Human in the loop for modelling food and biological systems: a novel perspective coupling artificial intelligence and life science

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HUMAN IN THE LOOP FOR MODELLING FOOD AND BIOLOGICAL SYSTEMS: A NOVEL PERSPECTIVE COUPLING ARTIFICIAL INTELLIGENCE AND LIFE SCIENCE

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KEYWORDS
Human expertise, modelling, interactive learning, agri-food systems, visualization, optimization, machine learning

ABSTRACT
Since centuries, agriculture, food and biological systems are strongly linked to human expertise, albeit such knowledge has been capitalized and shared often at a local level, only. Since the beginning of the last century, swept away by productivism, modern agriculture and food production have put cumulated human knowledge aside. Facing new challenges like sustainability in a changing context, holistic approaches cannot be managed “manually” ab initio and there is a clear need for computing decision-support tools to tackle these new issues. Moreover, new approaches should be built centred on humans and for humans. The heart of our purpose is to shift the focus again on human and local expertise, guided by powerful computing interactive systems.

INTRODUCTION

Since centuries, agriculture, food and biological systems are strongly linked to human expertise, albeit such knowledge has been capitalized and shared often at a local level, only. Scientific and technical experts have tried to study complex food and biological systems for a while. Generally lot of heterogeneous experiments have been achieved in different conditions and statistical analysis allows extracting various characteristic features leading to a local or partial understanding of the system in the mind of the expert. Nevertheless the task is far more complex if a global understanding of those systems is needed, even if experts have sometimes partial intuitions on it (Perrot et al., 2011))(Van Mil et al., 2014)(Perrot et al., 2016). The heart of our purpose in this paper is to shift the focus on human, intuitions and local expertise, guided by powerful computing interactive systems.

If we refers to the cognitive human behavior, as it is described in the community of intelligent systems (Lucentini and Goodwin, 2015), a point widely studied is the cognitive architectures and the way that data is captured from the environment, stored and further processed. Basically, cognitive architectures refer to two paradigms: symbolic and sub-symbolic. It gives the possibility to infer, for some aspects, like experts decision for process management, data exploration, fault tolerance, learning, systematicity and so on, how the human behavior will be. It is just a question of analyzing if an architecture is based on a symbolic, sub-symbolic or mixed approach.
Symbols, as described by (Lucentini and Goodwin, 2015), “are entities which make reference to another objects by means of a totally arbitrary convention, a law or a class. They are a widely used form of representation, for example the word car is a symbol for a real car, because there is a convention that the word car in a specific language refers to those types of elements”. The sub-symbolic level, is not using symbols as the symbolic one and is more a “bottom-up” approach emerging from neuronal connections, non explicitly conscientize by the experts.

Our challenge for this article is to present experiences led in our laboratory to guide through man machine interactions, the emergence of a model integrating symbolic and sub-symbolic human knowledge. It is dedicated to food and biological complex systems.

HUMAN IN THE LOOP

For our approach, we rely on the ability of experts to create patterns giving them the possibility to reason in an uncertain environments. Indeed, experts, faced with complexity when coping with their dynamic environment and constraints, develop a considerable ability to focus their attention and organize the space of reasoning around dynamic patterns, based more on experience than on rules (Ballester et al., 2008). Such patterns are scripts that embody in an efficient way knowledge of viable stereotyped event sequences. For example, it has been described in (Sicard et al., 2011) applied to a cheese biological ecosystem: the process is represented in the expert's mind in the form of chronological standard change patterns and drift from standard trajectories that lead to defects on the cheese, like bad odours or bacterial contaminations. This mechanism of information aggregation allows the experts to anticipate the appropriate system state to intervene in, and, if needed, to correct early drift trajectories. The experts are thus able to manage a certain amount of complexity in an uncertain environment. In multiscale living biological global systems, patterns are organized in space and time (various land parcels and climatic conditions for example for agronomic problematics such wine, wheat crop..., various space and growth time for living ecosystems for example food, marine or gut ecosystems).

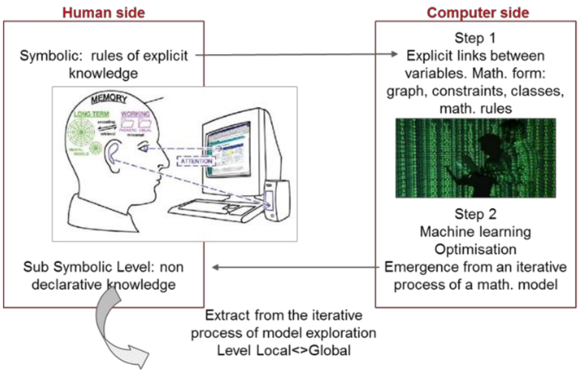

Figure 1: An approach of human integrated in the computing loop. A first step is delivered by the expert from his symbolic knowledge and integrated by the computer side in the form of explicit links, graphs, rules,…A second step emerge from the iterative interaction between human and computer through a model exploration at different level after a computing step of calculus.

One of the efficient coding mechanisms used by experts is the cognitive mechanism of 'chunk' recognition (Chase and Simon, 1973). A 'chunk' is a grouped set of clustered variables, closely related to each other, taken from a situation and associated to each other. Chunks are used to describe a part of a standard trajectory, directly linked to a particular state, which could require to be stabilized or corrected. These variables are acquired through the perceptions of experts. For example, winemakers anticipate the quality of their wine using mental chunks based on their perception of the quality of the soil of a parcel and its localisation, the way the grapevine has been conducted, etc. Nevertheless, chunks are not easy to handle as they are not usually in the form of explicit knowledge and sometimes refer to the subsymbolic level of the expert cognition. As a consequence, very often they are not exploited as functional knowledge to create computational models suitable for decision making. Some of the patterns can be explicit on a graph or in the form of rules. For the subsymbolic ones, our hypothesis is that it can emerge from the exploration of the result of a model if relevant computing tools and visualisation techniques are implemented for man-machine interactions.

We propose a parallel between the approaches of computational cognitive (Sun, 2008)(Mc Clelland, 2009) developed to model human cognition devoted to symbolic and sub-symbolic levels and the computing tools we develop to embed human in the computing loop. From this parallel, the idea is to build a tool able to deal with and integrate those different levels of human knowledge into the loop of modeling. Every simulation model is here a way to embed a part of the human knowledge on a biological system. The challenge of this paper is more precisely to present different studies were the use of computational models in this spirit is developed. It is based on human, machine learning, optimization and visualization. The purpose, more than a compilation of studies is to enhance our vision of "the human in the loop" through different experimentations. We thus focus on the knowledge available at the different level of human cognition. We observe symbolic and sub-symbolic levels and especially the mental patterns the experts have in mind. We exemplify this approach on a series of systems like in cheese ripening process, wheat culture management, wine odor prediction or bacteria freeze drying. Two axes are explored: food and biological systems exploration and food and biological properties

The approach tested and experimented (figure 1) is an approach coupling (1) an algorithm enabling the effective description of the human symbolic knowledge in the form of rules, classes or links between variables or classes (step 1) ;(2) an approach of machine learning including a crucial optimisation step proposing different alternative of representation (step 2) explored iteratively through a visual interface. The idea is to open from this iterative exploration process the door to the sub-symbolic knowledge emergence. Two ingredients are important for that: the way we use optimisation and visualization techniques.

OPTIMISATION AND EMERGENCE

The idea of optimisation takes its roots in the 16th and 17th centuries notion of “modernity”, when philosophers where advertising the issue of becoming “owner and master” of nature (“Discours de la méthode” (Descartes,1637), in a mathematical framework (Galilée (Martin, 2002)). Thanks to modern computation capabilities, managing and predicting natural phenomena becomes more and more a reachable challenge. However optimality, in any domain, raises various fundamental questions, in particular regarding the purpose of optimisation (are we able to address the appropriate issues with the help of modern computational tools?) and the methods (are we able to address the right issues with the right tools?).

A subsidiary question is also: Do we not believe too much in computation? Improvement may be another perspective, more appropriate, in particular for an interactive/iterative process of problem solving involving human knowledge.

In this work, we revisit the use of stochastic optimisation heuristics and in particular Evolutionary Algorithms, exploited in an iterative and interactive context, to better address complex questions. Evolutionary Algorithms (EAs) are stochastic methods that copy, in a very abstract manner, the principles of natural evolution that let a population of individuals be progressively adapted to its environment (Goldberg, 1989). This progression results in an improvement of the fitting of the individuals to its environment, this can be exploited as an optimisation heuristic: an optimal adaptation is reached asymptotically.

An EA considers populations of potential solutions exactly like a natural population of individuals that live, fight, and reproduce, but with a natural environment pressure replaced by an artificial optimization pressure. Reproduction consists of generating new individuals-solutions using the so-called genetic operators that, by analogy with nature, are called mutation if they involve one individual, or crossover if they involve two parent solutions. A fitness function, computed for each individual, is used to drive the selection process, is thus improved, and ultimately optimized by the EA.

In an interactive context, an improvement scheme seems adequate and enough, as the optimisation aim is often not fixed and varies with interactions with experts. Additionally, EA are convenient for building interactive schemes; there is actually a large interest of the community into interactive EA (IEA). Interactions with the optimisation/improvement EA may take place at various levels (interactive evaluation of results, reformulation of optimisation function, modification of current solutions, interactive tuning of the parameters of the algorithm).

VISUALIZATION TECHNIQUES

Visualization is a field of computer science concerned with the creation and study of visual representations of data (Card et al., 1999). It makes use of our powerful visual cortex and wealth of experience to reach insights from data, amplified through human-computer interaction. For a visualization to be interactive, it needs to support human input to control some aspects of the visual display. Additionally, a good interaction response rate needs to be met to ensure real-time perception of task execution.

Visualization can be a valuable asset in the context of modelling. For example, creating robust computational models necessitates tools to explore the behaviour of models and tune their underlying representations, but not only. From our experience visualization can empower modelling by bringing in:

- human-computer interaction methodologies that facilitate the study of the visible and hidden roles humans play in modelling (Lutton et al., 2016);
- more intuitive representations of often complex multiscale models (Chabin et al., 2017). These visualizations can facilitate collaboration between the various stakeholders involved in the modelling process (e.g. data owners, domain experts, modellers, decision makers); and
- interactive tools to explore the behaviour of the constructed models, and ultimately allowing for enrichment and modification (Sacha et al., 2016).

EXPERIENCES OF HUMAN IN THE LOOP:

Food and biological system exploration

Explore to find a camembert-type cheese ripening viable trajectory.

This experiment was led under the frame of a french ANR project (INCALIN) and a FP7 European project (DREAM). The challenge was to work with the experts and a distributed high performance calculation structure to discover relevant viable trajectories of cheese ripening (Sicard et al., 2012). The viability study is achieved on a space dimension of 5: Two control variables: relative humidity and temperature of the ripening chamber; Three state variables: the cheese mass, cheese surface temperature and respiration rco2. The trajectories are considered relevant if the cheese are in a given target of sensory quality at the end of the process of ripening and if the ripening time is reduced.

In a first step (see Step 1, figure 1) explicit knowledge is described by the experts in terms of a constraint set, a subset of the three dimensional state space: cheese mass, cheese surface temperature and respiration level (see article (Sicard et al., 2012)). It can be represented as a tube including all the values in which the state variables should stay at each time. The bound values stem from the experimental limits and the legal norms (viability tube represented figure 2).

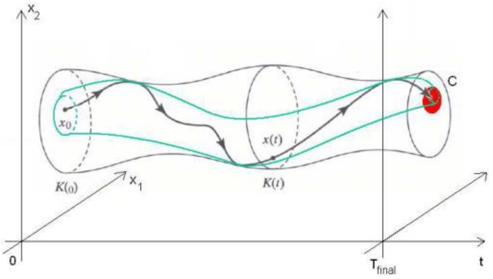

Figure 2: Viability tube of the ripening process of a camembert type cheese (upon Sicard et *al.*, 2009).

In a second step (Step 2, figure 1), 45 654 840 simulations are performed on a computing cluster of calculus and a Pareto front of the results is explored visually by the experts. On the basis of this first exploration, new constraints are proposed, emerging from the visual exploration of the experts, and a new Pareto front is explored and iteratively, till a satisfying solution is found by the experts.

This exploration applied to a cheese ripening process, has led us to find an original viable trajectory for the industry, satisfying the manufacturing constraints while maintaining the quality target for the ripening process. This trajectory has a 8-day ripening time, whereas the standard is 12 days. This trajectory was validated on a ripening pilot. The microbial equilibrium was preserved so as the cheese sensory properties (see figure 3).

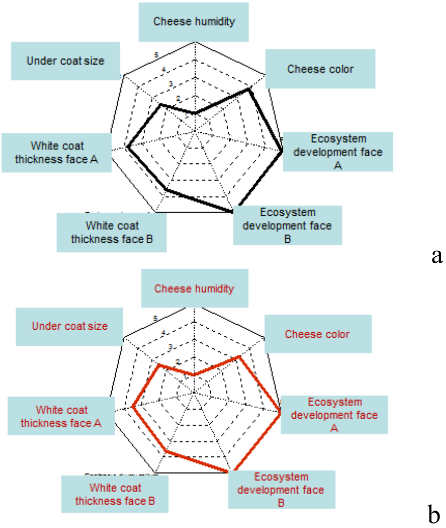

Figure 3: The cheese sensory evaluation after having tested the emergent trajectory following the exploration experiments: -a- in black: cheese sensory evaluation at the end of the ripening process for the classic trajectory (day 12); -b-in red: cheese sensory evaluation at the end of the ripening process for the classic trajectory (day 8). The cheese sensory characteristics for the two trajectories (classic and optimized) are almost the same.

Explore to find sustainable strategies for wheat culture.

We organised a Pareto front visual exploration session to help a domain expert investigate various fertilization strategies for wheat growth. Our expert had a research question pertaining to azote fertilisation strategies. In particular, she wanted to find strategies that work well regardless of the climate or the weather. To achieve this, in a first step we constructed a Pareto front from simulation files produced by the expert using an existing soil crop model called Azodyn (Jeuffroy et al., 1999). This model takes soil characteristics and predicts the consequences of azote (N) fertiliser management strategies, in terms of daily crop growth, yield, grain protein content and N losses to the environment. The Pareto front was constructed by maximising yield, and both minimising loss and the final N dose. These objectives were selected by the experts, to help them answer their research question. In a second step, the exploration session was carried out iteratively using a large tactile display (figure 4) and an interactive visualization system coupled to an evolutionary algorithm (Cancino Tionca et al., 2012)(Boukhelifa et al., 2017) (figure 5).

Besides helping the expert answer their research question, the objectives of this workshop were three-fold: (a) to get feedback and evaluate our approach of interactive model exploration, (b) to collect data on expertise related to each application domain, and (c) to establish opportunities for automatic learning and user interaction leverage points.

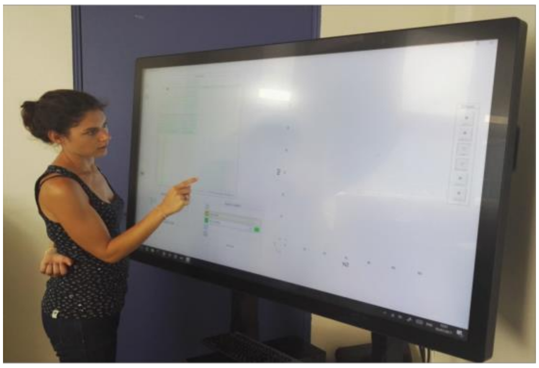

Figure 4: Model exploration session with a domain expert using interactive visualization.

During this exploration session, the domain expert reported finding interesting fertilisation strategies that she did not investigate previously (thus new research questions). More interestingly, in collaboration with this domain expert, we were able to generate decision rules for the different fertilisation strategies that she explored. In the future, we plan to test these rules, by generating a new dataset based on the new findings, and re-launching the simulation and exploration. We have also gathered a rich dataset on interactive model exploration (videos, notes and log files), which we plan to analyse.

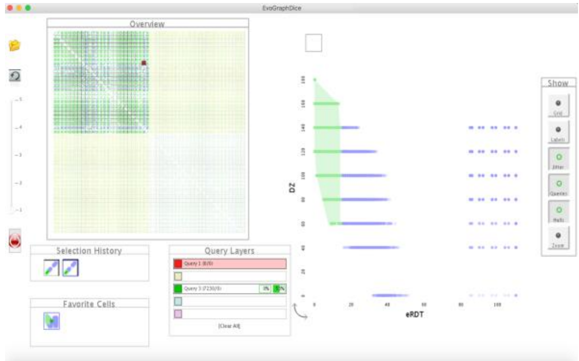

Figure 5: EvoGraphDice: The visualization tool we used for the exploration session. In this view the expert selected a view showing yield versus. Azote doze. The green selection corresponds to favorable fertilization strategies according to the ‘yield’ criteria.

Food and Biological properties prediction

Predict flavor of red wine

In food science, sensory properties are important and not always easy to predict. For example the analysis of the aromatic component of food products is usually performed by separating, identifying and quantifying the molecules included in an extract. Such well-established procedure provides a list of key odorants but does not give any information about the perceptual influence of mixed compounds. This is a major problem for the prediction of the food overall sensory profile on the basis of its chemical content. To solve this issue, we developed an approach of “human in the loop”, applied to the prediction of the odor of 16 red wines (Roche et al., 2017). We worked with experts, sensory databases and computational tools coupling fuzzy logic and genetic algorithms for fuzzy model parameters optimization. This model queries analytical and sensory databases in order to predict the flavor profile (figure 6).

In a first step (see Step 1, figure 1) explicit knowledge is initially described by a panel of 4 experts (flavorists) in the form of rules. They were asked to describe in basic odor qualities 4 to 15 sensory descriptors useful to characterize red wines but not specific to it (e.g. bell pepper, blackcurrant fresh, cherry cooked, cherry stone, strawberry fresh). Basic odor qualities are also linked to analytical data by the experts in the form of ontologies (A. Roche, N. Perrot, T. Thomas-Danguin, “Odor perceptual space: From odorant descriptors to odor qualities”, in writing).

In a second step (see step 2, figure 1), a model is proposed linking all the knowledge in a model coupling ontologies, fuzzy reasoning to compute the rules proposed by the flavorits and a genetic algorithm performing an optimization of the fuzzy rules parameters using a data basis collected during experiments. It estimates the intensity of each sensory descriptor for a wine on the basis of its composition in terms of odor active compounds. After several iterations with experts, a final model is proposed to predict the wine sensory properties. Applied to a series of datasets on 16 red wines. The results of prediction are in good agreement with the actual values with the two projections on the first two principal components of a PCA, statistically significantly correlated (Monte-Carlo test p = 0.003).

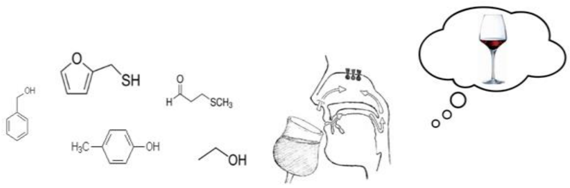

Figure 6: From analytical data to flavor perception of red wines: a question of human in the loop.

Predict and discover knowledge of a multiscale involved process: a "theory building tool" applied to bacteria freeze drying

In many real-world modelling case studies, the amount of data available is often not enough to apply fully automated tools such as black-box machine learning algorithms. At the same time, additional knowledge on the problem is usually available, in the form of implicit proficiency developed by experts of the domain. In such situations it is fundamental to allow human users to interact with the machine learning tools, and make their knowledge explicit. LIDEOGRAM (Life-based Interactive DEvelopment Of GRAphical Models) (Chabin et al., 2017) is a tool implementing this specific vision: The goal is to provide experts with a design tool for modelling complex system processes. In LIDEOGRAM, each non-input variable for a case study is modelled as a mathematical formula dependent on other variables in the problem. Interacting with a graphical representation of the system, users are involved in three steps: In a first step (see step 1, figure 1), sets of variables and classes grouping some or all the variables can be created, and a first graph of links between those variables and classes can be proposed. Starting from the relationships described by the user-defined graph, in a second step (see step 2, figure 1), a machine learning approach based multi-linear regression will propose mathematical formulas, each one a different trade-off between complexity and fitting. This process ultimately creates a multi-scale model, where each part of the process is defined with respect to variables at a lower scale, following the dependencies given by the initial user-defined graph. In a final step, experts select mathematical formulas of their choice, iteratively, until a satisfactory result is reached. LIDEOGRAM has been successfully applied to a case study involving freeze-drying of bacteria, where a model developed interacting with a human expert was able to deliver better result than one obtained through a purely automatic approach (see Figure 7 for a screenshot of the interface used in the experiments).

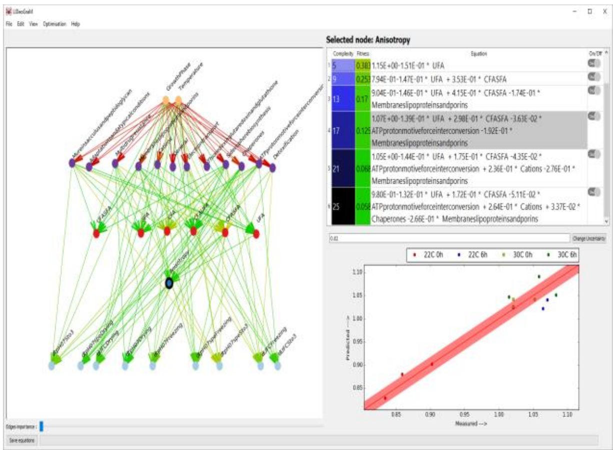

Figure 7: Screenshot of LIDeOGraM. The left side shows a graphical model representing the meanness of the local models obtained by symbolic multi-linear regression. The top-right part is the list of equations proposed for the selected node, and the bottom-right part shows a plot of the measured versus predicted data associated to the selected equation.

Computational models such a LIDEOGRAM are useful tools for hypothesis generation: through simulations, users can explore unseen scenarios, and ultimately exploit the model as a theory-building device (Sun, 2008). At the same time, this approach can be used to create new knowledge by summarizing information, in a process similar to chunking in cognitive models (Lucentini and Goodwin, 2015). While we advocate for the use of models to explore the implications of ideas, especially for assessing their sufficiency, optimality, and empirical adequacy, such explorations must nevertheless be carried out with care. Reaching broad conclusions from the shortcomings of particular models, in particular, is difficult: Even if a modeler can show that a model fits all available data perfectly, the work still cannot tell us that it correctly captures the processes in the tasks that it addresses (Mc Clelland, 2009).

CONCLUSIONS

In this paper, an approach centered on human and human embedded in the computing loop is presented. It is based on human, machine learning, optimisation and visualisation. Different studies were the use of computational models interacting with human are presented. Those experimentations, show clearly the value added of such a paradigm and open a road for future research in food and biological modelling.

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