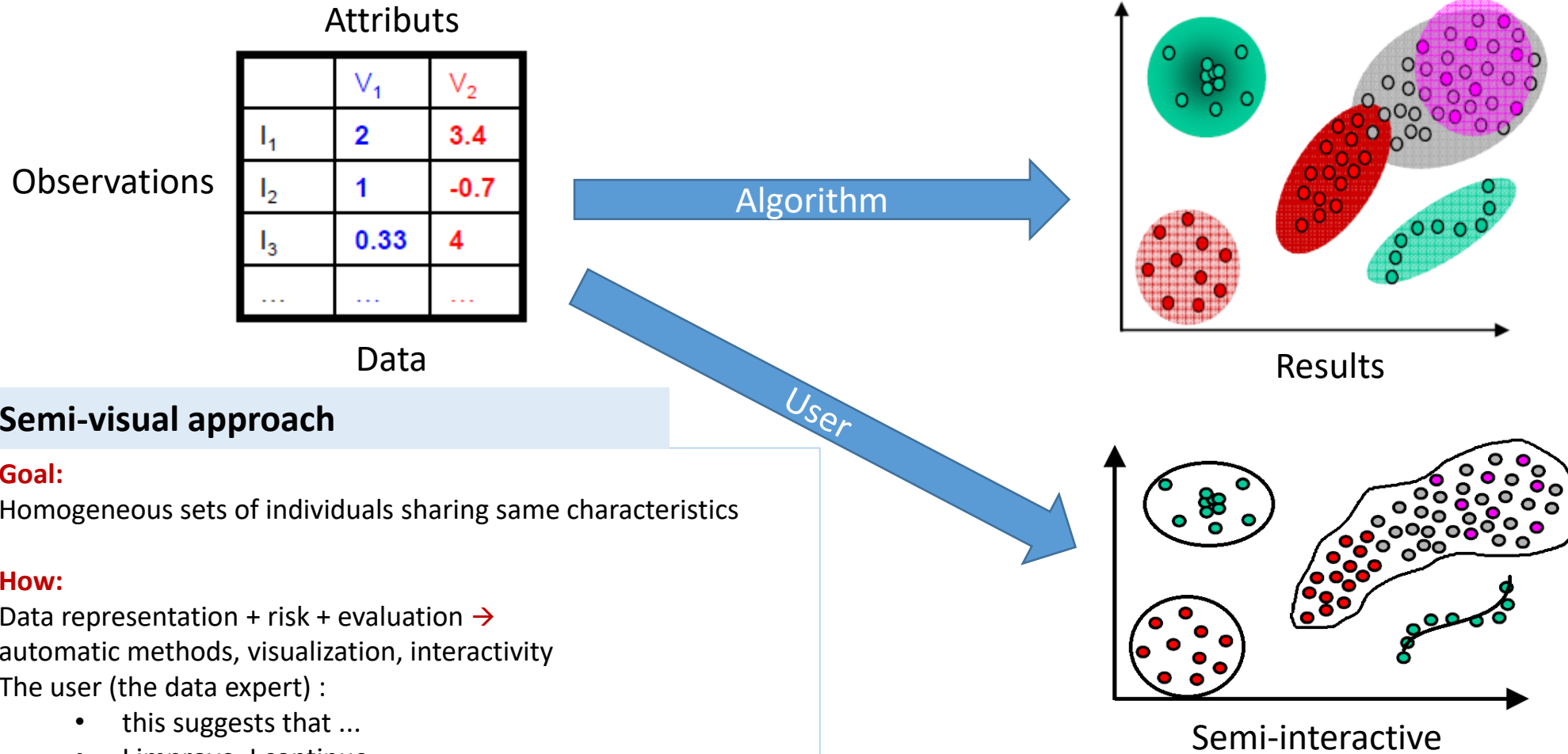


<http://www.kdnuggets.com/> (Décembre 2017)

<https://www.kdnuggets.com/2017/12/top-data-science-machine-learning-methods.html>

Visual Data methods : 38.3% → 5th position in 2011, 48.7% → 4th position in 2016
à 51% → 3rd position in 2017

Visual Data Mining



Visual Data Mining

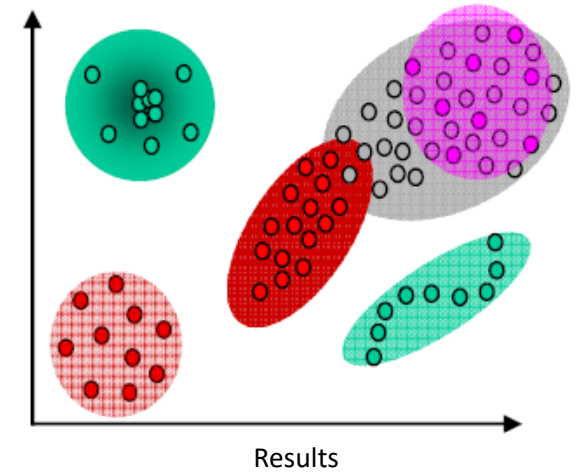
Observations,

	P Variables	
	V_1	V_2
x_1	2	3.4
x_2	1	-0.7
x_3	0.33	4
...	...	...

Data set E

$$f: R^p \rightarrow \{1, \dots, k\}$$

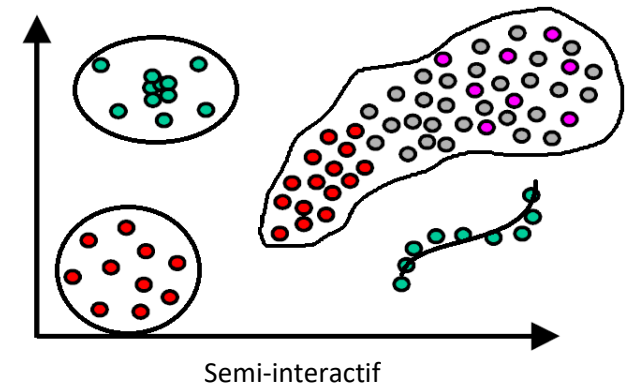
$$X \rightarrow C$$



$$Op: \{1, \dots, I\} \rightarrow \{1, \dots, I\}$$

$$C \rightarrow C'$$

$$Q(C') > Q(C)$$



Clustering evaluation:

- Minimize intra-classe inertia

$$I_{intra}(C_a) = \sum_{x_i \in C_a} d(x_i, x_a^*)^2$$

- Maximize inter-classe inertia

$$I_{inter}(C) = \sum_{i=2}^t \sum_{j < i} d(x_i^*, x_j^*)^2$$

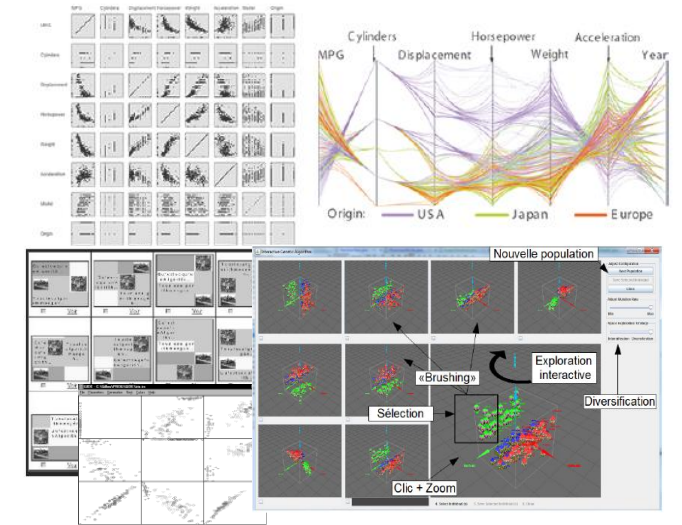
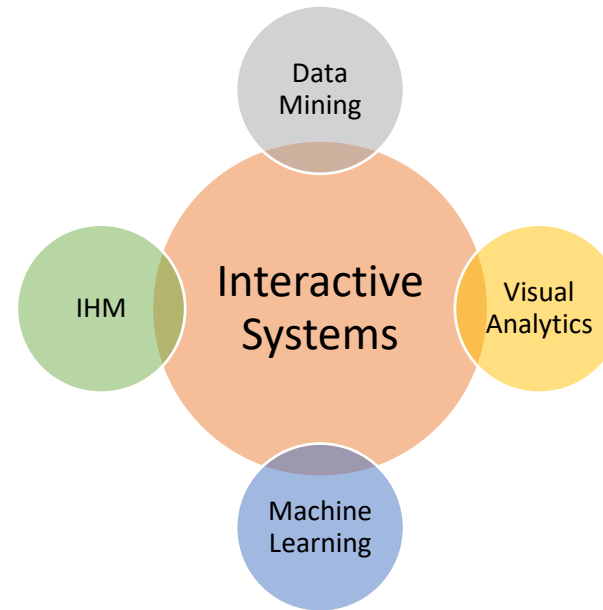
-

Interactives systems

Observations

Attributs		
	V_1	V_2
I_1	2	3.4
I_2	1	-0.7
I_3	0.33	4
...	...	...

Data



Differences

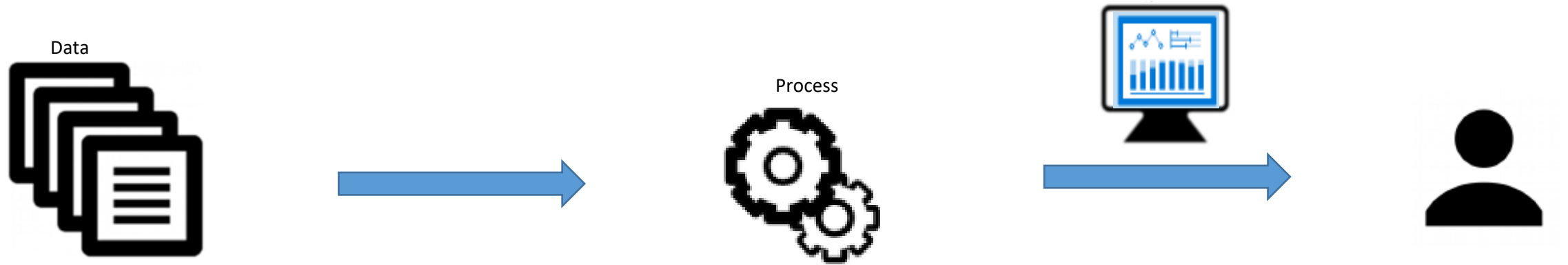
- Interactivity in the processus
- Interactivity steps
- Improve the model

Advantages

- Obtain better results
- Complex tasks to be automated
- Understand data and resluts
- Imply the user in the process

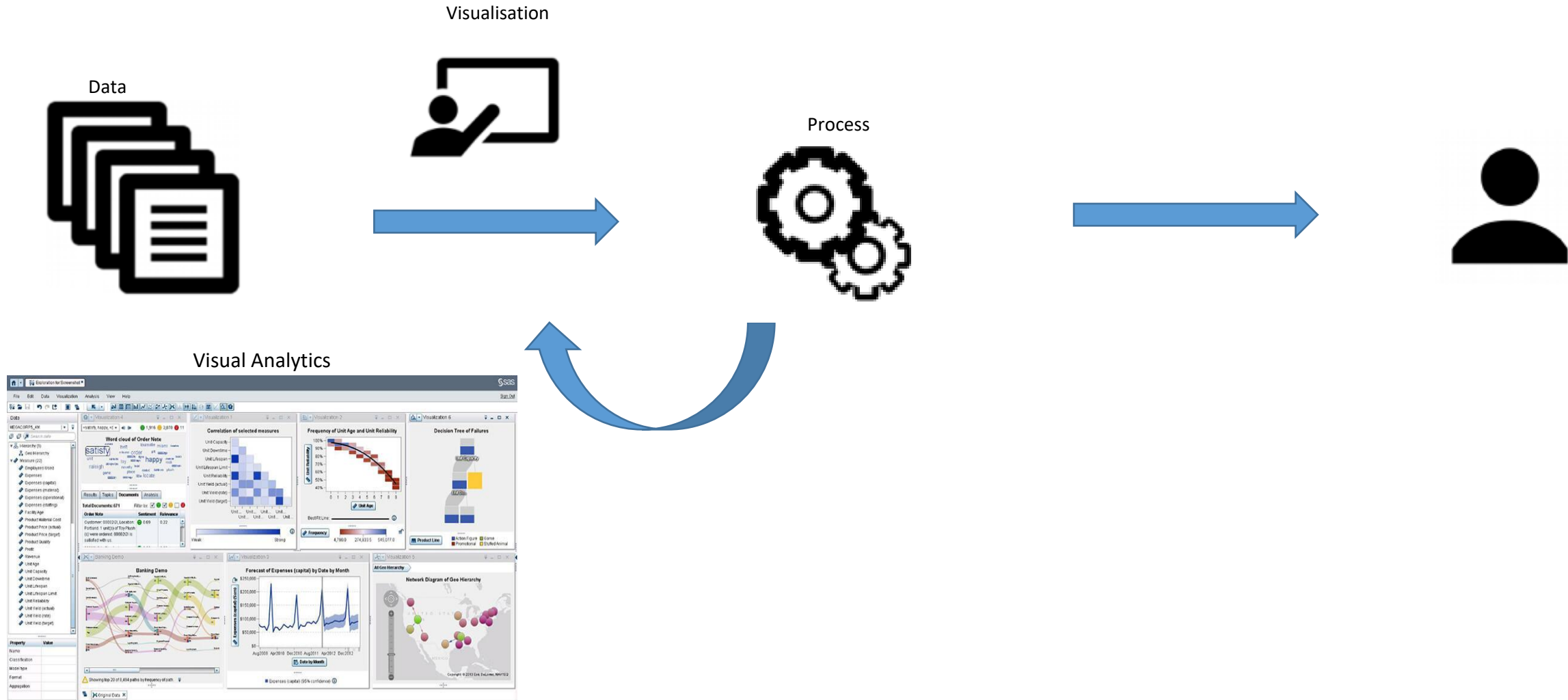
Human-In-The-Loop

Classical approach



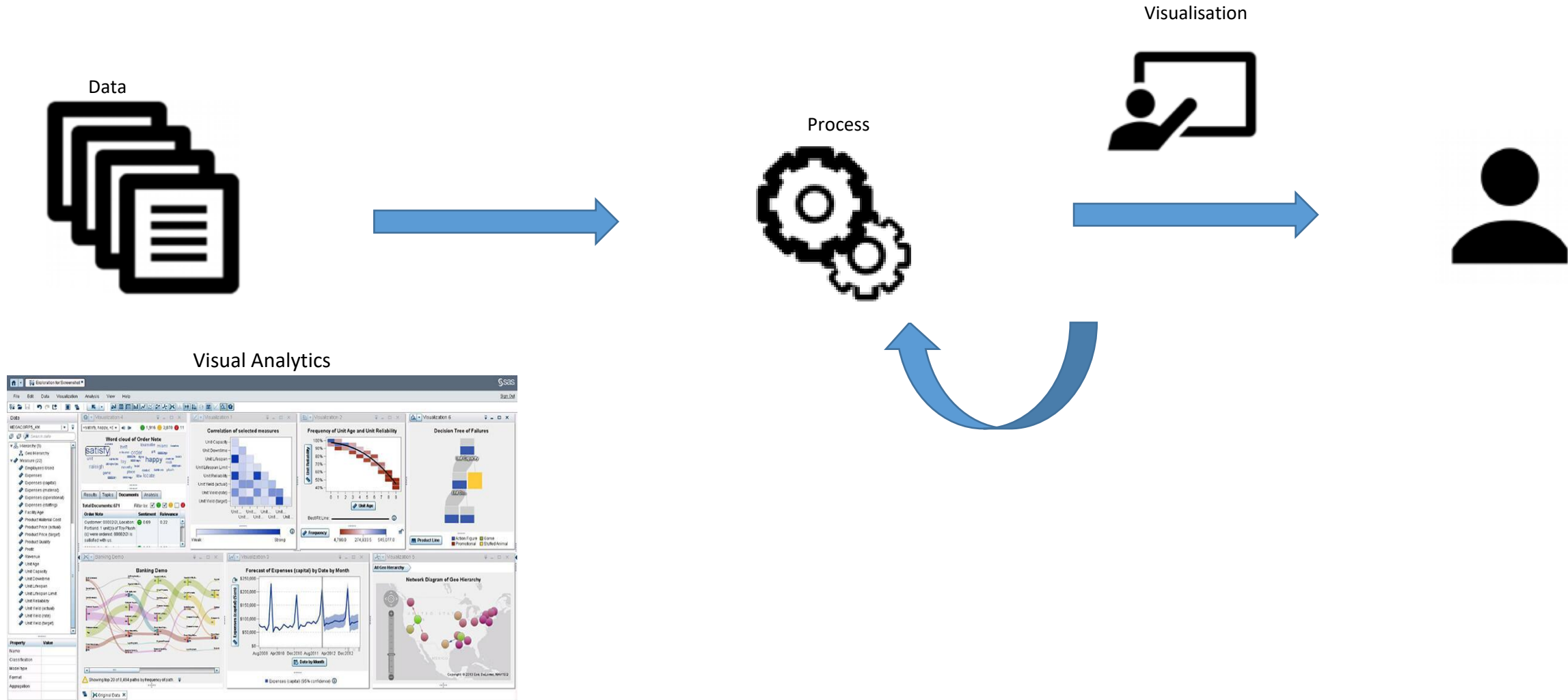
Human-In-The-Loop

Visual Analytics



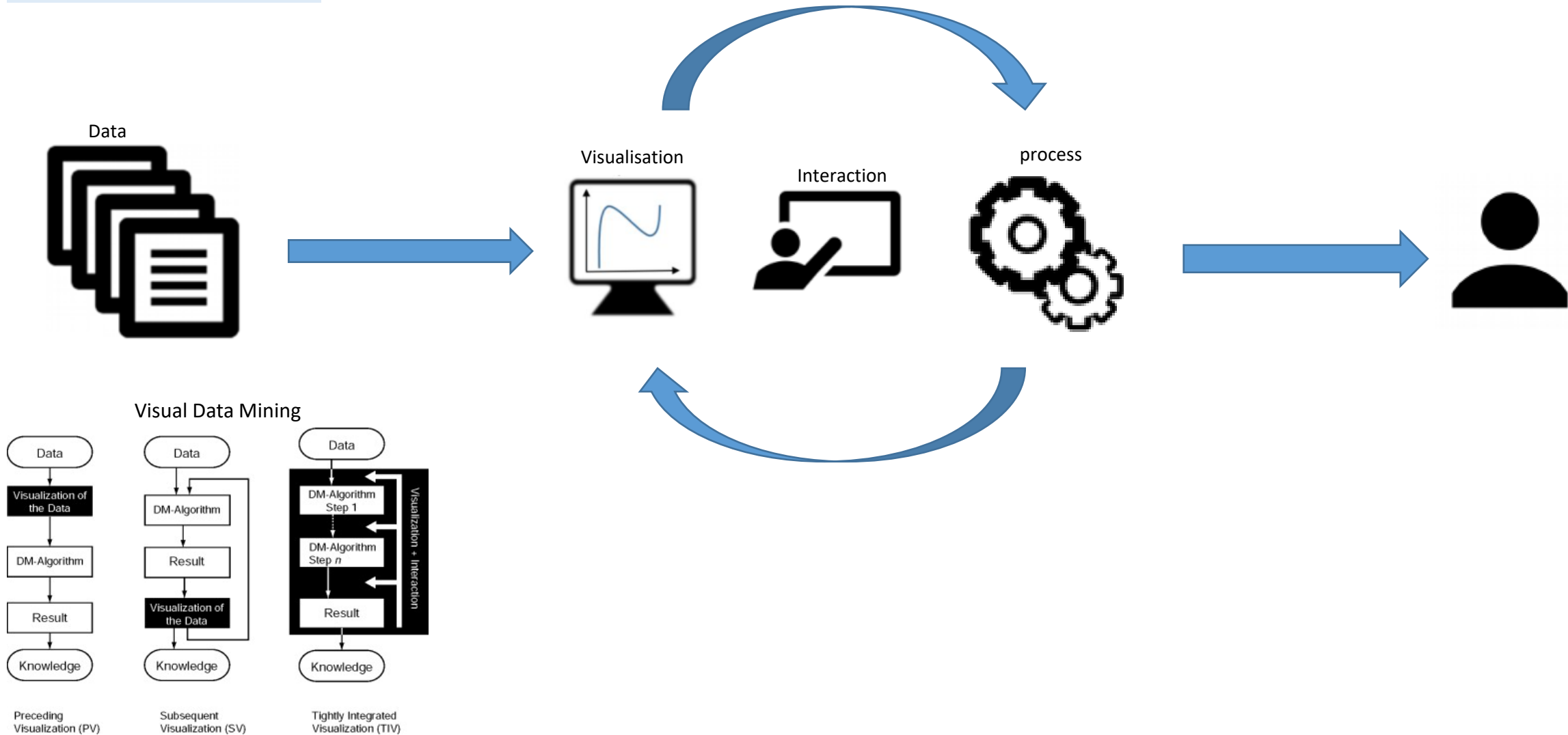
Human-In-The-Loop

Visual Analytics



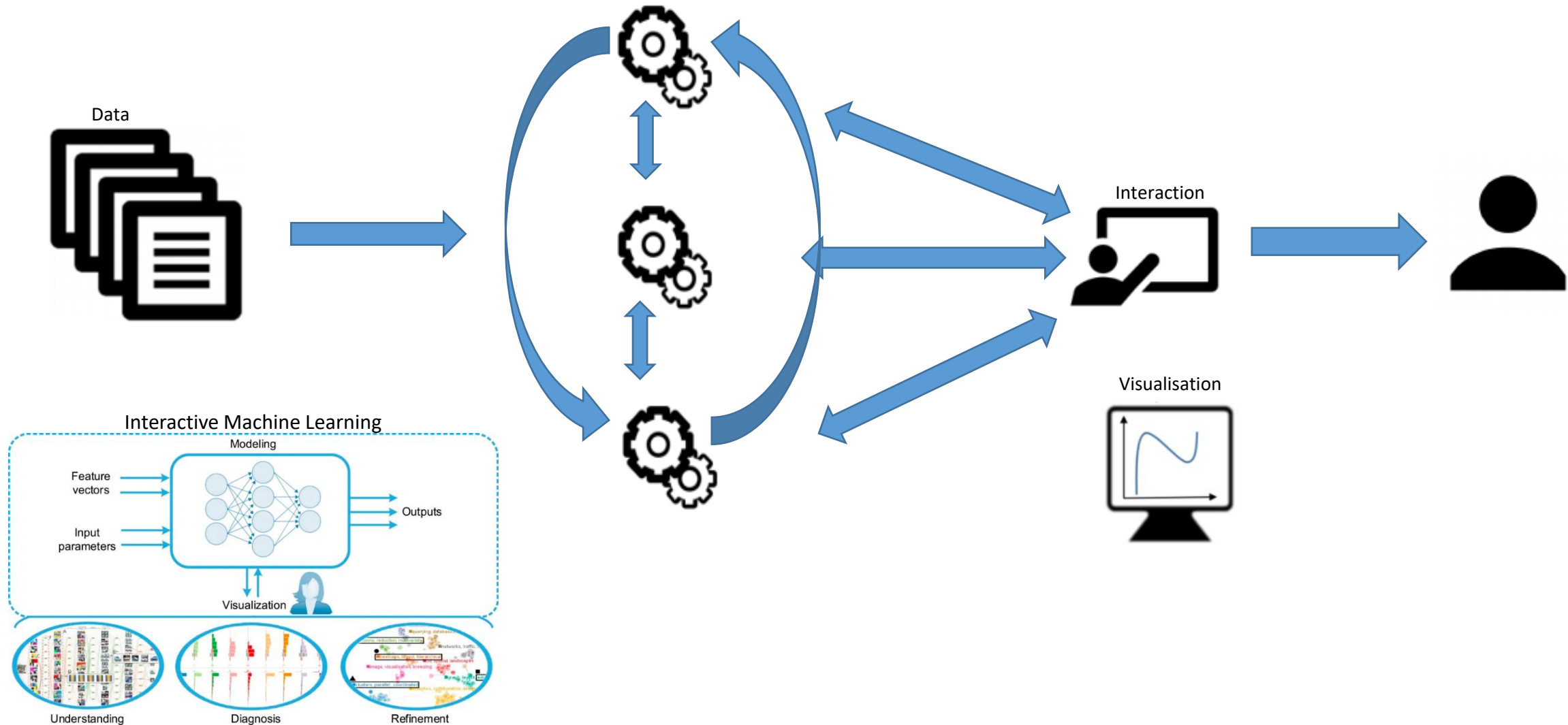
Human-In-The-Loop

Visual Data Mining



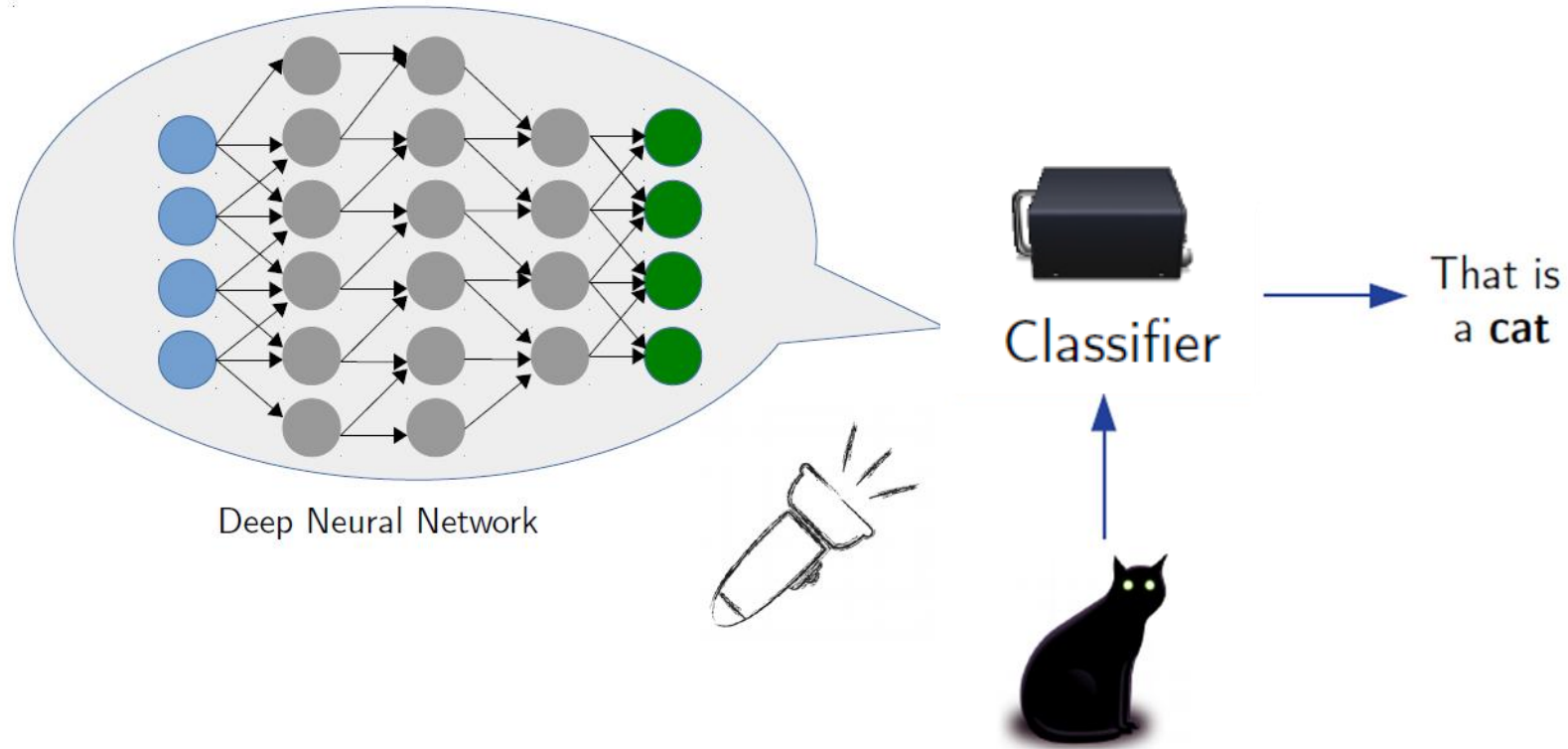
Human-In-The-Loop

Interactive Machine Learning



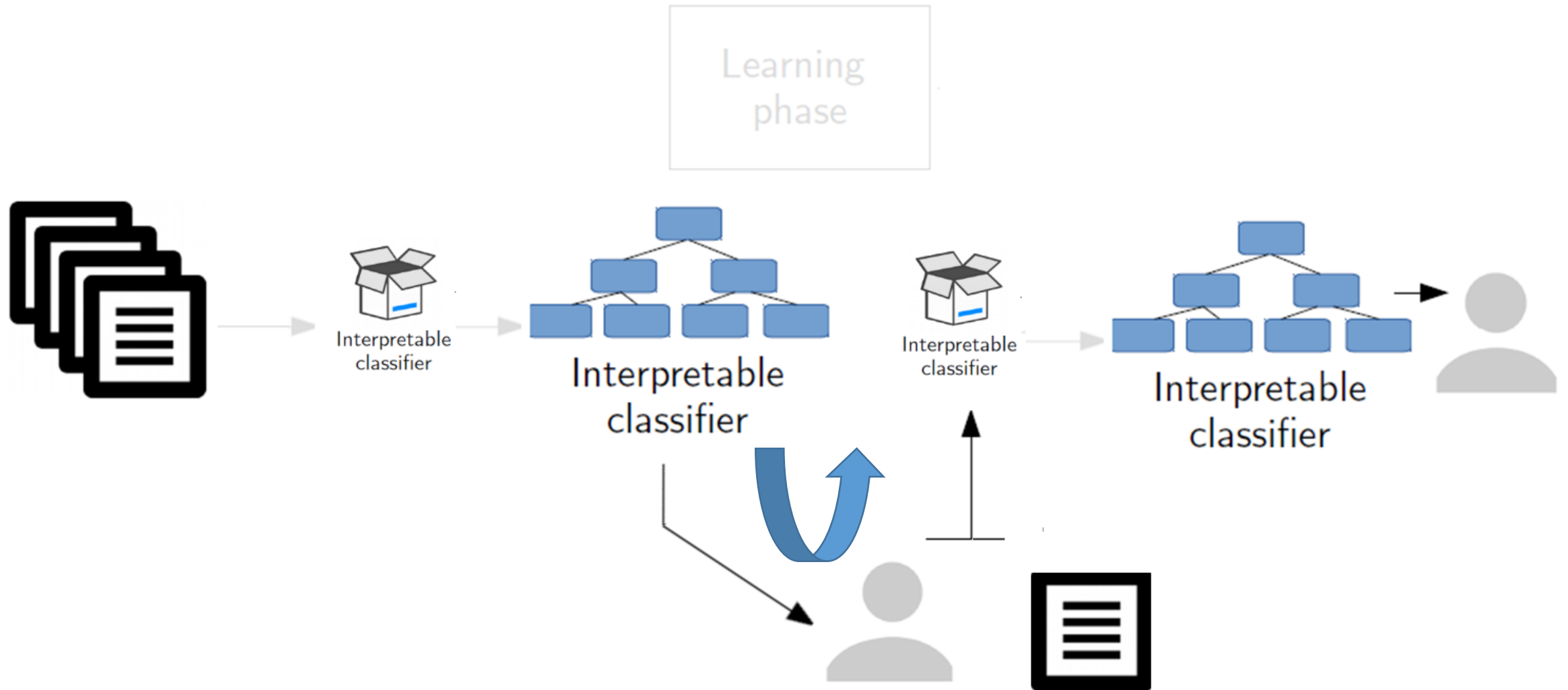
Interactive Machine Learning

Explicability interpretability of decision models and prediction



Interactive Machine Learning

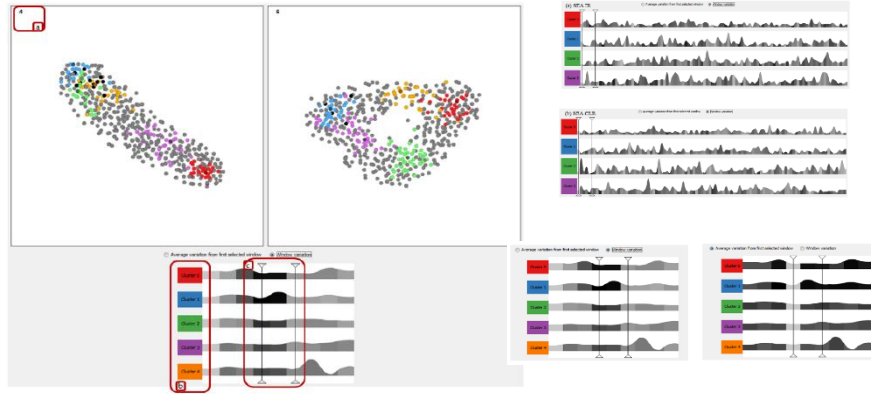
Explicability interpretability of decision models and prediction



3

Contributions

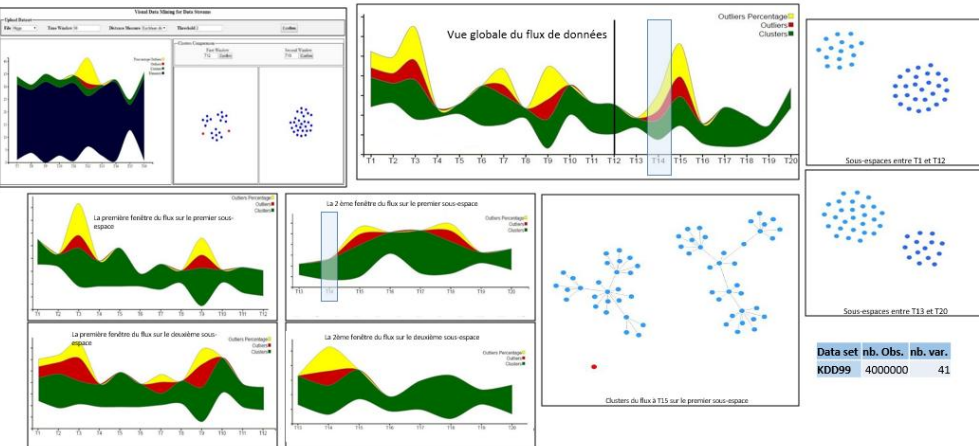
Human-In-The-Loop



Visual analytics

Visual Data Mining

Interactive Machine Learning



Data stream clustering

Neighborhood graphs

Temporal windows

Clustering

NNG:

distance < threshold
Connected component=
Clusters

Cluster

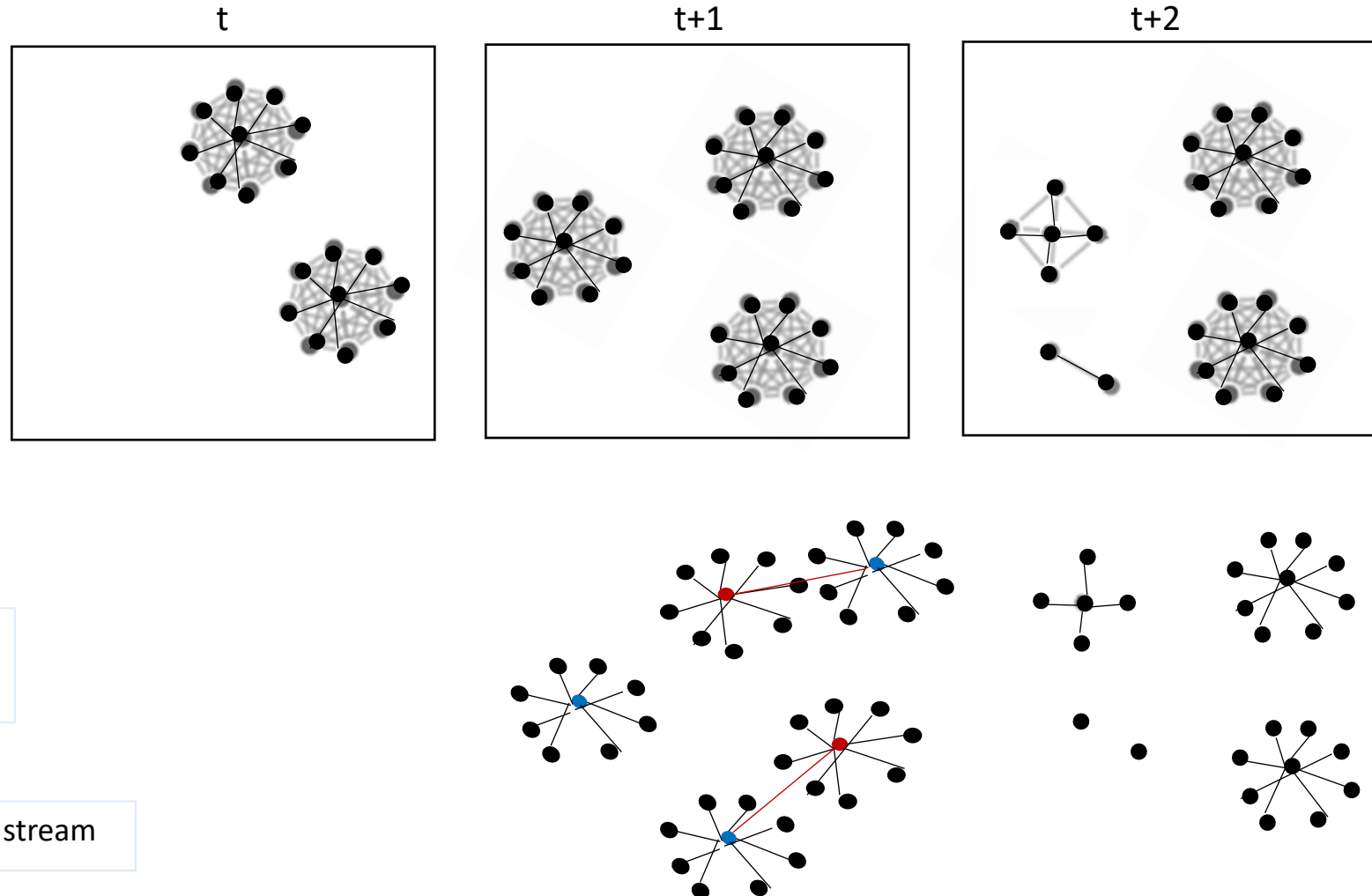
Centroid
neighbors

Stream

Centroids of $W(t+1)$ link with
nearest centroids of $W(t)$

Visualization

Incremental graph through the stream



Data stream clustering

Neighborhood graphs

Temporal windows

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NNG:

distance < threshold
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Cluster

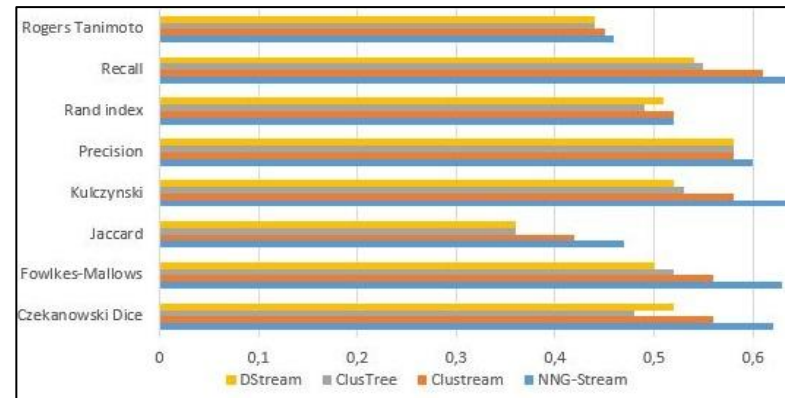
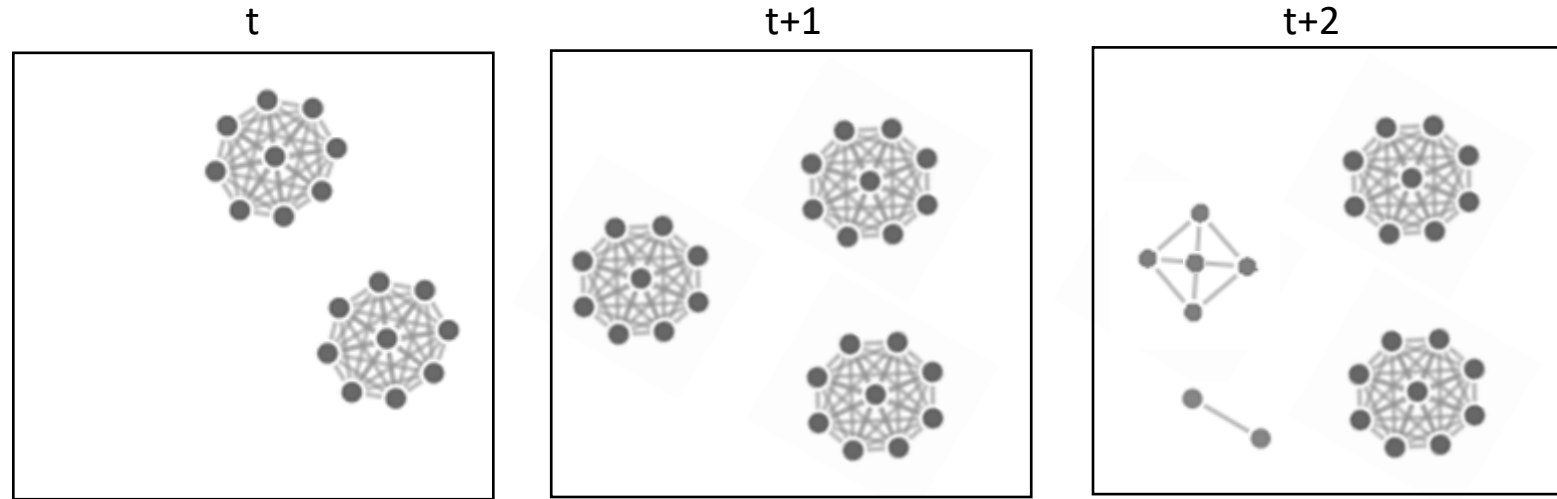
Centroid
neighbors

Stream

Centroids of $W(t+1)$ link with nearest
centroids of $W(t)$

Results:

- Comparison with the state of the art
- External evaluation indices
- Massive data sets



Data set	Type	nb. Obs.	nb. var.
Higgs	Numeric	11000000	28
Hepmass	Numeric	10500000	28
Susy	Numeric	5000000	0
KDD99	Heterogenous	4000000	41

Application:

Outliers detection on log files
Comparison: MCODE algorithm (Kontaki & al., 2011)

Data stream biclustering

Neighborhood graphs

Contr 2

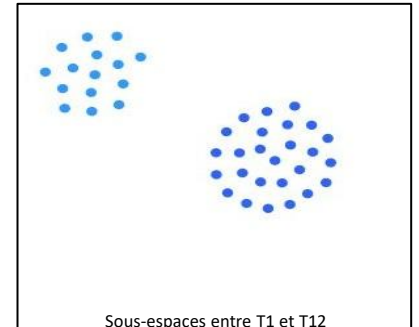
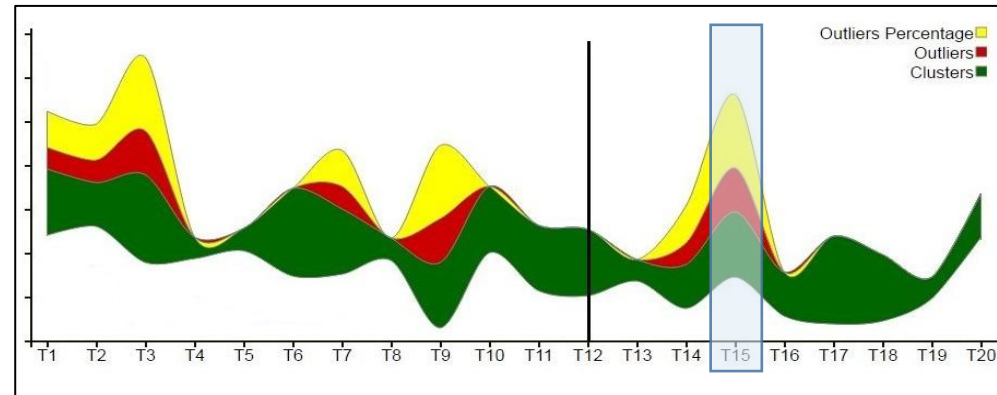
Data set	nb. Obs.	nb. var.
KDD99	4000000	41

Proposition:

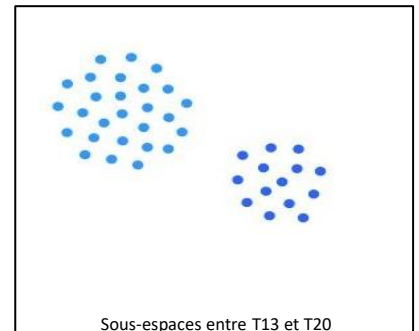
Neighborhood graphs clustering
On attributes then the observations

Contr 3

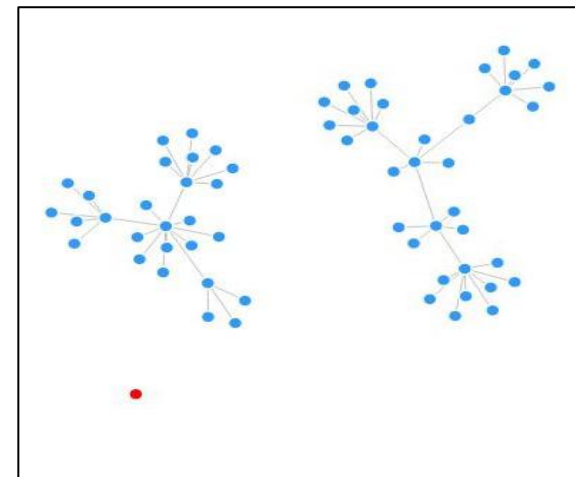
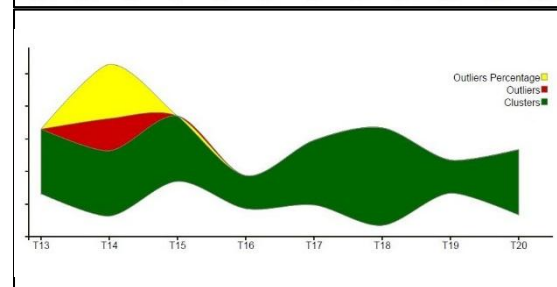
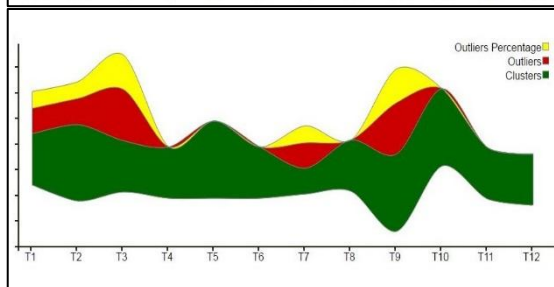
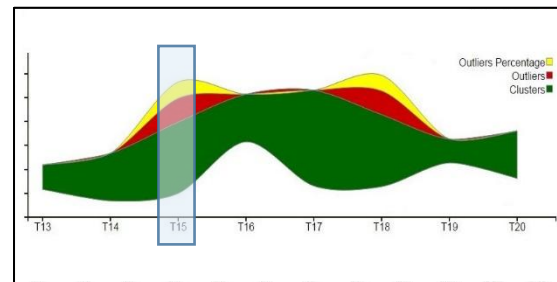
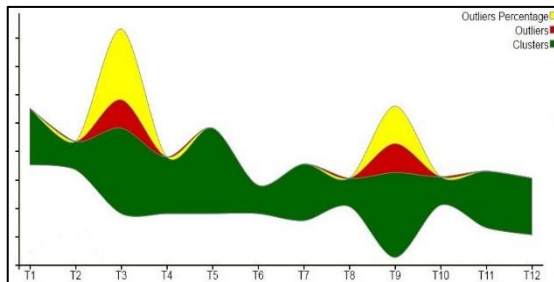
Visual exploration



Sous-espaces entre T1 et T12

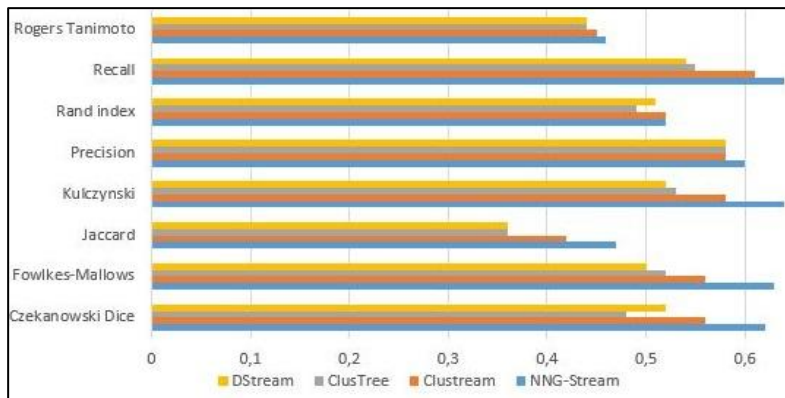
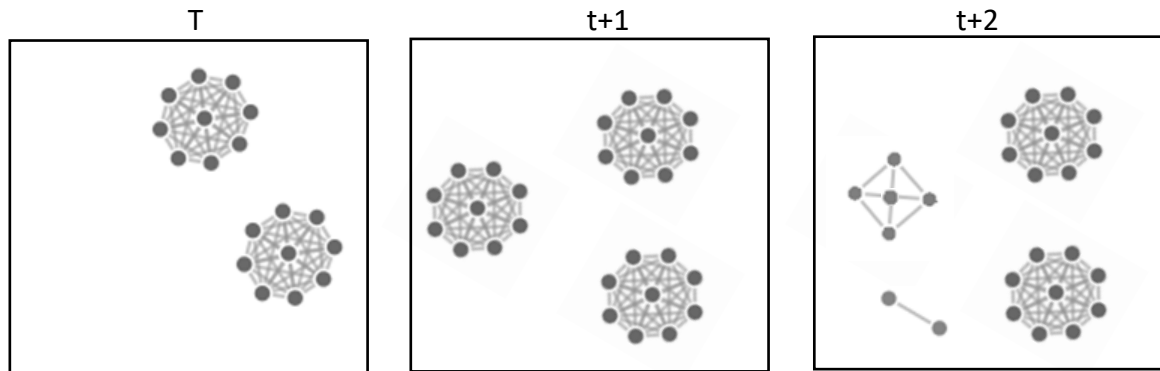


Sous-espaces entre T13 et T20

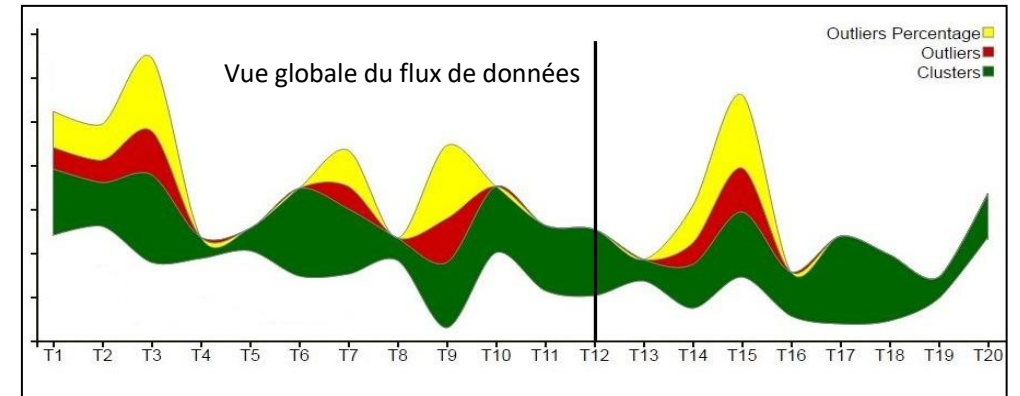


Data stream biclustering

Results and applications



Hepmass data set



Data set	Type	nb. Obs.	nb. var.
Higgs	Numeric	11000000	28
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KDD99	Heterogenous	4000000	41

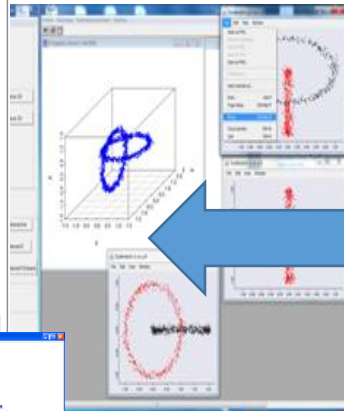
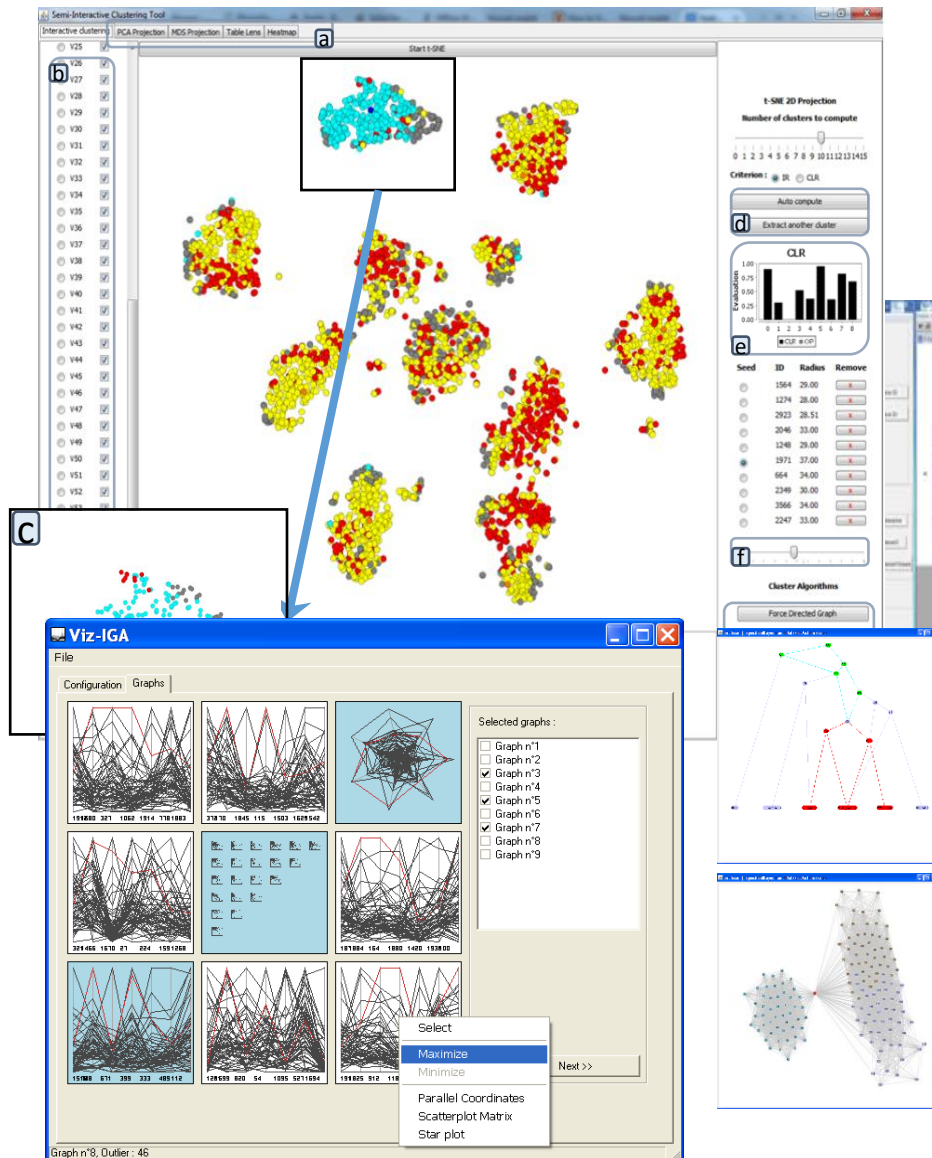
Application :

Detection of atypical behavior

Recording of network traffic events

A comparison with MCOB (Kontaki & al., 2011)

Human-In-The-Loop



Visual analytics

Visual Data Mining

Interactive Machine Learning



Clustering

Deterministic approach

Contr 1: cluster extraction

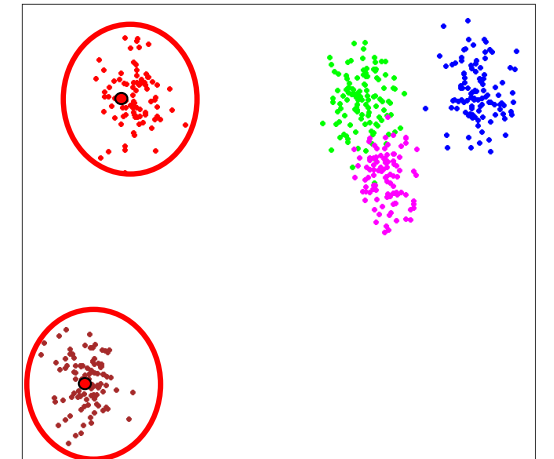
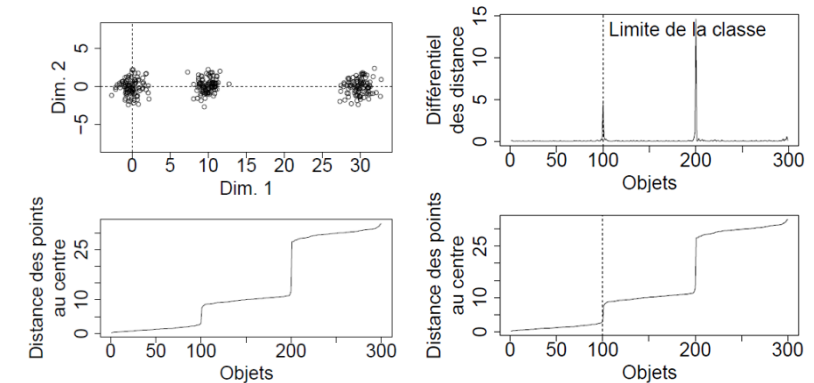
Extraction of a spherical cluster

- Cluster defined by a center
- Data distributed around the center
- Cluster radius (distance limit)

Automatic search of the cluster limit

- Calculating the distance of all objects at the given center
- sort the distances
- Finding the first steep increase in distance

→ Peak detection method (Palshikar, 2009):
evaluation measure applied to the distance
differential



... without knowing k

Deterministic approach

Contr 2: cluster evaluation

Compactness criterion of one cluster

- entire partition
- cluster evaluation based on the other clusters (Wemmert-Gançarski, 2000)

Inertia ratio IR: the ratio of the intra-class inertia by the total inertia of the data, normalized by the number of objects in the extracted cluster and the whole data set

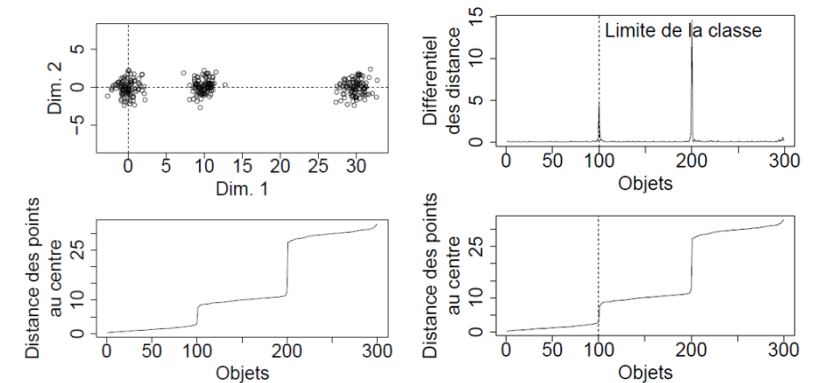
Cluster limit ratio CLR: the ratio between the distance of the last object of the extracted cluster and the first object outside the cluster.

OP: penalty for overlapping cluster to make sure that the extracted clusters are different

$$IR(C_k) = \frac{Card(D) \sum_{o \in C_k} d(o, c_k)^2}{Card(C_k) \sum_{o \in D} d(o, g)^2}$$

$$CLR(C_k) = \frac{\max_{o \in C_k} (d(o, c_k))}{\min_{o \notin C_k} (d(o, c_k))}$$

$$OP(C_k) = \lambda \frac{\sum_{o \in C_k} nb_o}{Card(C_k)}$$

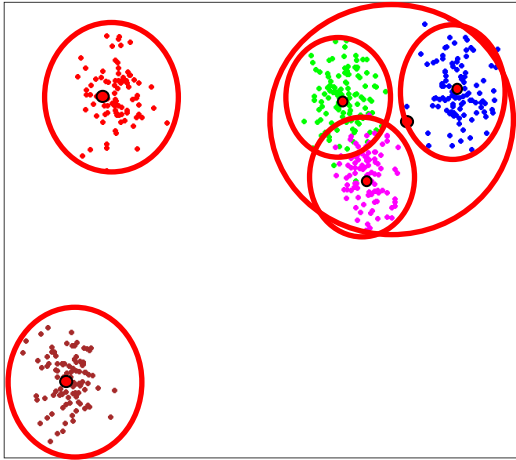


Contr 3: deterministic approach

- Combining cluster extractor (contr 1) with evaluation criterion (contr 2)
- First extracted are extracted in beginning (iterative extraction)
- Order is unique according to the criterion
- Allow overlapping

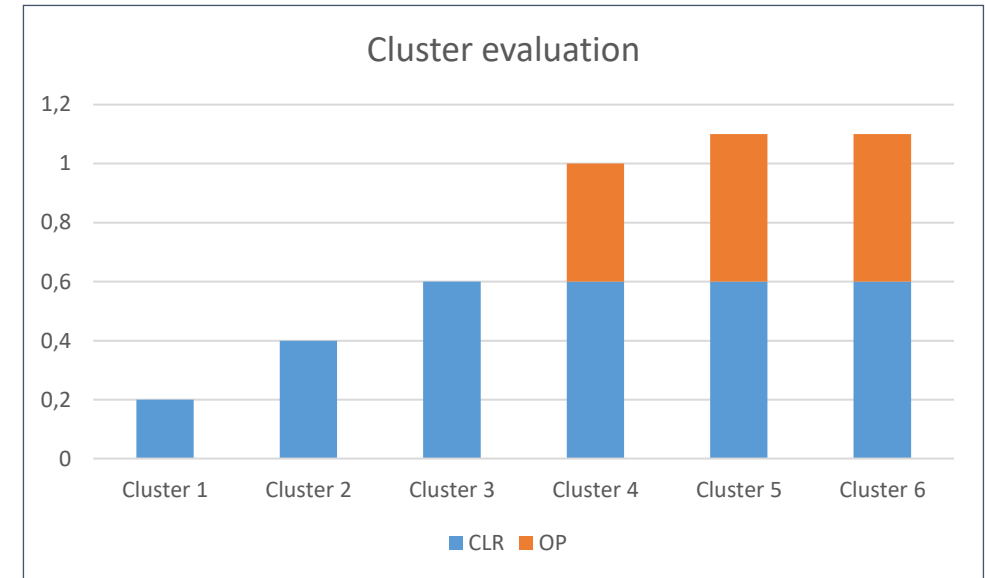
Iterative clustering

Iterative approach



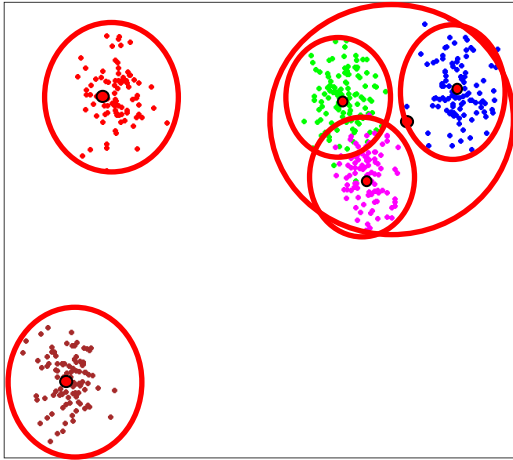
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$$OP(C_k) = \lambda \frac{\sum_{o \in C_k} nb_o}{Card(C_k)}$$



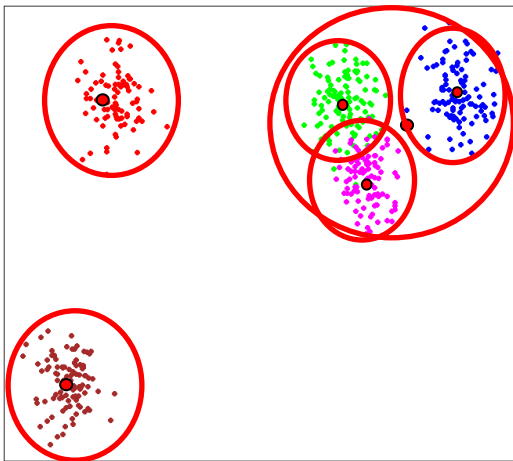
Iterative clustering

Iterative approach



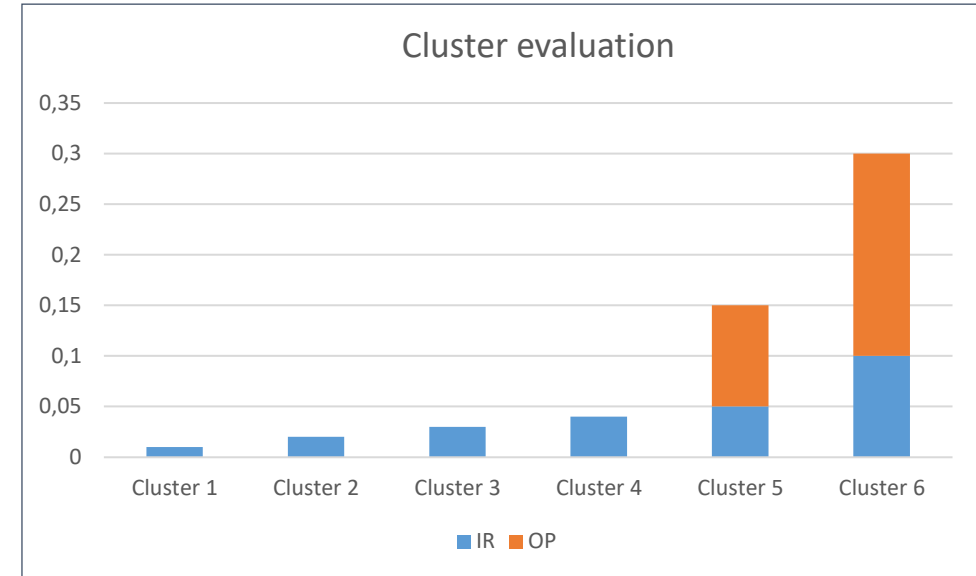
$$CLR(C_k) = \frac{\max_{o \in C_k} (d(o, c_k))}{\min_{o \notin C_k} (d(o, c_k))}$$

$$OP(C_k) = \lambda \frac{\sum_{o \in C_k} nb_o}{Card(C_k)}$$



$$IR(C_k) = \frac{Card(D) \sum_{o \in C_k} d(o, c_k)^2}{Card(C_k) \sum_{o \in D} d(o, g)^2}$$

$$OP(C_k) = \lambda \frac{\sum_{o \in C_k} nb_o}{Card(C_k)}$$



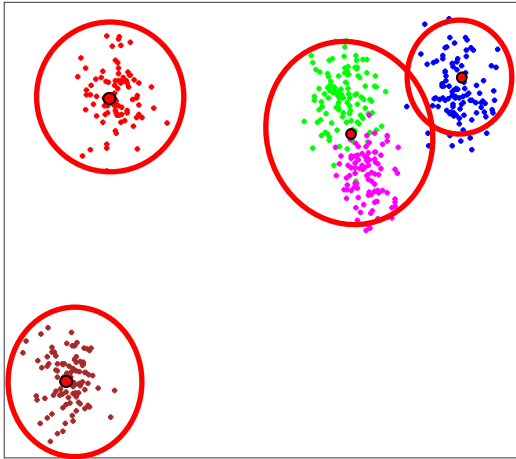
- *Iris de Fisher*, de l'UCI (150 obs., 4 var.) :
3 clusters
- **Accuracy**: mean of 100 executions
 - IR: 0.805
 - **CLR: 0.834**
 - K-means: 0.765

Data set	nb. Obs.	nb. var.
WaveFrom	5000	21
Optical Digit	5620	64
Sea Concept	6000	3
Statlog	6435	36
Ovarian	253	15154
Isolet	6238	616
Bicatyeast	419	70

Iterative clustering

Semi-interactive approach

Contr 4



- Active user
- Iterative clustering
- 2D projection
- Modify the automatic proposition
- Propose other centers
- Visual perception

→ Interactive clustering

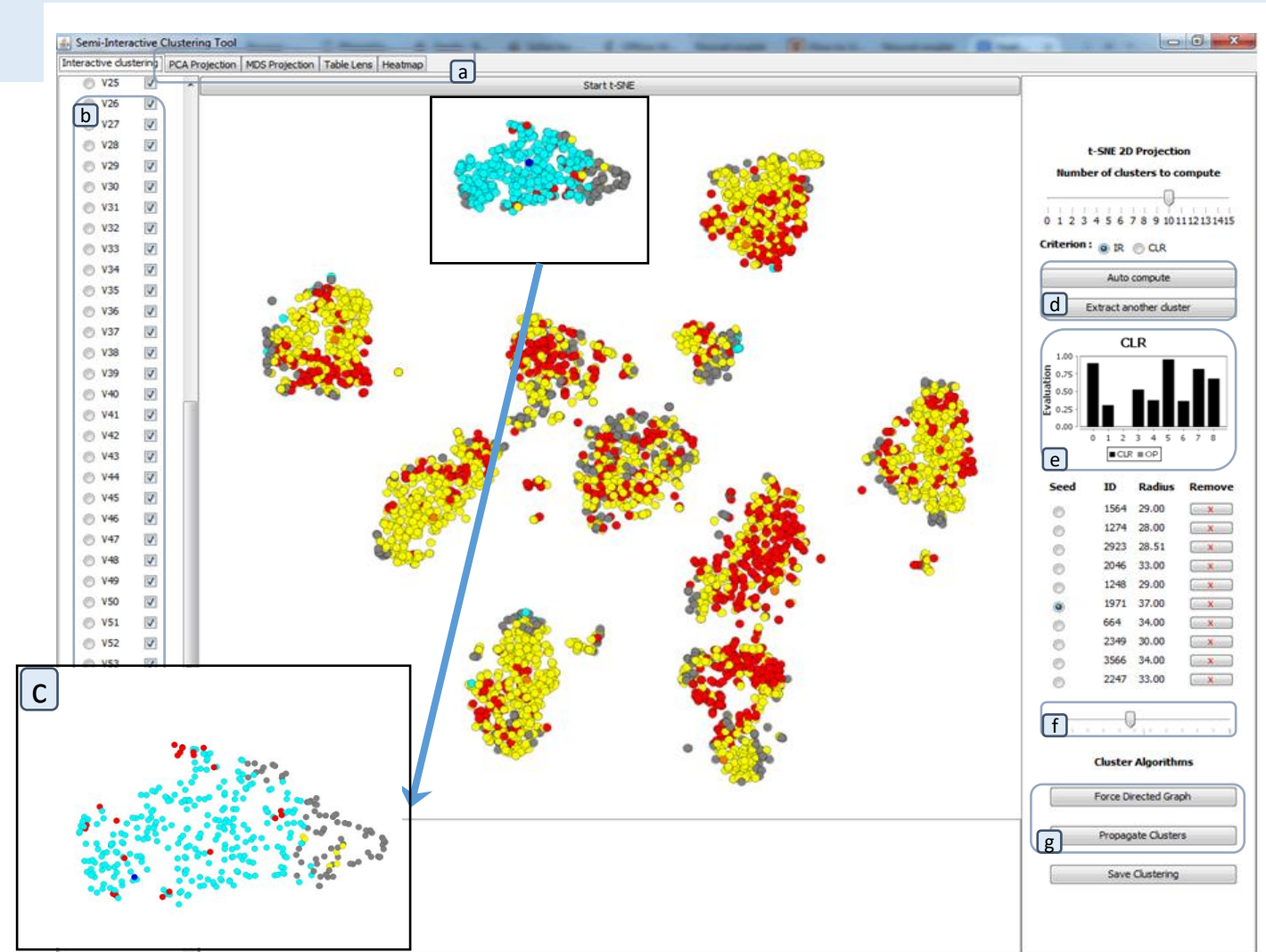
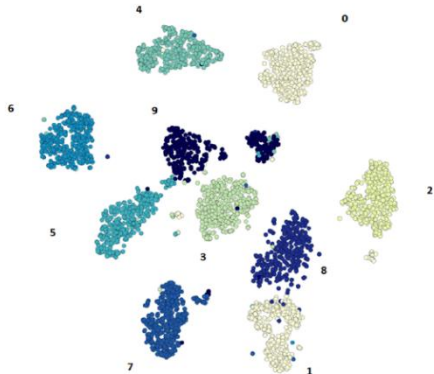
Iterative clustering

Semi-interactive approach

Contr 4

Data set :
OpticalDigits
5 620 obs.,
64 var.,
10 classes,
UCI ML Repository.

Optical Recognition of Handwritten number of 46 persons



Iterative clustering

Semi-interactive approach

User evaluation

11 participants (**Computer science**) Age 30-40
- 2 **information visualization** et **interaction**,
- 3 **data mining**

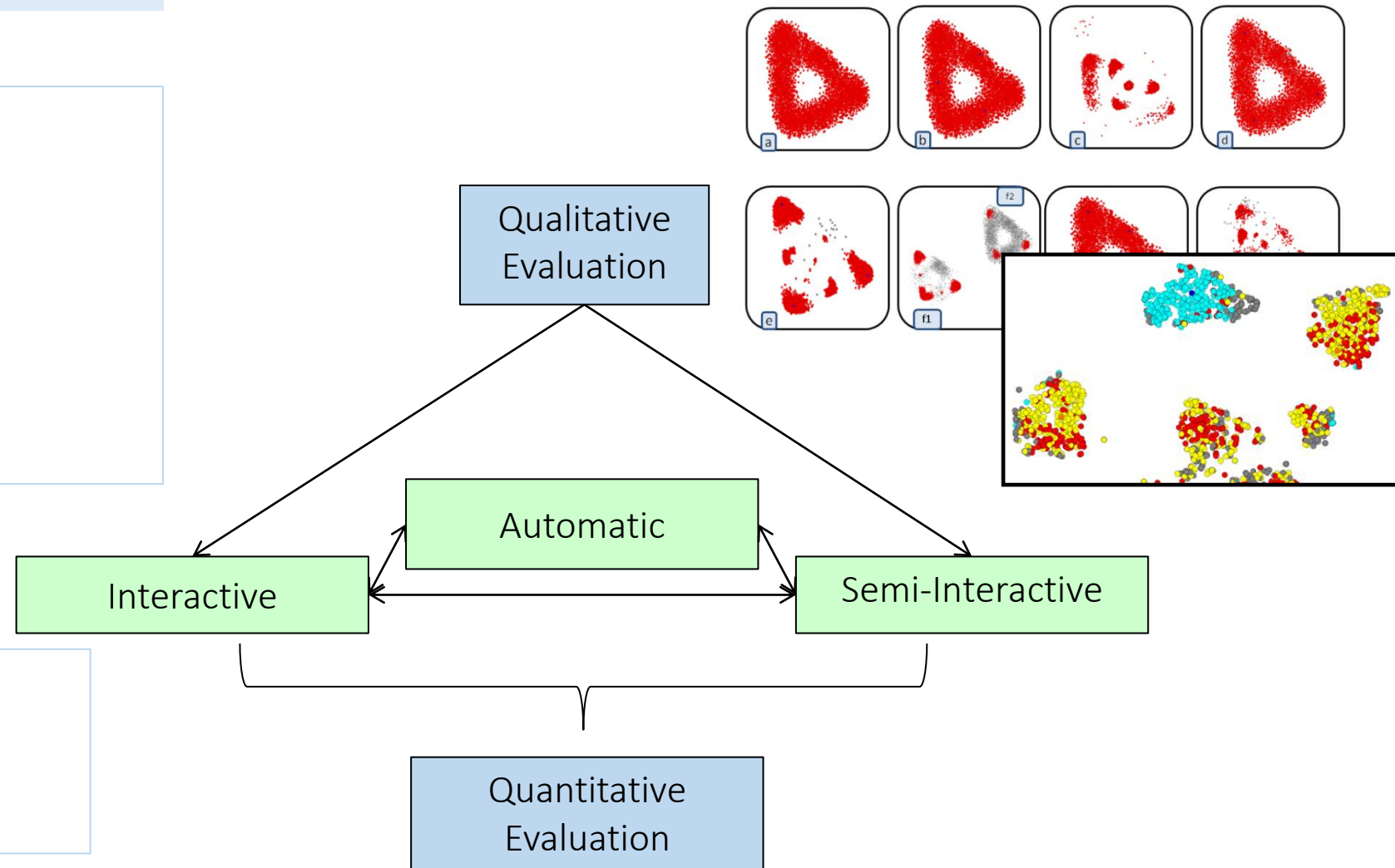
Protocol : 3 scenarios
- purely interactive
- semi-interactive
- purely automatic

clustering / real classes : external criterion

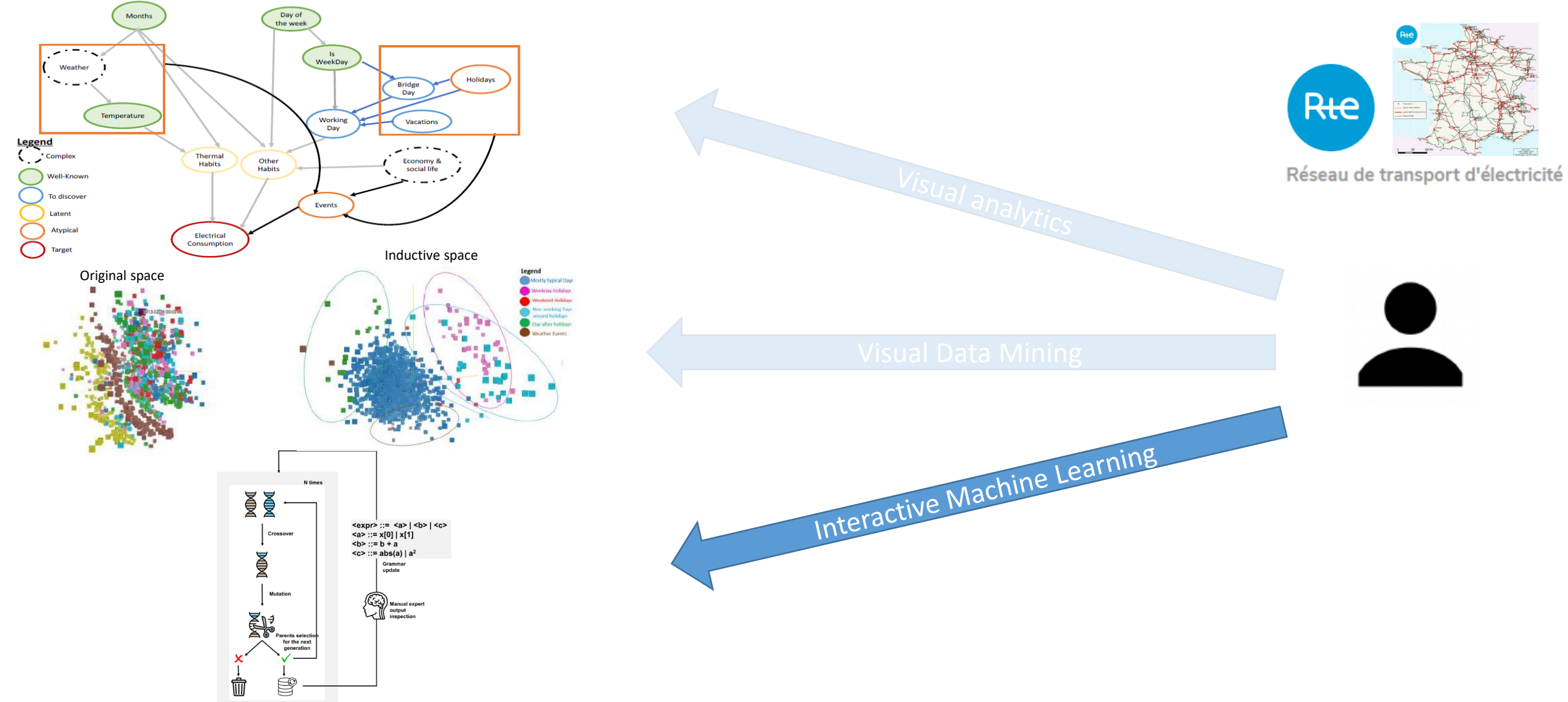
Statistical tests

Shapiro-Wilk test : normality
Student test : means

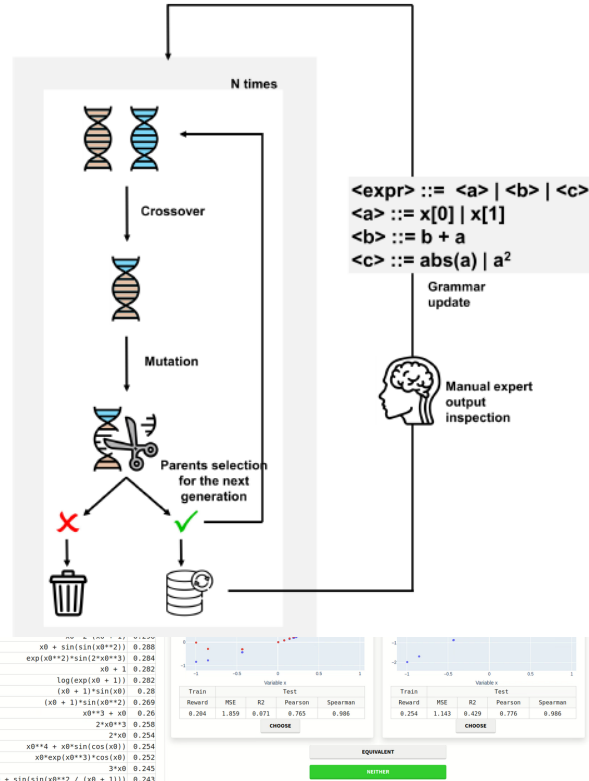
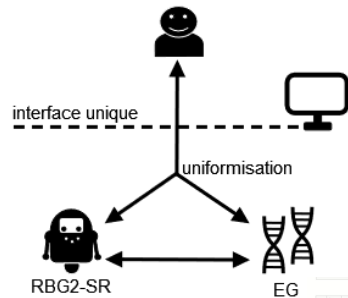
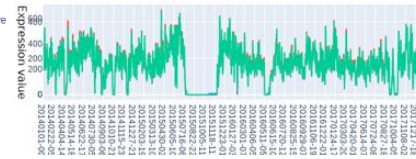
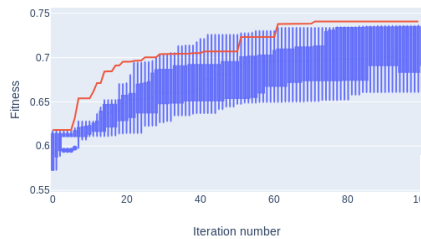
→ semi-interactive > automatic
semi-interactive > interactive



Human-In-The-Loop



Human-In-The-Loop



Visual analytics

Visual Data Mining

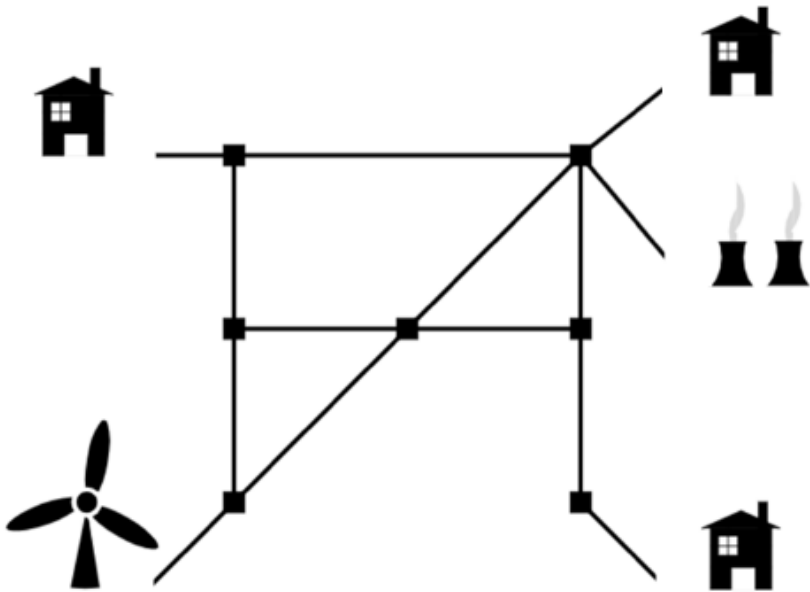
Interactive Machine Learning

4

French power grid application

Interactive Machine Learning

Explicability interpretability of decision models and prediction



*if ($connected_{or}^{line_i}$) then (watch feature₁)
else (watch feature₂)*

$$\sqrt{(p_1 + p_2)^2 + (q_1 + q_2)^2}$$

$$\frac{\sqrt{p^2 + q^2}}{v} \quad \sqrt{p^2 + q^2}$$

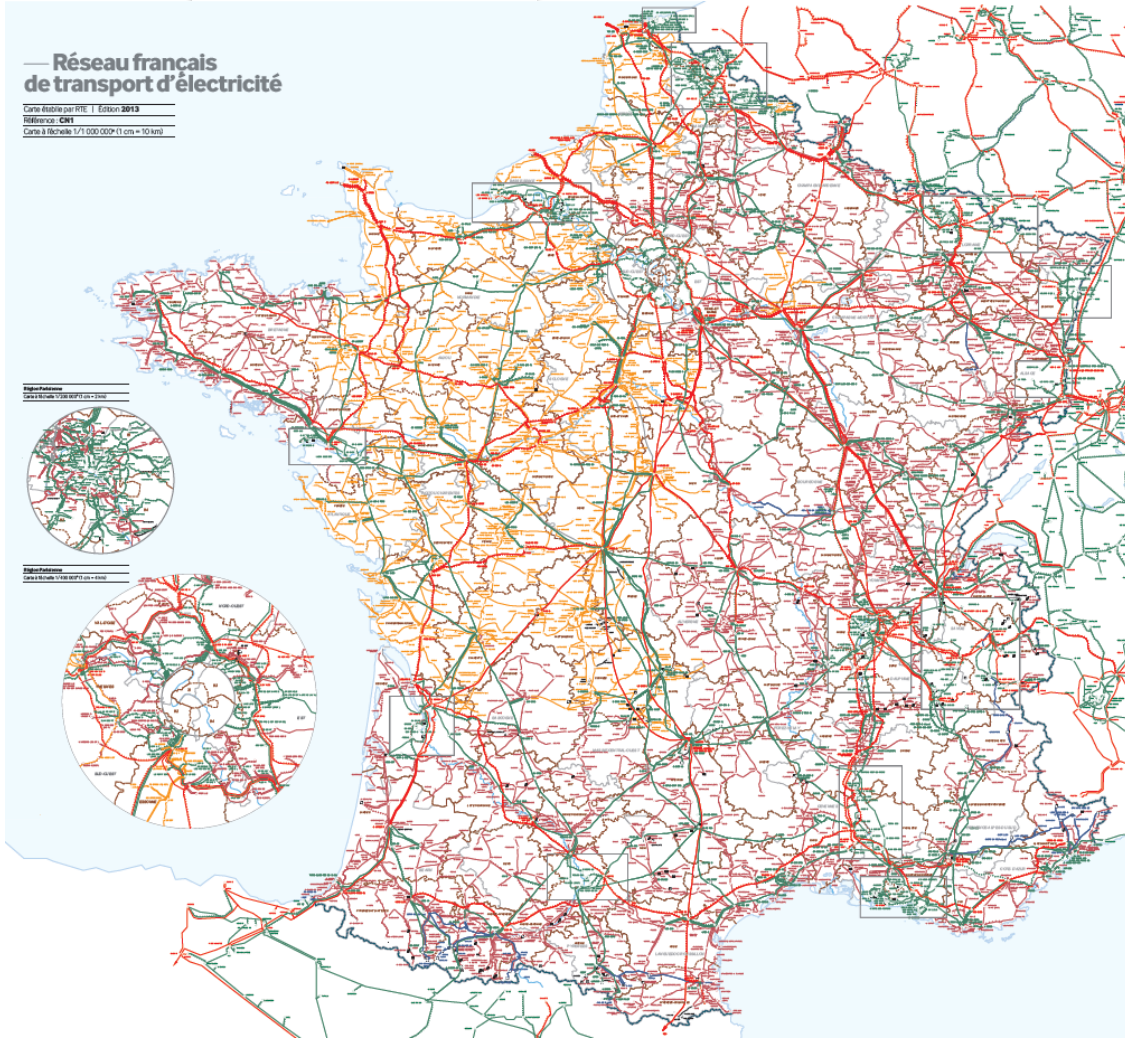
$$i_{frontier_1} - abs(i_{frontier_2})$$

- Linear feature extraction is often misinterpreted or overinterpreted
- Non linear methods are even harder to be interpreted for non machine learning experts



Réseau de transport d'électricité

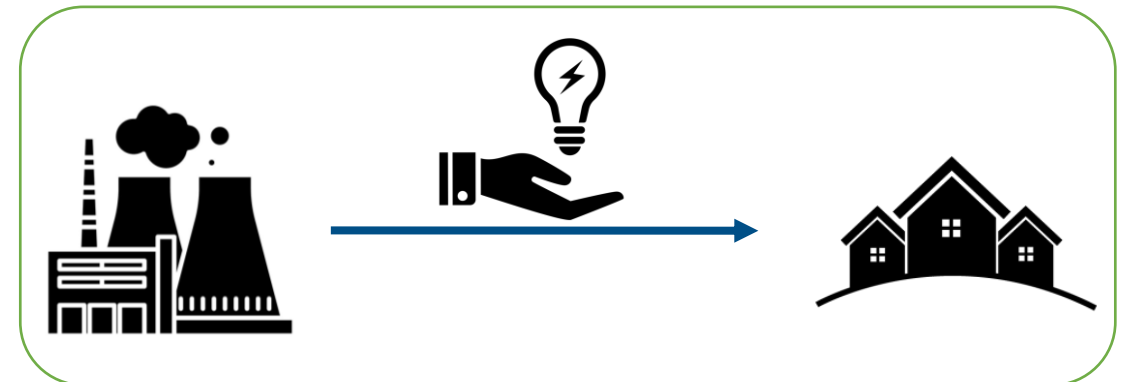
IML for the french power grid



French electrical power grid
(source RTE)

The French high-voltage power grid is made of 100,000 kilometers power lines and interconnected to 6 European countries

Rte (Réseau de transport d'Electricité) responsible for its operation, maintenance and development



Motivation: monitoring the power grid



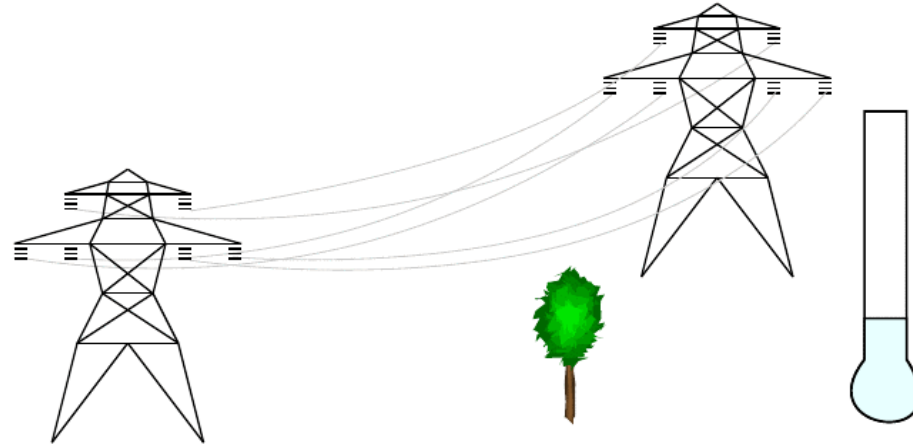
Rte Control room

Anticipated increase in the difficulty to operate the grid (renewable, cross-border exchanges, etc.)

Need for synthesis in the information provided to operators

There will always be operators to "*drive*" the network.

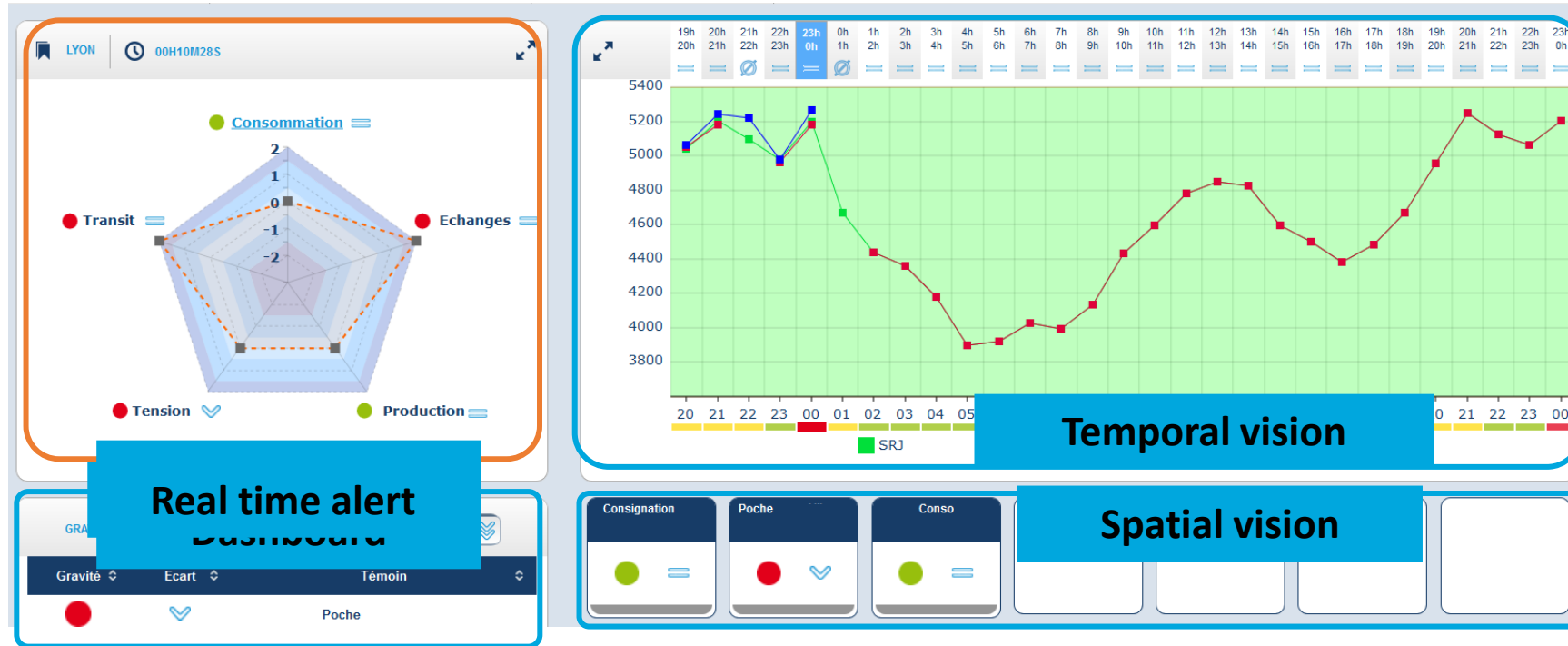
Study of electrical transits



A thermal limit is the physical threshold above which a short circuit can occur, which would endanger people in the vicinity and could damage equipment

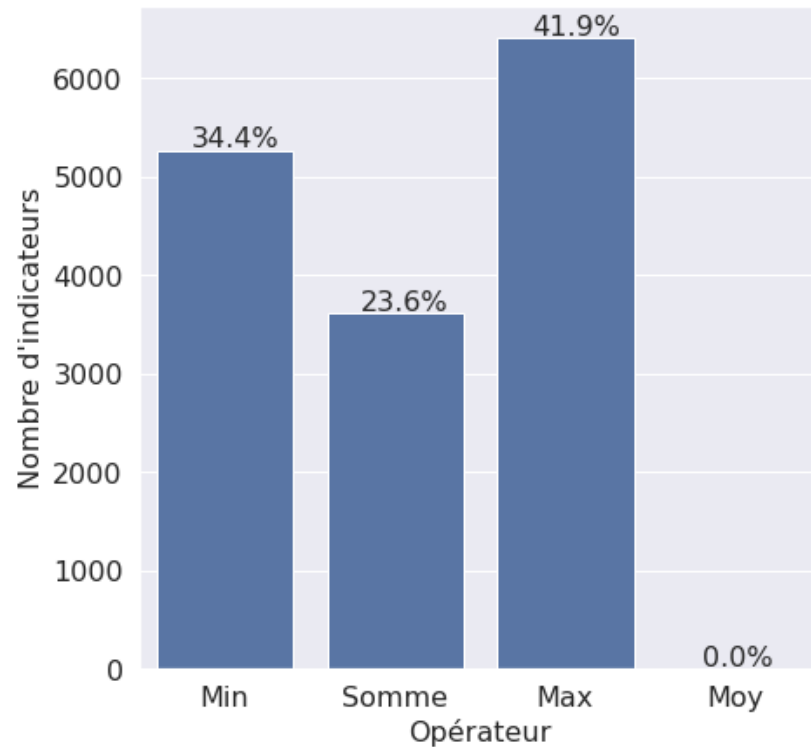
Create indicators with a physical meaning, in order to summarize the state of the network to operators

COMPARE Industrial Software

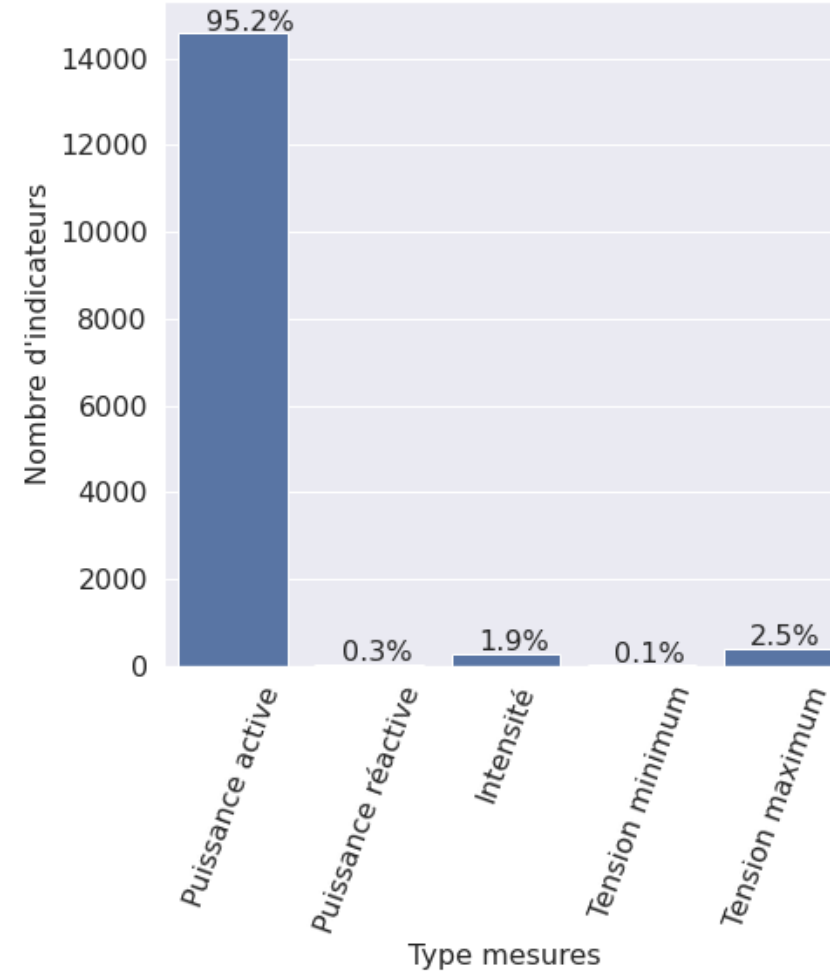


- Created by RTE to summarize the state of a zone to dispatchers and identify the origin of a constraint
- Powered by forecasting and measured data on the grid
- Commissioned in 2014
- Approximately 200 users

Indicators created manually by experts



$$\max(p_{production_1}, p_{production_2})$$



Statistics of existing indicators (October 2019)

Industrial constraints

Create indicators with a physical meaning, in order to summarize the state of the network to operators and going beyond the existing



Propose ***interpretable*** solutions for experts



Take into account expert ***knowledge*** and physics aspect



Reusability



Minimize ***expert user*** involvement

Objective

Definition:

Find a mathematical expression f between a set of observations $X \in \mathbb{R}^{M \times D}$ with D variables and M observations, and a target variable $y \in \mathbb{R}^M$:

$$f(x)=y \text{ such that } f \text{ is } \textit{interpretable} \text{ by a human}$$

- **Interpretability** is characterized by two elements:
 - The physical (or trade) **sense**
 - The **legibility (readability)** of the function
- A symbolic expression created will be used as an indicator

Symbolic regression

Definition:

Find a mathematical expression f between a set of observations $X \in \mathbb{R}^{M \times D}$ with D variables and M observations, and a target variable $y \in \mathbb{R}^M$:

$$f(x) = y$$

Multiple methods for regression

- Genetic Programming (Koza, 1990)
- Divide and conquer : AIFeynman (Udrescu et al., 2020)
- Deep neural networks (Biggio et al., 2020)
- Basic expansion: FFX (McConaghy, 2011)

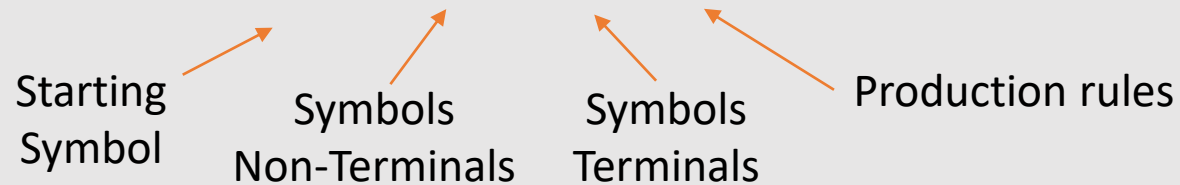
Interpretability criterion: Use of grammatical structure

Definition of a grammar

Definition

Non-contextual grammar G (Chomsky, 1959) is a tuple :

$$G = (\sigma_{start}, \sigma_{nt \in NT}, \sigma_{t \in T}, \rho) \text{ where } \rho \text{ is } \sigma_{NT} ::= rule_1 \mid .. \mid rule_K$$



Language $L(G)$ with symbolic expressions $f \in L$ to represent physical constraints and expert knowledge

Grammar guided symbolic regression

- Grammatical evolution (O'Neill and Ryan, 2001),
- Programmatically Interpretable reinforcement learning (Verma et al., 2018)

Chomsky, N. (1959). On certain formal properties of grammars. *Information and control*, 2(2):137–167.

O'Neill, M. et Ryan, C. (2001). Grammatical evolution. *IEEE Transactions on Evolutionary Computation*, 5(4):349–358.

Verma, A., Murali, V., Singh, R., Kohli, P. et Chaudhuri, S. (2018). Programmatically Interpretable Reinforcement Learning. In *Proceedings of the ICML*, pages 5045–5054

Generating an expression from a grammar

Grammar Example

$\langle expr \rangle ::= \langle a \rangle \mid \langle b \rangle$

$\langle a \rangle ::= \langle c \rangle * \langle c \rangle \mid \langle c \rangle / \langle c \rangle$

$\langle b \rangle ::= \langle c \rangle + \langle c \rangle \mid \langle c \rangle - \langle c \rangle$

$\langle c \rangle ::= x_0 \mid x_1 \mid x_2 \mid x_3 \mid x_4 \mid x_5$

Generate expression " $x_1 + x_4$ "

- Symbole courant :

$\langle c \rangle$

- Règles grammaticales choisies :

- Itération 1 : $\langle expr \rangle ::= \langle b \rangle$
- Itération 2 : $\langle b \rangle ::= \langle c \rangle + \langle c \rangle$
- Itération 3 : $\langle c \rangle ::= x_1$
- Itération 4 : $\langle c \rangle ::= x_4$

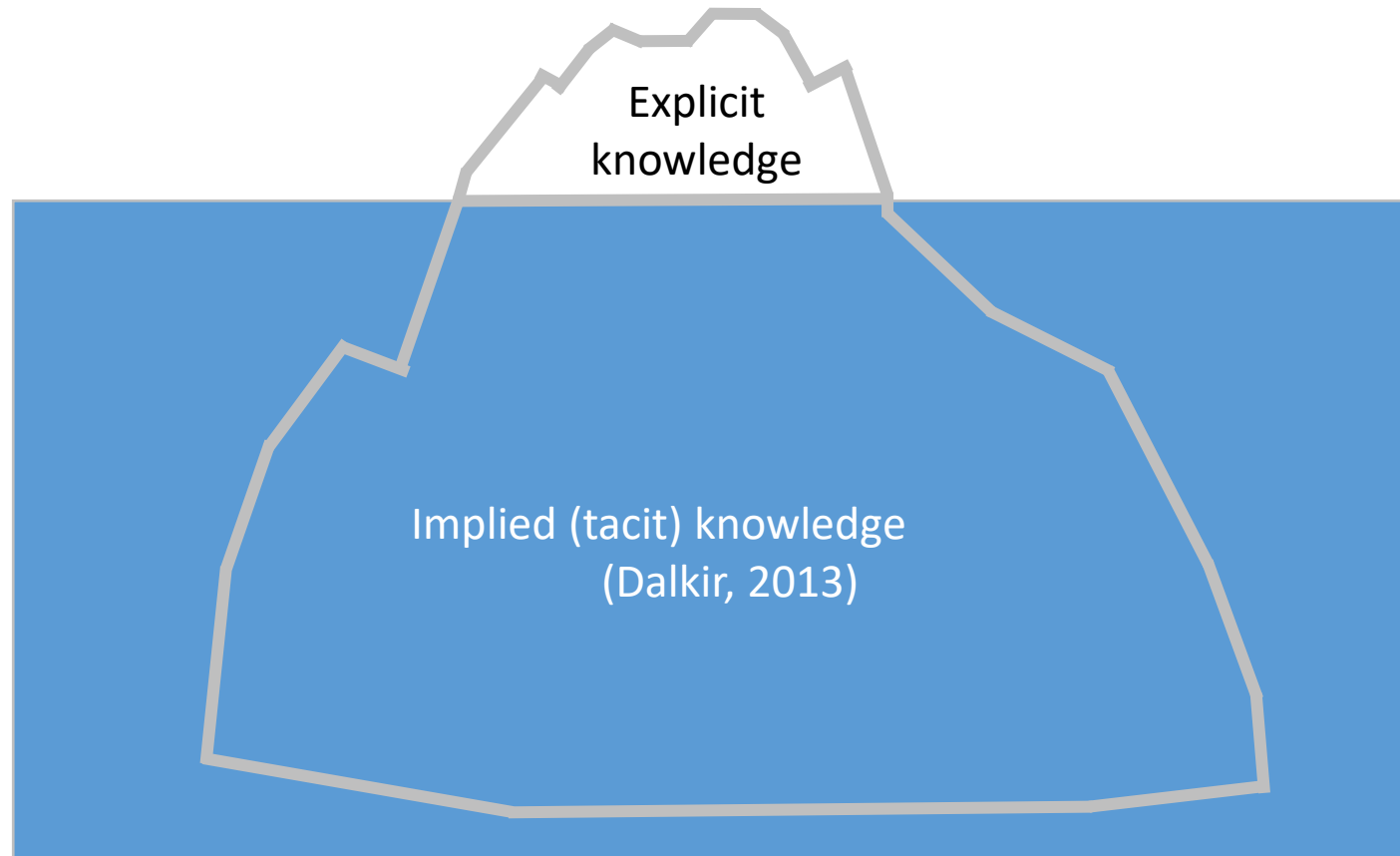
- Liste de symboles à remplacer :

$\square$

- Expression construite :

" $x_1 + x_4$ "

Knowledge Elicitation



Objectives

Preliminary issues

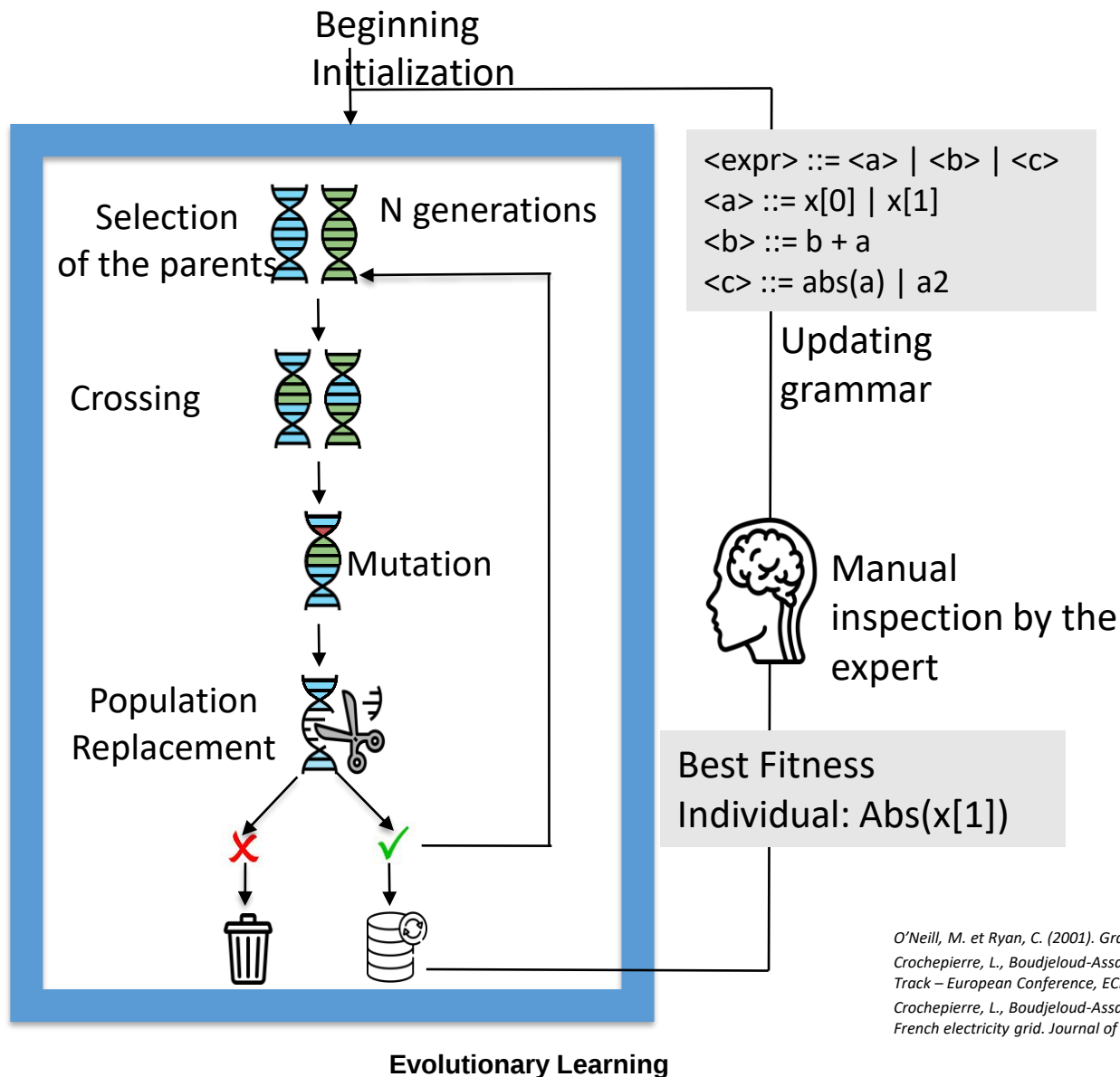
- How can knowledge be represented on the electricity network?
- How do you learn from indicators while using this knowledge?
- What method should be considered to comply with the industrial constraints mentioned?

Selected direction

- Representation of knowledge in the form of grammar
- Learning by evolutionary algorithms
- Compliance with the constraints of interpretability, reusability and knowledge taking into account



Proposed Approach: Interactive Grammatical Evolution



- Learning based on grammatical evolution(O'Neil, 2001)
$$fitness(y, y_{hat}) = pearson(y, y_{hat}) + 10^{-8} \times profondeur_individu$$
- Analysis of best-fit individuals
- Collect expert feedback between learnings
- Incremental grammar improvement between training sessions

O'Neill, M. et Ryan, C. (2001). Grammatical evolution. *IEEE Transactions on Evolutionary Computation*, 5(4):349–358.

Crochepierre, L., Boudjeloud-Assala, L. et Barbesant, V. (2020). Interpretable Dimensionally-Consistent Feature Extraction from Electrical Network Sensors. In *Applied Data Science Track – European Conference, ECML PKDD 2020, Proceedings*, pages 444–460.

Crochepierre, L., Boudjeloud-Assala, L. and Barbesant, V. (2021). Interactive approach to extracting interpretable and explanatory variables for the management of constraints in the French electricity grid. *Journal of New Information Technologies, Knowledge Extraction and Management, RNTI-E-37*:373–380.

Updating grammar

$\langle \text{expr} \rangle ::= \langle p \rangle \mid \langle q \rangle \mid \langle i \rangle \mid \langle v \rangle$

$\langle p \rangle ::= \langle p \rangle - \langle p \rangle \mid \langle \text{pop} \rangle(\langle p \rangle, \langle p \rangle) \mid \langle \text{pvar} \rangle$

$\langle q \rangle ::= \langle q \rangle - \langle q \rangle \mid \langle \text{pop} \rangle(\langle q \rangle, \langle q \rangle) \mid \langle \text{qvar} \rangle$

$\langle v \rangle ::= \langle v \rangle - \langle v \rangle \mid \langle \text{pop} \rangle(\langle v \rangle, \langle v \rangle) \mid \langle \text{var} \rangle$

$\langle i \rangle ::= \langle i \rangle - \langle i \rangle \mid \langle \text{pop} \rangle(\langle i \rangle, \langle i \rangle) \mid \langle i_frontiervar \rangle$

$\langle \text{pop} \rangle ::= \text{sum} \mid \text{minimum} \mid \text{maximum}$

Initial grammar

- New Units
- New Operations
- Physical Relationships
- Additional knowledge (e.g. output units)

User-Suggested Enhancements

Update

$\langle \text{expr} \rangle ::= \langle p \rangle \mid \langle s \rangle \mid \langle i \rangle \mid \langle f \rangle * \langle \text{expr} \rangle \mid \langle p \rangle / \langle v \rangle$

$\langle p \rangle ::= \langle p \rangle - \langle p \rangle \mid \langle \text{pop} \rangle(\langle p \rangle, \langle p \rangle) \mid \langle \text{sop} \rangle(\langle p \rangle) \mid \langle p_var \rangle$

$\langle q \rangle ::= \langle q \rangle - \langle q \rangle \mid \langle \text{pop} \rangle(\langle q \rangle, \langle q \rangle) \mid \langle \text{sop} \rangle(\langle q \rangle) \mid \langle q_var \rangle$

$\langle v \rangle ::= \langle v \rangle - \langle v \rangle \mid \langle \text{pop} \rangle(\langle v \rangle, \langle v \rangle) \mid \langle \text{sop} \rangle(\langle v \rangle) \mid \langle v_var \rangle$

$\langle i \rangle ::= \langle s \rangle / \langle v \rangle \mid \langle \text{pop} \rangle(\langle i \rangle, \langle i \rangle) \mid \langle \text{sop} \rangle(\langle i \rangle) \mid \langle i_frontier_var \rangle$

$\langle p2 \rangle ::= \langle p \rangle * \langle p \rangle \mid \text{square}(\langle p \rangle)$

$\langle q2 \rangle ::= \langle q \rangle * \langle q \rangle \mid \text{square}(\langle q \rangle)$

$\langle v2 \rangle ::= \langle v \rangle * \langle v \rangle \mid \text{square}(\langle v \rangle)$

$\langle s \rangle ::= \text{sqrt}(\langle p2 \rangle + \langle q2 \rangle) \mid \langle v \rangle * \langle i \rangle$

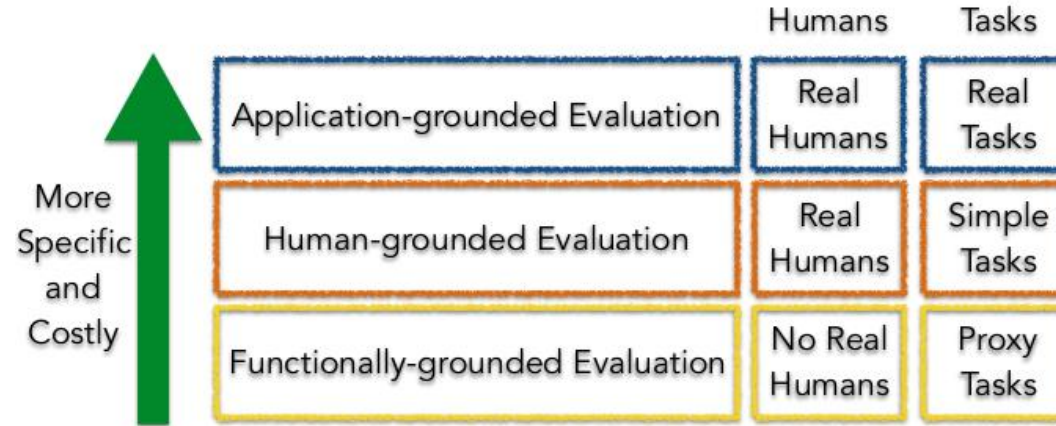
$\langle f \rangle ::= \langle f \rangle * \langle f \rangle \mid \langle p \rangle / \langle p \rangle \mid \langle q \rangle / \langle q \rangle \mid \langle v \rangle / \langle v \rangle$

$\langle \text{pop} \rangle ::= \text{sum} \mid \text{minimum} \mid \text{maximum}$

$\langle \text{sop} \rangle ::= \text{abs} \mid \text{neg} \mid \text{pos}$

Final grammar

Interpretability assessment



Taxonomy of Method Interpretability Evaluation
(Doshi-velez and Kim, 2017)

2-step interpretability assessment

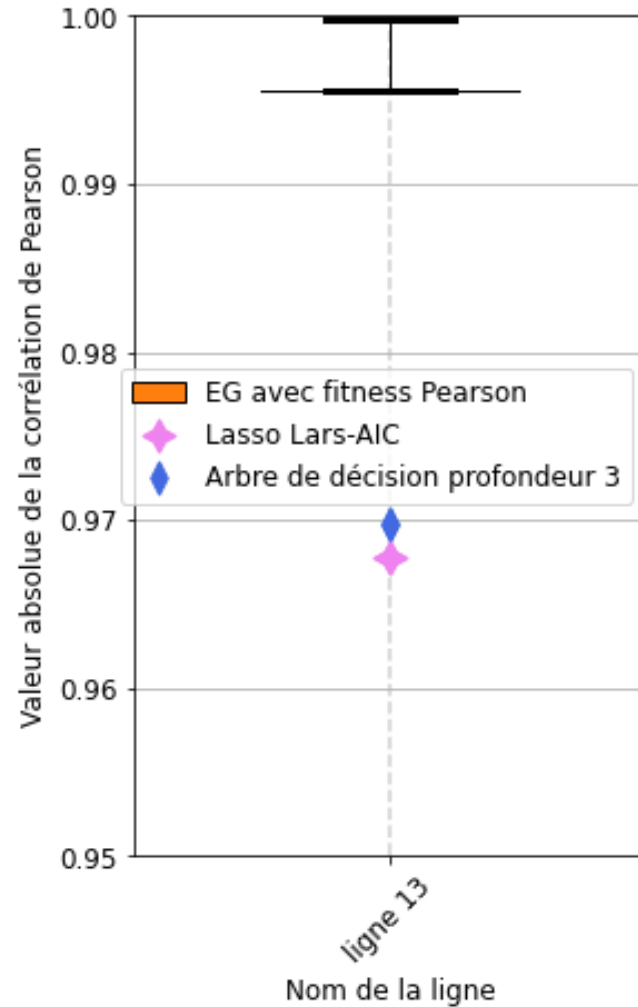
- "Functionally-grounded": comparison of scores with other interpretable methods: LASSO (Zou et al., 2007), Decision tree (Breiman et al., 1984)
- "Human-grounded": analysis of best fitness expressions in output

Doshi-Velez, F. et Kim, B. (2017). Towards a rigorous science of interpretable machine learning. arXiv preprint arXiv :1702.08608.

Zou, H., Hastie, T. et Tibshirani, R. (2007). On the "degrees of freedom" of the lasso. The Annals of Statistics, 35(5):2173–2192.

Breiman, L., Friedman, J. H., Olshen, R. A. et Stone, C. J. (1984). Classification and Regression Trees. Chapman and Hall/CRC.

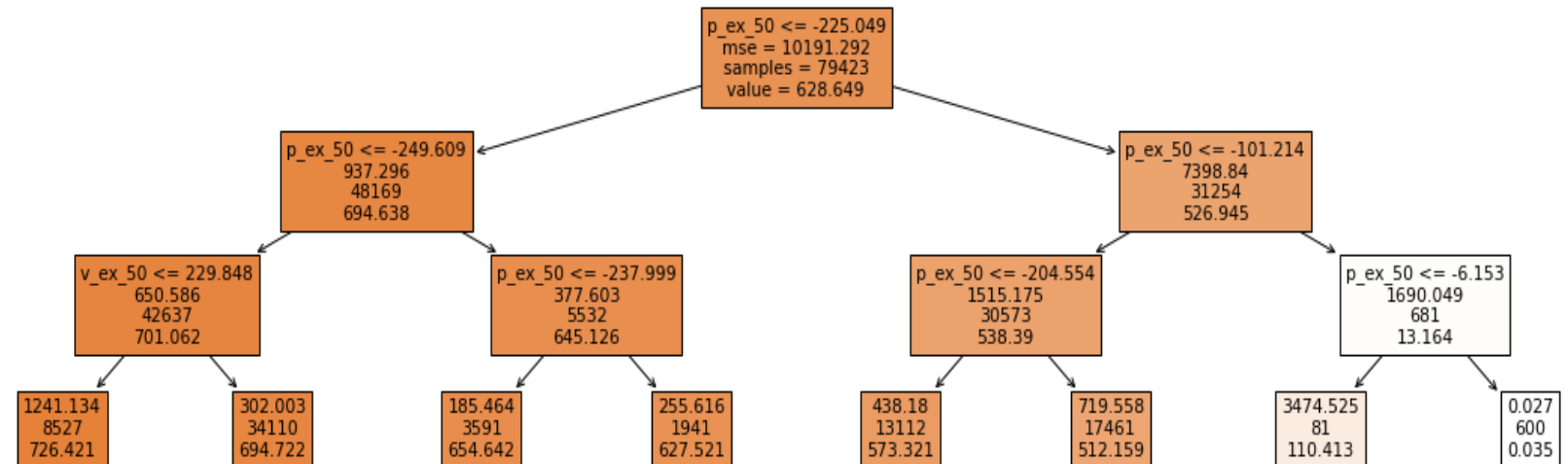
Focus on line 13



- Best expression EG :

$$\frac{\sqrt{p_{ex_50}^2 + q_{ex_50}^2}}{v_{ex_50}}$$

- Best score for decision tree



- LASSO

$$0.68 \ p_{ex_10} + 0.01 \ p_{ex_20} + 0.0009 \ p_{ex_61} + 0.14 \ p_{or_74}$$

"Human-grounded" evaluation

Expressions identification

- User-proposed unit validation

variations autour de $\sqrt{p^2 + q^2}$ tel que $\sqrt{(p_1 + p_2)^2 + (q_1 + q_2)^2}$

- Aggregation of variables with a unit useful for explaining transits

sum, min, max d' une liste de variables de puissance active p

- Identifying a global phenomenon: border transit

$i_{frontière_1} - i_{frontière_2}$

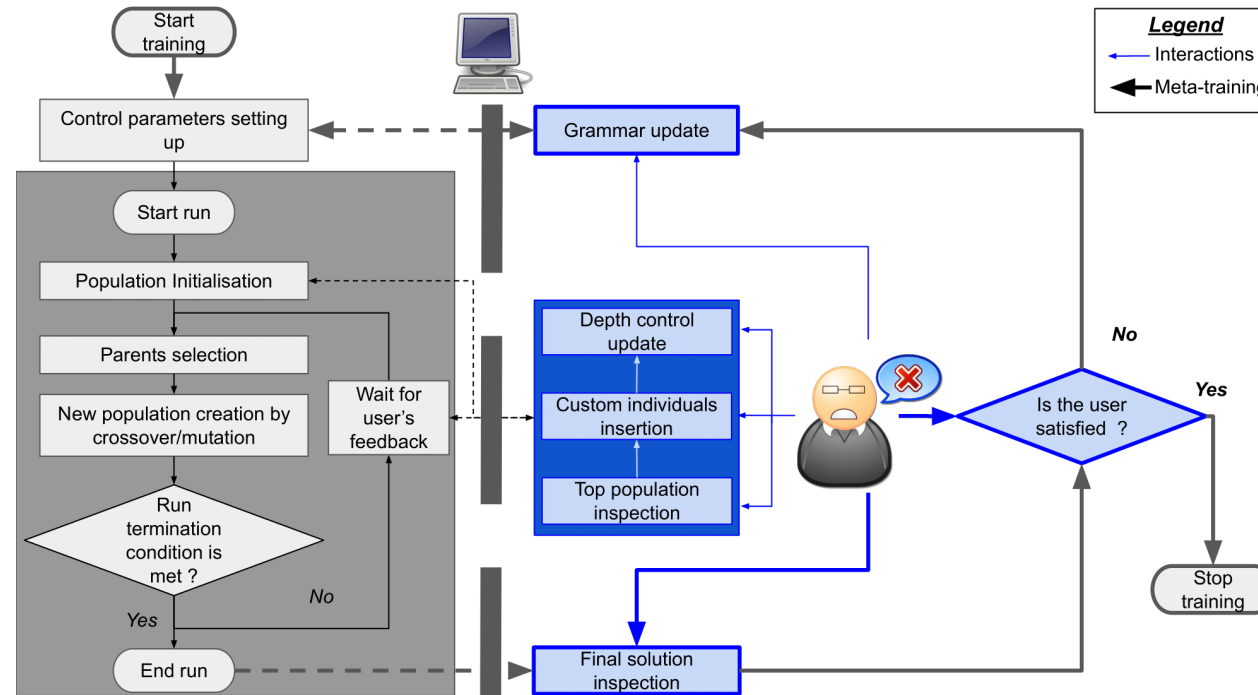
- Introducing topological variables

if(ligne₁ est connectée) then {sous_expression₁} else {sous_expression₂}

Expert comment

- Relevant correlation above 0.8 (human acceptance threshold)
- Threshold of 0.9 to use expressions as they are
- Interest in intervening during learning

Multi-level interaction platform



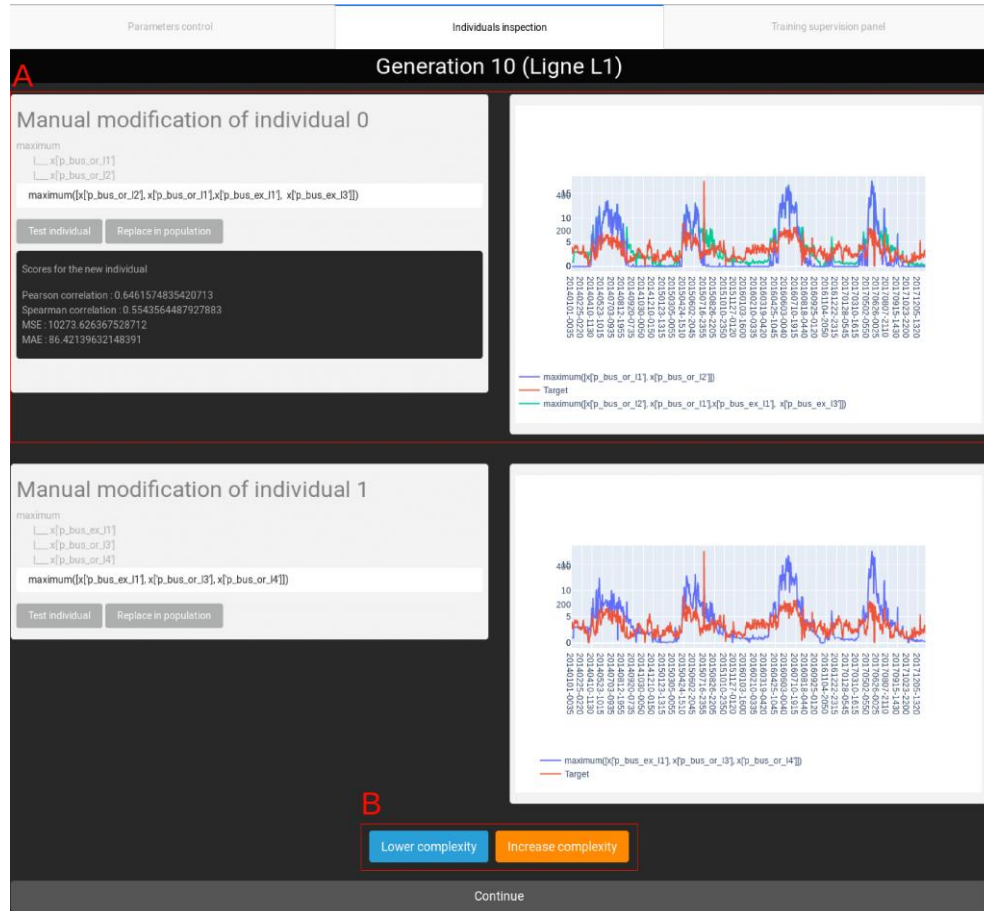
Multi-level interactivity (Crochepierre et al., 2022)

- During training: inspection by the expert and addition of individuals
- Between two learnings: integrating expert comments into the grammar

Implementation de l'interface :

- Dash Plotly Library in Python

Interactions with genetic individuals



Inspection of individuals

- Tree representation
- Error metrics (correlations, EQMs, ...)
- Time series representation

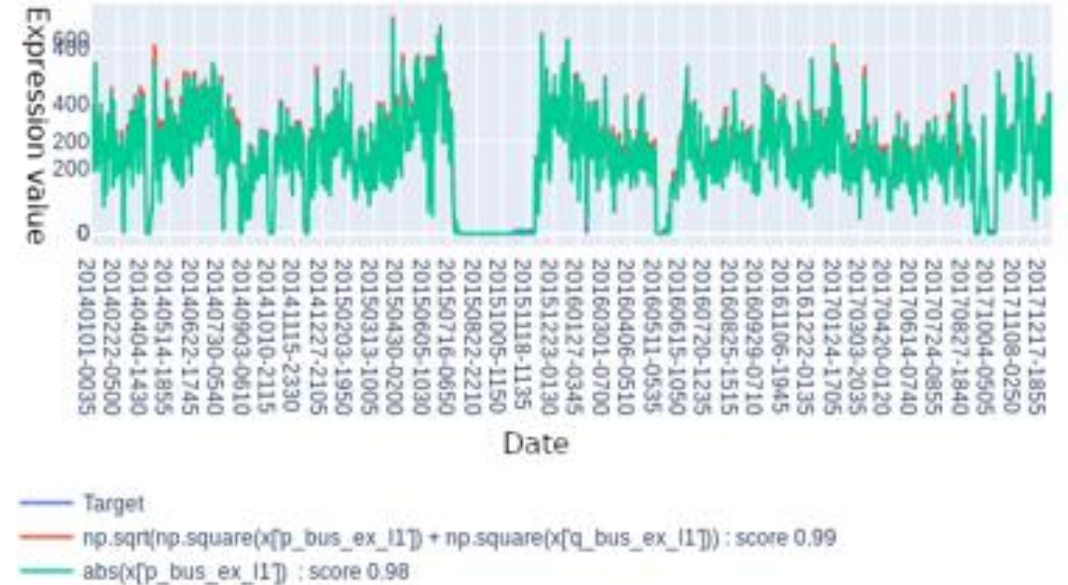
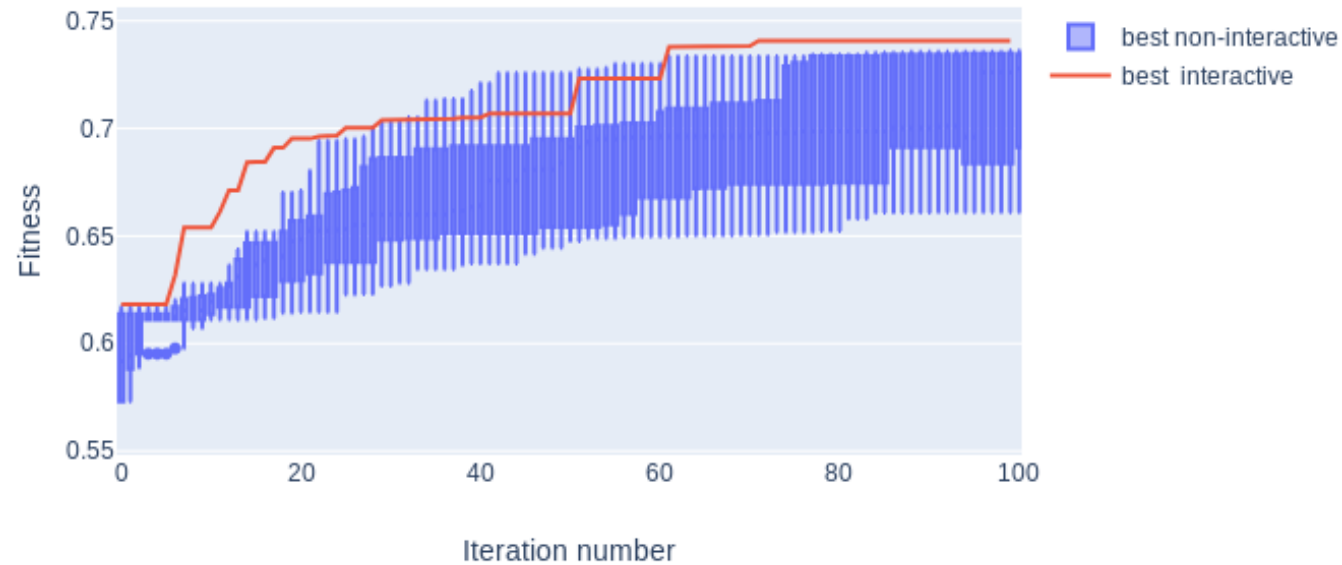
Individual Update

- Text representation
- Comparative test with the initial individual
- Replacement if relevant

Comparison between individuals

- By score and time series

Usage scenarios



Improved performance

- Achieve the best results in fewer iterations
- Discover new expressions

Reduced complexity

- Set preferences between visually similar individuals with identical scores
- Choosing the best balance between error and complexity
- Some more complex lines are more difficult to model
- All the rules of grammar are considered equiprobable

Objectives

Preliminary issues

- How to orient research in the grammatical space?
- How do you learn from indicators while using this knowledge?
- What method should be considered to comply with the industrial constraints mentioned?

Selected direction

- Reinforcement Learning
- Definition of a Markov decision-making process
- Compliance with the constraints of interpretability, reusability and knowledge taking into account



Markov Decision Process definition

Definition (Crochepierre et al, 2022)

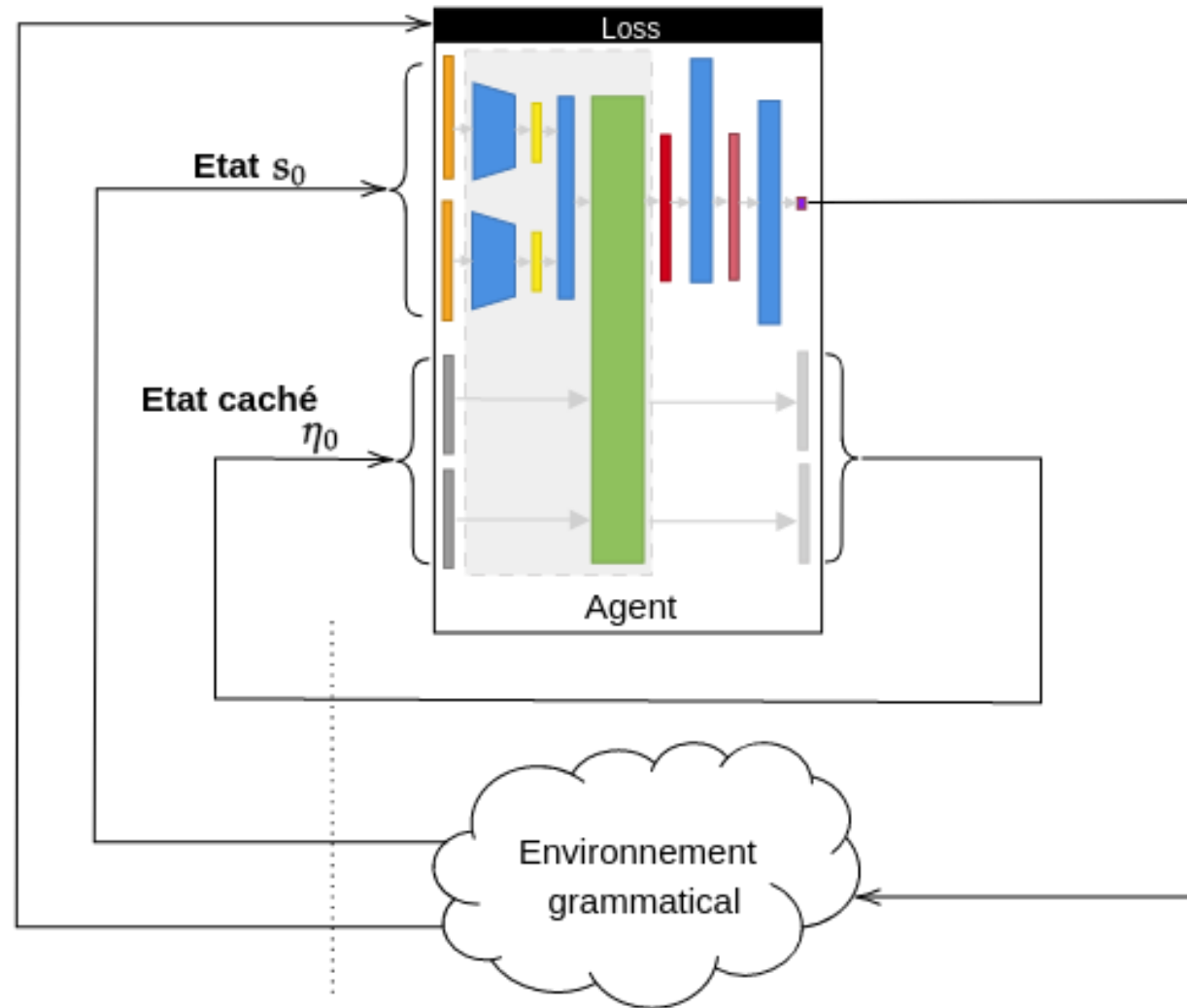
- ▷ State : information on expression under construction
- ▷ Action : selection of a grammatical rule in G
- ▷ Reward : $R(f) = \frac{1}{1+EQM(y, f(x))}$

Learning distribution of grammar rules G

- Neuronal agent π_θ with REINFORCE (Williams, 1992)
- Risk-seeking policy gradient (Petersen et al., 2021)

$$J_\theta = \mathbb{E}_{f \sim \pi_\theta} [\log(P_\theta(f)) R(f) | R(f) > R_\varepsilon]$$

Architecture neuronale



Agent neuronal et environnement de renforcement

Evaluation of the method

Symbolic Regression Benchmarks

- Nguyen : 10 fonctions (Uy et al., 2011)
- Keijzer: 15 functions (Keijzer, 2003)
- Pagie: 1 function (Pagie, 1997)
- Vladislavleva : 8 fonctions (Vladislavleva, 2009)

Comparison with state-of-the-art methods

- Grammatical Evolution (GE): without updating the grammar
- Probabilistic Model Building Genetic Programming (GB-LGP): updating the grammar according to the proportion of rules present in the best individuals

Results

- A benchmark discarded
- Bilateral Mann-Whitney U-test: best score on 22 of 33 benchmarks
- Lower average MSEs
- More Expressions Discovered Accurately

Méthode	U test	EQM moyenne	# solutions exactes découvertes
EG	+3/ ~ 5/ - 25	1,7	0
GB-LGP	+1 / ~ 3 / - 29	11,4	0 à 7
RBG2-SR	+22/ ~ 7/ - 4	6.09×10^{-1}	4 à 14

Comparison of EQM scores, U-test and number of exact functions discovered on 33 benchmarks (30 learnings)

Autres évaluations

- Définition de l'état étudié par ablation

$$s_h = (a_h^{past}, a_h^{parent}, a_h^{siblings}, d_h, \sigma_h, m_h, \eta_h)$$

- Meilleur compromis erreur-complexité sur le jeu de données Airfoil

Objectives

Preliminary issues

- How can implicit knowledge be integrated into learning?
- Is it possible to reduce the number of user interactions?
- What method should be used to comply with the four industrial constraints?

Selected direction

- Learning on user preferences
- Switching between the REINFORCE algorithm and the use of preferences
- Compliance with the four constraints



Algorithm description

Learning from human preferences on pairs of symbolic expressions

$$f_1 > f_2, (f_1, f_2) \sim \pi_\theta$$

3 strategies

- Preferences sorted into 3 categories (Kuhlman *et al.*, 2018)
- Preferences on pairs (Christiano *et al.*, 2017)
- Direct suggestion for solutions

Objective function

$$J_\theta = \mathbb{E}_{\substack{(f_1, f_2) \sim \pi_\theta \\ R(f_1) > R(f_2)}} [\log(P_\theta(f_1))(R(f_1)) - \log(P_\theta(f_2))(R(f_2)) | R(f_{i, i \in \{1, 2\}}) > R_\varepsilon]$$

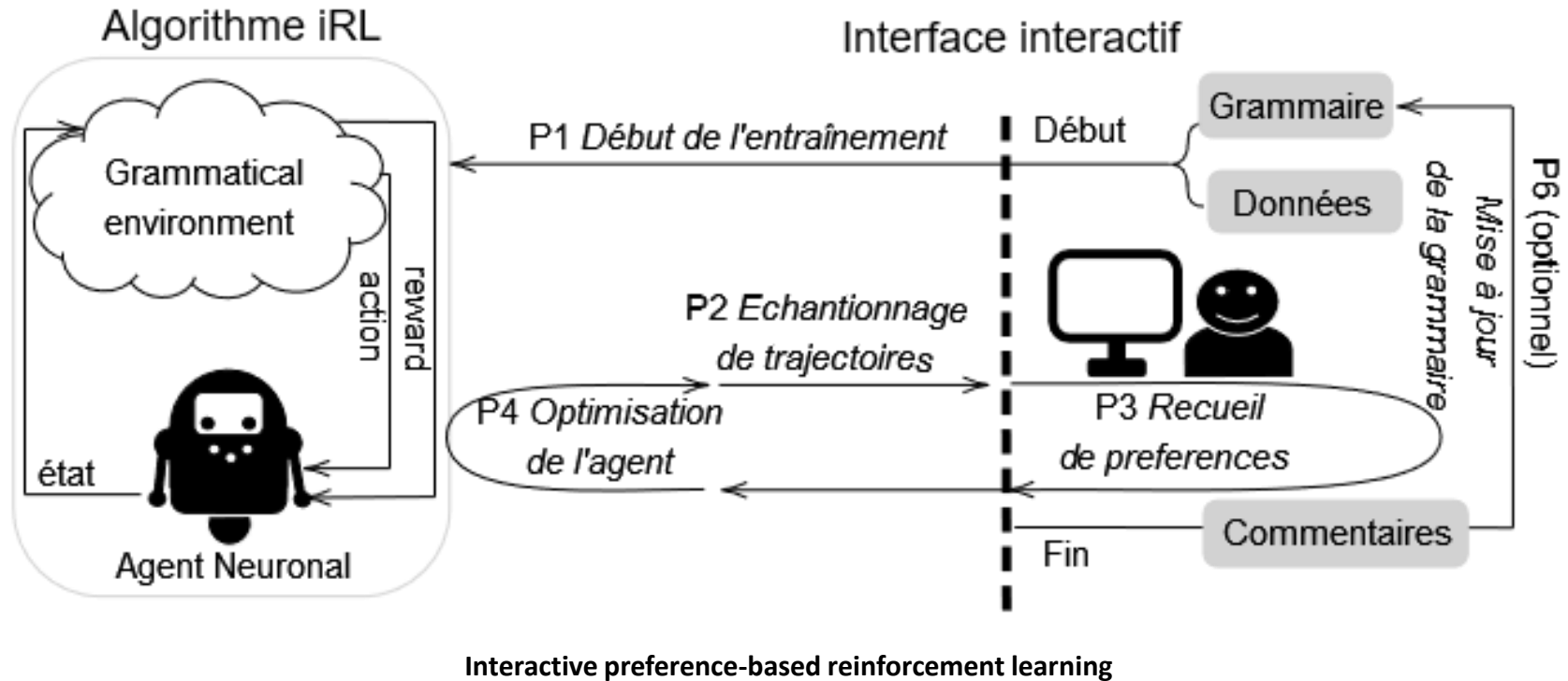
Alternate use of objectives with/without interaction

Wirth, C., Akrou, R., Neumann, G., Fürnkranz, J. et al. (2017). A survey of preference-based reinforcement learning methods. *Journal of Machine Learning Research*, 18(136):1–46.

Christiano, P. F., Leike, J., Brown, T. B., Martic, M., Legg, S. et al. Amodio, D. (2017). Deep Reinforcement Learning from Human Preferences. In *Advances in Neural Information Processing Systems*, volume 30, pages 4299–4307

Kuhlman, C., Valkenburg, M. V., Doherty, D., Nurbekova, M., Deva, G., Phyto, Z., Rundensteiner, E. A. et al. Harrison, L. (2018). Preference-driven Interactive Ranking System for Personalized Decision Support. In *Proceedings of the 27th ACM International Conference on Information and Knowledge Management, (CIKM 2018)*, pages 1931–1934.

Platform Overview



Applications

Symbolic regression benchmark (Uy et al., 2011):

- The target symbolic expression is known to the research team but not to the user
- Visual and score-based exploration
- A priori knowledge (or not) of the solution

Application to power system :

- Symbolic expression exact target unknown
- Exploratory task, representative of the industrial objective
- Data simulated with Grid2Op * library on an IEEE14 network

Tab 1 – Categorical Preferences

VISUALIZE EXPRESSIONS

Reinforcement Based Grammar Guided Symbolic Regression with Preference Learning

NEW TRAINING

Categorical preferences	Preference pairs	Solution suggestion
Best expressions Selection by filter (top solutions) All remaining String to select APPLY SELECTION × $2 \cdot x_0 \cdot (x_0 + 1)$ (score 0.692) × $-x_0^{**2} + \exp(2 \cdot x_0)$ (score 0.616) × $(x_0 + 1)^{**2}$ (score 0.541) × $\exp(2 \cdot x_0)$ (score 0.475) × $\exp(x_0^{**2} + x_0)$ (score 0.437) × $2 \cdot x_0 + 1$ (score 0.396) × $x_0^{**2} \cdot (x_0^{**2} + 3 \cdot x_0) + x_0$ (score 0.392) × $\exp(x_0)$ (score 0.342) × $x_0^{**2} + x_0 + 1$ (score 0.339) × $x_0^{**2} + \exp(2 \cdot x_0)$ (score 0.303) × $x_0^{**2} \cdot (x_0 + 1)$ (score 0.296) × $x_0 + 1$ (score 0.282) × $\log(\exp(x_0 + 1))$ (score 0.282) × $x_0^{**3} + x_0$ (score 0.26) × $2 \cdot x_0^{**3}$ (score 0.258) × $2 \cdot x_0$ (score 0.254) × $3 \cdot x_0$ (score 0.245) × $2 \cdot x_0^{**2}$ (score 0.236) × $\log(\exp(x_0))$ (score 0.212) × x_0 (score 0.212) × $-x_0 + \exp(x_0)$ (score 0.209) × x_0^{**3} (score 0.207) × $\exp(x_0^{**2})$ (score 0.206) × $-x_0^{**2} + \exp(x_0^{**2})$ (score 0.202)	Average expressions Selection by filter (middle solutions) Select filter type String to select APPLY SELECTION Select...	Bad expressions Selection by filter (low solutions) Contains sin cos APPLY SELECTION × $x_0^{**2} + x_0 + \sin(\sin(x_0))$ (score 0.404) × $\exp(x_0^{**2}) + \sin(\sin(\sin(x_0)))$ (score 0.305) × $\exp(\sin(x_0))$ (score 0.302) × $x_0 + \sin(\sin(x_0^{**2}))$ (score 0.288) × $\exp(x_0^{**2}) \cdot \sin(2 \cdot x_0^{**3})$ (score 0.284) × $(x_0 + 1) \cdot \sin(x_0)$ (score 0.28) × $(x_0 + 1) \cdot \sin(x_0^{**2})$ (score 0.269) × $x_0^{**4} + x_0 \cdot \sin(\cos(x_0))$ (score 0.254) × $x_0 \cdot \exp(x_0^{**3}) \cdot \cos(x_0)$ (score 0.252) × $x_0 + \sin(\sin(x_0^{**2} / (x_0 + 1)))$ (score 0.243) × $x_0 + (\sin(x_0^{**2}) + \exp(-x_0^{**2})) \cdot \sin(\exp(x_0^{**2})) / \cos(x_0^{**2}) + 1$ (score 0.234) × $x_0^{**2} \cdot \exp(\cos(x_0))$ (score 0.225)

Tab 2 – Preference Pairs

id	Expression	Reward
245	$2 \cdot x_0 \cdot (x_0 + 1)$	0.692
853	$-x_0^{**2} + \exp(2 \cdot x_0)$	0.616
149	$(x_0 + 1)^{**2}$	0.541
985	$\exp(2 \cdot x_0)$	0.475
155	$\exp(x_0^{**2} + x_0)$	0.437
954	$x_0^{**2} + x_0 + \sin(\sin(x_0))$	0.404
711	$2 \cdot x_0 + 1$	0.396
145	$x_0^{**2} \cdot (x_0^{**2} + 3 \cdot x_0) + x_0$	0.392
573	$\exp(x_0)$	0.342
747	$x_0^{**2} + x_0 + 1$	0.339
800	$\exp(x_0^{**2}) + \sin(\sin(\sin(x_0)))$	0.305
697	$x_0^{**2} + \exp(2 \cdot x_0)$	0.303
783	$\exp(\sin(x_0))$	0.302
257	$x_0^{**2} \cdot (x_0 + 1)$	0.296
115	$x_0 + \sin(\sin(x_0^{**2}))$	0.288
846	$\exp(x_0^{**2}) \cdot \sin(2 \cdot x_0^{**3})$	0.284
753	$x_0 + 1$	0.282
443	$\log(\exp(x_0 + 1))$	0.282
870	$(x_0 + 1) \cdot \sin(x_0)$	0.28
7	$(x_0 + 1) \cdot \sin(x_0^{**2})$	0.269
585	$x_0^{**3} + x_0$	0.26
199	$2 \cdot x_0^{**3}$	0.258
3	$2 \cdot x_0$	0.254
342	$x_0^{**4} + x_0 \cdot \sin(\cos(x_0))$	0.254
253	$x_0 \cdot \exp(x_0^{**3}) \cdot \cos(x_0)$	0.252
884	$3 \cdot x_0$	0.245
699	$x_0 + \sin(\sin(x_0^{**2} / (x_0 + 1)))$	0.243



Tab 3 – Suggestion of expressions

[VISUALIZE EXPRESSIONS](#)

Reinforcement Based Grammar Guided Symbolic Regression with Preference Learning

[NEW TRAINING](#)

Categorical preferences	Preference pairs	Solution suggestion
Choose an expression to compare with 2*x0 + 1 (score 0.396) ✕ Suggest an expression (x[:, 0] + (x[:, 0] <2_args_op> <f>)) Select... + - * /		Grammar reminder <f> ::= (<f> <2_args_op> <f>) (<var_and_1> <2_args_op_with_1> <var_and_1>) <1_arg_op> (<f>) <varname> <varname> ::= (- x[:, <varidx>]) x[:, <varidx>] <var_and_1> ::= (- x[:, <varidx>]) x[:, <varidx>] 1 <2_args_op_with_1> ::= + * <2_args_op> ::= + - * / <1_arg_op> ::= np.cos np.sin np.exp np.log <varidx> ::= 0

VALIDATE AND CONTINUE

Preliminary interaction

User Profile

- User U1: No knowledge of the form of the function
- User U2: Knowledge of the polynomial form of the function
- User U3: Knowledge of the exact form of the function

Utilisateur	Nombre d'interactions	Retrouve la solution exacte
U1	15	✗
U2	21	✗
U3	16 et 26	✓

4 common strategies used by users

- Prefer expressions with the highest score
- Prefer the best performer most of the time (with a random probability $p \in \{0.2, 0.5, 0.8\}$)
- Avoid cos/sin operations
- Avoid cos/sin/exp operations

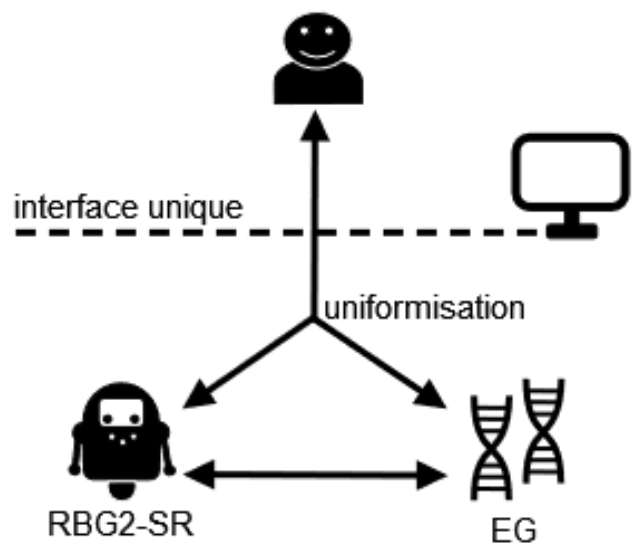
Results of the simulations

- Error reduced by an order of magnitude with QR1 interactivity: it is possible to reduce the error by preferences
- Optimal interaction frequency of 5 QR2: it is possible to solicit the user only at certain time steps

Fréquence d'interaction	EQM moyenne ($\pm$ écart-type)	R2 moyenne ($\pm$ écart-type)
Référence	$1,62 \times 10^{-2} (\pm 1,6 \times 10^{-2})$	$9,92 \times 10^{-1} (\pm 8,2 \times 10^{-3})$
1	$6,57 \times 10^{-2} (\pm 8,91 \times 10^{-2})$	$9,67 \times 10^{-1} (\pm 4,45 \times 10^{-2})$
2	$6,14 \times 10^{-2} (\pm 2,09 \times 10^{-2})$	$9,69 \times 10^{-1} (\pm 1,04 \times 10^{-1})$
5	$7,21 \times 10^{-3} (\pm 8,93 \times 10^{-2})$	$9,96 \times 10^{-1} (\pm 4,46 \times 10^{-3})$
10	$1,14 \times 10^{-2} (\pm 1,79 \times 10^{-2})$	$9,94 \times 10^{-1} (\pm 8,92 \times 10^{-3})$
15	$8,56 \times 10^{-3} (\pm 1,03 \times 10^{-2})$	$9,96 \times 10^{-1} (\pm 5,12 \times 10^{-3})$
20	$1,13 \times 10^{-2} (\pm 1,71 \times 10^{-2})$	$9,94 \times 10^{-1} (\pm 8,57 \times 10^{-3})$

Comparaison des scores d'EQM et R2 avec et sans (baseline) interactivité sur les données de la fonction f_{nguyen_4} (10 apprentissages)

Interactivity, RBG2-SR and EG



Evaluation of function f_{nguyen_4}

Algorithme	Fréquence d'interaction	EQM moyenne ($\pm$ écart-type)	R2 moyenne ($\pm$ écart-type)
RBG2-SR	-	$1.62 \times 10^{-2} (\pm 1.6 \times 10^{-2})$	$9.92 \times 10^{-1} (\pm 8.2 \times 10^{-3})$
EG	-	$1.48 \times 10^{-2} (\pm 1.6 \times 10^{-2})$	$9.93 \times 10^{-1} (\pm 6.5 \times 10^{-3})$
iRBG2-SR	5	$7.21 \times 10^{-3} (\pm 8.93 \times 10^{-3})$	$9.96 \times 10^{-1} (\pm 4.46 \times 10^{-3})$
	15	$8.56 \times 10^{-3} (\pm 1.03 \times 10^{-2})$	$9.96 \times 10^{-1} (\pm 5.12 \times 10^{-3})$
RBG2-SR + EG	-	$1.24 \times 10^{-2} (\pm 1.56 \times 10^{-2})$	$9.94 \times 10^{-1} (\pm 7.79 \times 10^{-3})$
i(RBG2-SR + EG)	5	$1.98 \times 10^{-2} (\pm 4.75 \times 10^{-2})$	$9.90 \times 10^{-1} (\pm 2.37 \times 10^{-2})$
	15	$1.11 \times 10^{-2} (\pm 1.47 \times 10^{-2})$	$9.94 \times 10^{-1} (\pm 6.98 \times 10^{-3})$
	25	$1.12 \times 10^{-2} (\pm 1.78 \times 10^{-2})$	$9.94 \times 10^{-1} (\pm 8.90 \times 10^{-3})$

Comparaison scores d'EQM et R2 (10 learning)

Assessment of this experience

Improved search in grammatical space through interactivity



Consideration of implicit knowledge



Decrease in error compared to the RBG2-SR approach



Reduction in the number of user requests

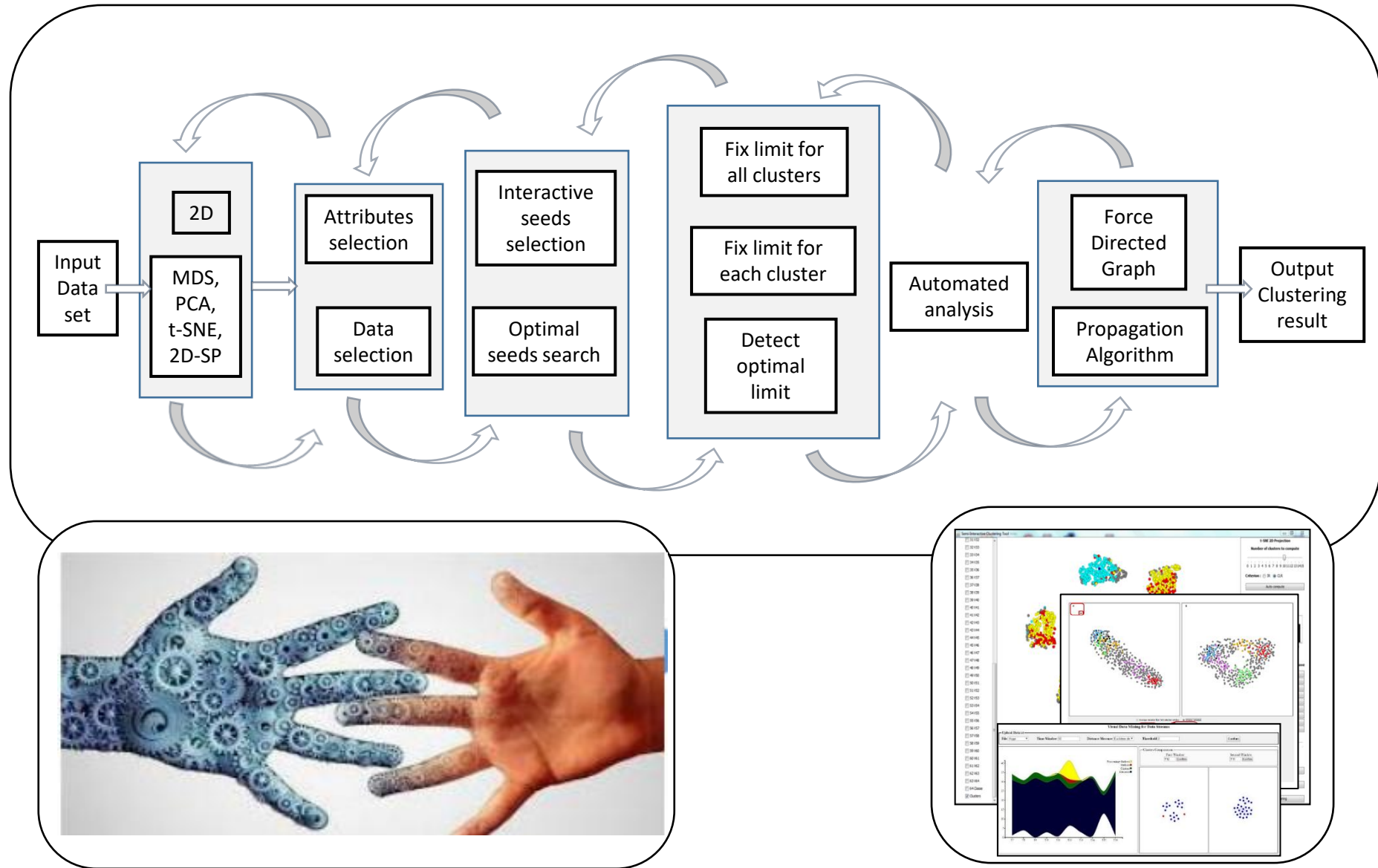
Preliminary results on a single function

- To be replicated on new data
 - Other Functions
 - Power grid data
 - Scaling up (larger network, real data, ...)
- Test new user behaviors
- Evaluate on a larger panel of users

5

Conclusion and Challenges

Conclusion



Answers

How to integrate the user constraints in the process?

Visual Data Mining

- Evaluation update through the clusters' modification

Interactive Machine Learning

- Grammar evaluation and updating

How to better guide the user in the process ?

Visual analytics

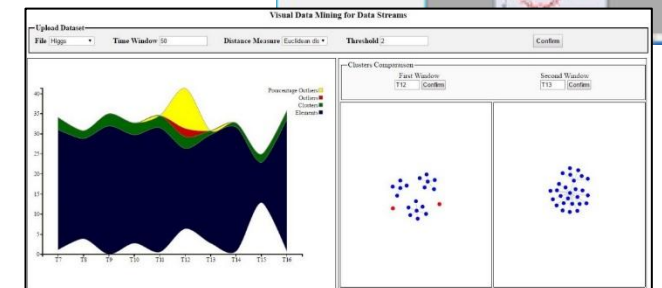
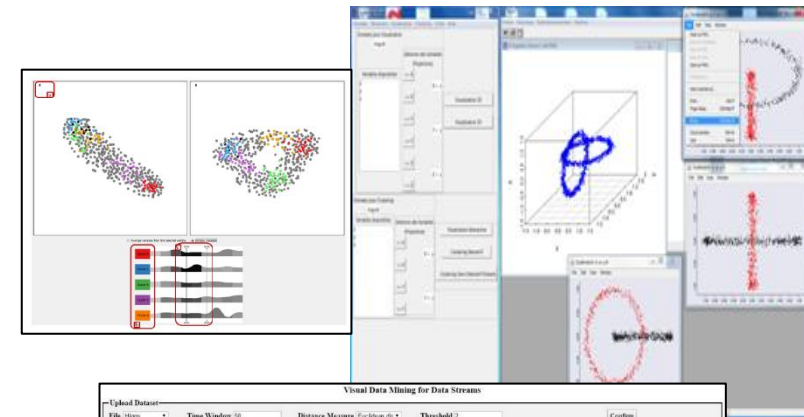
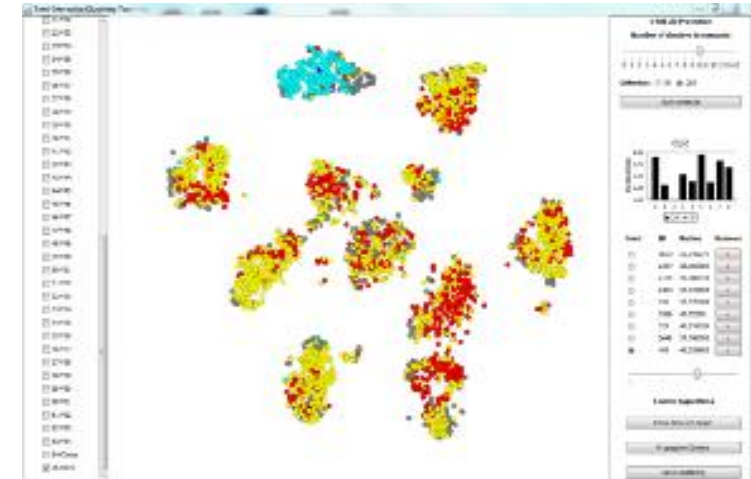
- Data stream visualization:
 - Change detection
 - Selected window exploration
 - Optimal subspaces to describe the data stream
- Select subspaces and visualize the associated themeriver

Visual Data Mining

- Evaluation update a each cluster modification
- Evaluation criterion of each extracted cluster

Interactive Machine Learning

- Extract interpretable explanation of a network constraint



How to avoid the visualization bias?

Cooperative approaches: automatic, visual & interactives

Challenges

Track 1: How to integrate the user in the process: exploration & processing

Challenge 1

Evaluation in visual data mining

- How to detect artefacts /How to evaluate the visualizations : subspace projections

Challenge 2

Interactive machine learning

- User interactions learning (IA) : model the user behavior
- How avoid the visual perception bias

Challenge 3

Semi-interactive approaches

- Cooperatives approaches automatics & visualizations: explanations, interpretability

Track 2: Massive and temporal data

Challenge 1

Visual data mining

- How to use all semi-interactive approaches advantages

Challenge 2

Data and associated difficulties

- times series, spatio-temporal data, symbolic data, complex data
- Different data: images, Graphs, omics, bioscience

