Explainable Machine Learning using Formal Concept Analysis

Mathematics and Statistics in Machine Learning

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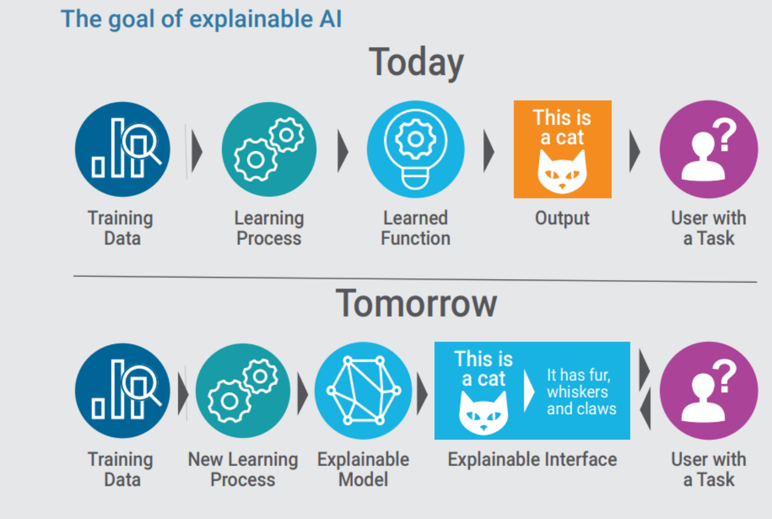
Introduction and motivation

- A Machine Learning or a Deep Learning model learns patterns from training data and predicts an outcome for an instance or maps an instance to a class.
- In a black box model:
  - The learned data patterns are not evident.
  - The reasons why a model decided an outcome are not clear.
- In order to make these models trustworthy and therefore acceptable, it is necessary to augment the model with **explanations** of its decisions.

  XAI is born.



https://www.datanami.com/2018/05/30/opening-up-black-boxes-with-explainable-ai/

How to *explain*?

The main natural strategies used to address the problem of XAI:

- Directly using interpretable models (decision trees, logic rules. . .).
- *Post hoc* explaining, by argumenting/explaining the result once it is obtained. Usually, local explanations.

Some remarks:

- A good explanation has to be simple, easy to understand, and faithful (accurate), conveying the true cause of the event.
- The design of representations that support the articulation of the explanations is required.

Goal

To present a language (Formal Concept Analysis) that incorporates syntax (symbolic representation) and semantics, allowing to reason and perform inference.

Foundations of Formal Concept Analysis

- Formal **context**: $\mathbb{K} = (G, M, I)$.

	small	medium	large	near	far	moon	no_moon
Mercury	×			×			×
Venus	×			×			×
Earth	×			×		×	
Mars	×			×		×	
Jupiter			×		×	×	
Saturn			×		×	×	
Uranus		×			×	×	
Neptune		×			×	×	
Pluto	×				×	×	

Table 1: G is the set of objects (planets), M is the set of the attributes or properties, and I is the incidence relationship.

- Derivation operators: for $A \subseteq G, B \subseteq M$, define

$$A^{\uparrow} = \{m \in M : gIm \, \forall g \in A\}$$

$$B^{\downarrow} = \{g \in G : gIm \, \forall m \in B\}$$

For instance:

$$\{\text{Venus}, \text{Mars}\}^{\uparrow} = \{\text{small}, \text{near}\}$$

$$\{\text{far}, \text{moon}\}^{\downarrow} = \{\text{Jupiter}, \text{Saturn}, \text{Uranus}, \text{Neptune}, \text{Pluto}\}$$

They form a **Galois connection**, so their composition is a **closure operator**.

$$\{\text{no\_moon}\}^{\downarrow\uparrow} = \{\text{small}, \text{near}, \text{no\_moon}\}$$

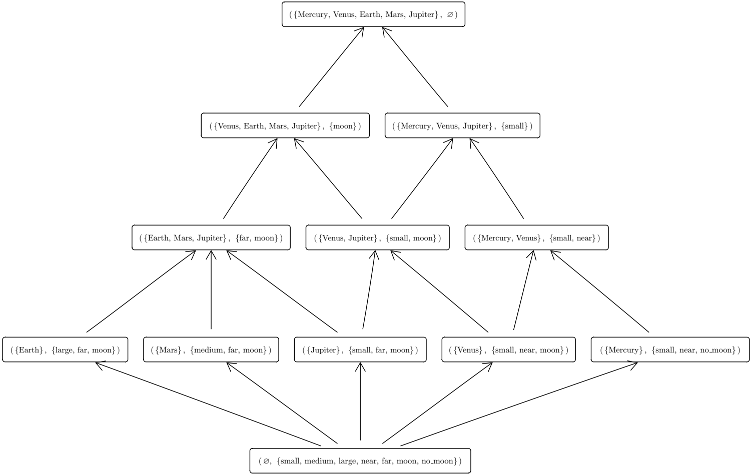
All planets with *no moon* are also *small* and *near* the Sun, and share no other attributes.

- (Formal) **Concept**: $(A, B) \in 2^G \times 2^M$ such that $A^\uparrow = B$ and $B^\downarrow = A$.

	small	medium	large	near	far	moon	no_moon
Mercury	×			×			×
Venus	×			×			×
Earth	×			×		×	
Mars	×			×		×	
Jupiter			×		×	×	
Saturn			×		×	×	
Uranus		×			×	×	
Neptune		×			×	×	
Pluto	×				×	×	

Table 2: A maximal rectangle is a formal concept

- The $\subseteq$ order in 2^G can be extended to a partial order in the set of concepts: this gives the **concept lattice**.



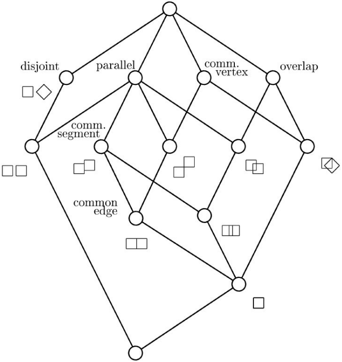
- **Attribute implications** are formulas $A \Rightarrow B$ with $A, B \subseteq M$ whose meaning is "all objects that have the attributes in A, also have the attributes in B".

$$
\begin{array}{rrcl}
1: & \{\text{no\_moon}\} & \Rightarrow & \{\text{small}, \text{near}\} \\
2: & \{\text{far}\} & \Rightarrow & \{\text{moon}\} \\
3: & \{\text{near}\} & \Rightarrow & \{\text{small}\} \\
4: & \{\text{large}\} & \Rightarrow & \{\text{far}, \text{moon}\} \\
5: & \{\text{medium}\} & \Rightarrow & \{\text{far}, \text{moon}\} \\
6: & \{\text{medium}, \text{large}, \text{far}, \text{moon}\} & \Rightarrow & \{\text{small}, \text{near}, \text{no\_moon}\} \\
7: & \{\text{small}, \text{near}, \text{moon}, \text{no\_moon}\} & \Rightarrow & \{\text{medium}, \text{large}, \text{far}\} \\
8: & \{\text{small}, \text{near}, \text{far}, \text{moon}\} & \Rightarrow & \{\text{medium}, \text{large}, \text{no\_moon}\} \\
9: & \{\text{small}, \text{large}, \text{far}, \text{moon}\} & \Rightarrow & \{\text{medium}, \text{near}, \text{no\_moon}\} \\
10: & \{\text{small}, \text{medium}, \text{far}, \text{moon}\} & \Rightarrow & \{\text{large}, \text{near}, \text{no\_moon}\}
\end{array}
$$

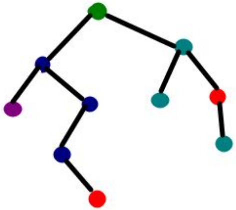
Remarks

We can use logic tools (e.g. Armstrong's rules) to perform inference.
With FCA, we have the syntax and the semantics to represent explanations and methods (algorithms) to extract and reason with them.

Use cases I. Ensembles of decision trees



Concept Lattice



Decision Tree

Dudyrev, E., & Kuznetsov, S. O. (2021). Summation of Decision Trees. In FCA4AI@ IJCAI (pp. 99-104).

Belohlavek, R., et al. (2009). Inducing decision trees via concept lattices. Int. J. of general systems, 38(4), 455-467.

The problem arises when using ensembles of decision trees (*boosting*, random forests...):

- Each tree represents only a part of the variables (attributes)
- There may be missing data

The solutions so-far:

1. Build a **large decision semilattice** able to capture and mimic the ensemble (reproducing faithfully its predictions).

   Dudyrev, E., & Kuznetsov, S. O. (2021). Summation of Decision Trees. In FCA4AI@ IJCAI (pp. 99-104).

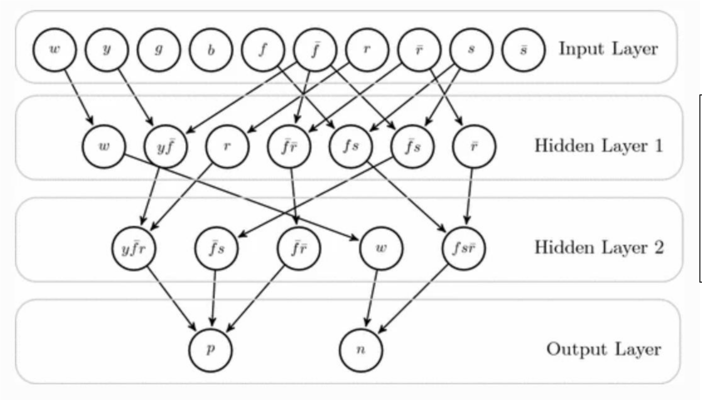
2. Generate **conceptual views** on the ensemble: several lattices that capture different standpoints, such as local and global properties.

   Hanika, T., & Hirth, J. (2023). Conceptual views on tree ensemble classifiers. International Journal of Approximate Reasoning, 159, 108930.

FCA gives us all the tools to interpret and manage these structures.

Use cases II. Deep learning and neural networks.

Kuznetsov, S. O., Makhazhanov, N., & Ushakov, M. (2017). On neural network architecture based on concept lattices. In ISMIS 2017, Warsaw, Poland (pp. 653-663).



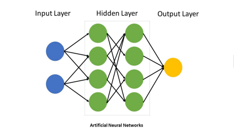
All attributes

Connections as in the concept lattice

One neuron per class

Hasanah, N., Imai, S., & Nobuhara, H. (2010). Application of formal concept analysis for rule mining in artificial neural networks. In SCIS & ISIS SCIS & ISIS 2010 (pp. 670-675).

time	n.risk	n.event	survival	std.err	lower 95% CI	upper 95% CI
5	23	2	0.913	0.0588	0.8049	1
8	21	2	0.8261	0.079	0.6848	0.996
9	19	1	0.7826	0.086	0.631	0.971
12	18	1	0.7391	0.0916	0.5798	0.942
13	17	1	0.6957	0.0959	0.5309	0.912
18	14	1	0.646	0.1011	0.4753	0.878
23	13	2	0.5466	0.1073	0.3721	0.803
27	11	1	0.4969	0.1084	0.324	0.762
30	9	1	0.4417	0.1095	0.2717	0.718
31	8	1	0.3865	0.1089	0.2225	0.671
33	7	1	0.3313	0.1064	0.1765	0.622
34	6	1	0.2761	0.102	0.1338	0.569
43	5	1	0.2208	0.0954	0.0947	0.515
45	4	1	0.1656	0.086	0.0598	0.458
48	2	1	0.0828	0.0727	0.0148	0.462



TRAINING

time	n.risk	n.event	survival	std.err	lower 95% CI	upper 95% CI
5	23	2	0.913	0.0588	0.8049	1
8	21	2	0.8261	0.079	0.6848	0.996
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48	2	1	0.0828	0.0727	0.0148	0.462

USE TRAINED NETWORK TO BUILD FORMAL CONTEXT

	≤ 36	≤ 48	≤ 60	≤ 42	≤ 60	≤ 78	≤ 53	≤ 72	≤ 91
S1			X			X			X
S2			X			X			X
S3		X			X				X
S4			X	X				X	
S5		X				X		X	
S6		X			X			X	
S7		X		X					X
S8		X		X				X	
S9	X			X			X		
S10	X				X		X		

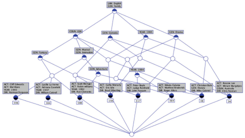
$$
\begin{aligned}
\{\text{no\_moon}\} &\Rightarrow \{\text{small}, \text{near}\} \\
\{\text{far}\} &\Rightarrow \{\text{moon}\} \\
\{\text{near}\} &\Rightarrow \{\text{small}\} \\
\{\text{large}\} &\Rightarrow \{\text{far}, \text{moon}\} \\
\{\text{medium}\} &\Rightarrow \{\text{far}, \text{moon}\}
\end{aligned}
$$

Use cases III. Recommendation systems.

Diaz-Agudo, B., et al. (2019). Explanation of recommenders using formal concept analysis. In ICCBR 2019 (pp. 33-48).

Movie Id.	Movie title	Director	Genre	Actors	Year	Rating
594	Snow White and the Seven Dwarfs	William Cottrell	Animation, Family, Fantasy, Musical	Adriana Caselotti Lucille La Verne	1937	5.0
596	Pinocchio	Norman Ferguson	Animation, Family, Fantasy, Musical	Mel Blanc Cliff Edwards	1940	4.5
588	Aladdin	Ron Clements	Adventure, Animation, Comedy, Family, Fantasy, Musical, Romance	Robin Williams Scott Weinger	1992	5.0
364	The Lion King	Roger Allers	Adventure, Animation, Drama, Family, Musical	Matthew Broderick Niketa Calame	1994	5.0
317	The Santa Clause	John Pasquin	Comedy, Drama, Family, Fantasy	Judge Reinhold Peter Boyle	1994	3.5
34	Babe	Chris Noonan	Comedy, Drama, Family	Miriam Margolyes Roscoe Lee Browne	1995	4.0
158	Casper	Brad Silberling	Comedy, Family, Fantasy	Eric Idle Cathy Moriarty	1995	3.0
48	Pocahontas	Mike Gabriel	Adventure, Animation, Drama, Family, History, Musical, Romance	Christian BaleIrene Bedard	1995	5.0

	DIRECTOR						GENRE									ACTORS												YEAR	
id	John Lasseter	Kevin Smith	Mel Gibson	Michael Caton-Jones	Peter Farrelly	Tim Burton	Adventure	Animation	Biography	Comedy	Drama	Family	Fantasy	History	War	Eric Stoltz	James Robinson	Jason Mewes	Jeff Anderson	Jim Varney	Johnny Depp	Lauren Holly	Liam Neeson	Martin Landau	Mhairi Calvey	Teri Garr	Tom Hanks	1994	1995
223		X								X								X	X									X	
231					X					X												X				X		X	
235						X			X	X	X										X			X				X	
110			X						X		X			X	X		X								X				X
151				X			X		X							X							X						X
1	X						X	X		X		X	X							X							X		X



GEN: Comedy → GEN: Family, LAN: English
"All your high scored movies that have GEN: Drama have also GEN: Family and LAN: English"
GEN: Animation, GEN: Musical → COUN: USA
"All your high scored movies that have GEN: Animation and GEN: Musical have also COUN: USA"
GEN: Adventure → *GEN: Animation, GEN: Musical*
"All your high scored movies that have GEN: Adventure *have also GEN: Animation and GEN: Musical"*
GEN: Romance → GEN: Adventure
"All your high scored movies that have GEN: Romance have also GEN: Adventure"
GEN: Drama → GEN: Family
"All your high scored movies that have GEN: Drama have also GEN: Family"
...

USER MODELLING

EXPLANATIONS GENERATION

"This movie is recommended to you because of the GEN: Comedy property" (property-style)

"The recommended movie shares the property GEN: Comedy with 588, 317, 34, 158" (Extent of concept) (item-style)

"The recommended movie shares the property YEAR: 1995 with 34, 48, 158" (Extent of concept) (item-style)

Some tools

https://upriss.github.io/fca/fcasoftware.html

Formal Concept Analysis Software

FCA Topics page on Github

Downloadable software:

- Tockit, Score, ToscanaJ, Tupleware at sourceforge, (Manual, etc)
- ConExp Concept Explorer (Java) at sourceforge (the source code can be found in the cvs). Apparently this software does not work with OpenJDK.
- ConExp FX a partial reimplementation of ConExp by Francesco Kriegel
- ConExp-NG, packaged release download, reimplementation of ConExp by Robert Jäschke's students, (uses FcaLib), Fcatools
- Conexp-clj by Daniel Borchmann
- Galicia
- FcaStone format conversion software and command-line lattice generation
- Camelis (Logical Information System based on FCA)
- Christian Lindig's Colibri (Java or ML), Concepts (in C) its github clone
- concepts.py Dominik Endres' implementation in Python.
- Python FCA Tool (developed at HSE, Russia). Python code for exploration developed by A. Revenko: MIW.
- Python implementation: concepts by S. Bank
- GALACTIC. A set of python3 packages for studying Formal Concept Analysis by K. Bertet, C. Demko and others.
- Coron System (data mining software)
- Csx2tikz (XSLT conversion from ToscanaJ format to tikz/LaTeX)
- Eclipse's Relational Concept Analysis
- FCA4J (A jar containing a set of Java algorithms to compute concept lattice, Iceberg Lattice, AOC-poset, Duquenne-Guigues Basis)
- FCA algorithms
- FcaBedrock (tool for creating contexts from csv files)
- fcaR An FCA package written in R by D. Lopez and A. Mora
- FCART (Link: https://cs.hse.ru/en/ai/issa/proj_fcart) Formal Concept Analysis Research Toolbox (for PC).
- Griff by R. J. Cole
- In-Close (fast Formal Concept miner)
- LaTeX style file for FCA
- Lattice Miner
- Lattice Navigator (lattice visualisation and context editing, written in C#)
- OpenFCA (using C, .Net, Flash), Video demo
- QDFCA (command-line filter in Ruby)
- RCAExplore for Relational Concept Analysis.

Limitations of FCA??

It seems that FCA only deals with binary tabular data.
Scalings are procedures to transform *many-valued* contexts into binary form (back and forth).
But there are extensions to:

- Numerical intervals.
- **Fuzzy** values.
- Negative attributes (absence of properties) and missing information.

Fuzzy FCA can cope with imprecise or vague information, what helps in the modelling process for the explanation.

Conclusions

- We have presented the principal uses of FCA in the explainability of different ML techniques.
- FCA is able to represent the knowledge inside a dataset in two ways:
  - The concept lattice, which enables a hierarchical view of the dependencies
  - Implicational systems that, with the help of logic, allow us to infer and deduce new information
- These two representations are expressive enough to model and then to manage and represent the possible explanations of other less explainable ML techniques.
- The different extensions of FCA will further foster the ability to generate explanations (particularly in DL).

References

- Ganter, B., and S. Obiedkov (2016). *Conceptual Exploration.* Springer Berlin Heidelberg.
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