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Procedia

Social and Behavioral Sciences

Procedia - Social and Behavioral Sciences 228 (2016) 161 – 168

2nd International Conference on Higher Education Advances, HEAd´16, 21-23 June 2016, València, Spain

Assessing the Role of General Chemistry Learning in Higher Education

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Abstract

The inclusion of General Chemistry (GC) in the curricula of higher education courses in science and technology aims, on the one hand, to develop students' skills necessary for further studies and, on the other hand, to respond to the need of endowing future professionals of knowledge to analyze and solve multidisciplinary problems in a sustainable way. The participation of students in the evaluation of the role played by the GC in their training is crucial, and the analysis of the results can be an essential tool to increase success in the education of students and improving practices in various professions. Undeniably, this work will be focused on the development of an intelligent system to assess the role of GC. The computational framework is built on top of a Logic Programming approach to Knowledge Representation and Reasoning, complemented with a problem solving methodology moored on Artificial Neural Networks. The results so far obtained show that the proposed model stands for a good start, being its overall accuracy higher than 95%.

Peer-review under responsibility of the organizing committee of HEAd´16

Keywords: General Chemistry; Higher Education; Logic Programming; Knowledge Representation and Reasoning; Artificial Neural Networks

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Peer-review under responsibility of the organizing committee of HEAd´16
doi:10.1016/j.sbspro.2016.07.024

1. Introduction

Education is to be able to reason, to use one's ability to gain our spectrum of knowledge, which is nowadays increasingly dependent on science and technology (American Association for the Advancement of Science, 1990; National Research Council, 1996). The inclusion of *General Chemistry* (*GC*) in the curricula of higher education courses in the area of science and technology, intends to form future professionals with the necessary skills to analyze and solve problems in a sustainable way. Furthermore, another important goal that should be taken into account is related with the development of expertise required for the subsequent disciplines on course plans.

Indeed, the assessment of the role played by *GC* in different courses in higher education is an essential tool to increase the students' success and to improve good practices in various professional domains. The involvement of students in the evaluation of the role of *GC* in Higher Education courses is of utmost importance, since they are the aimed targets.

Artificial Intelligence based methodologies and techniques for problem solving in educational context are still considered a new paradigm and a promising challenge. A few studies that illustrate the applicability of these tools to different problems in educational field can be found in literature. Şen & Uçar (2012) used *Artificial Neural Networks* (*ANNs*) and *Decision Trees* (*DTs*), in order to study the students' achievements. Şen, Uçar & Delen (2012) developed models to predict secondary education placement test results using *DTs*, support vector machines, *ANNs* and logistic regression. Recent studies described the development of decision support systems based on soft computing approaches to evaluate the quality of learning (Neves *et al*., 2015) and potential situations of school dropout (Figueiredo, Vicente, Vicente & Neves, 2014; Neves, Figueiredo, Vicente & Vicente, 2016).

The present work reports on a computational framework that uses knowledge representation and reasoning techniques to set the structure of the information and the associate inference mechanisms. It will be centered on a *Logic Programming* (*LP*) based approach to knowledge representation and reasoning (Neves, 1984; Neves, Machado, Analide, Abelha, & Brito, 2007), complemented with a computational framework based on *ANNs* due to their dynamic characteristics like adaptability, robustness and flexibility (Cortez, Rocha, & Neves, 2004), which makes possible the handling of unknown, incomplete or even contradictory data or knowledge.

2. Background

2.1. Knowledge Representation and Reasoning

The *Logic Programming* (*LP*) paradigm has been used in knowledge representation and reasoning in different areas, such as Model Theory (Kakas, Kowalski, & Toni, 1998; Pereira & Anh, 2009), and Proof Theory (Neves, 1984; Neves *et al*., 2007). In this work the proof theoretical approach is followed in terms of an extension to *LP*. An Extended Logic Program is a finite set of clauses in the form:

$$
\begin{array}{l}
\{ \quad p \leftarrow p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m \\
\quad ?\,(p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m) \quad (n, m \geq 0) \\
\quad exception_{p_1} \quad \cdots \quad exception_{p_j} \quad (0 \leq j \leq k), \quad being\ k\ an\ integer \\
\} :: scoring_{value}
\end{array}
$$

where "*?*" is a domain atom denoting falsity, the p_i, q_j, and p are classical ground literals, i.e., either positive atoms or atoms preceded by the classical negation sign $\neg$ (Neves, 1984). Under this formalism, every program is associated with a set of abducibles (Kakas *et al*., 1998; Pereira & Anh, 2009), given here in the form of exceptions to the extensions of the predicates that make the program. The term $scoring_{value}$ stands for the relative weight of the extension of a specific *predicate* with respect to the extensions of the peers ones that make the overall program.

In order to evaluate the knowledge that can be associated to a logic program, an assessment of the *Quality of Information (QoI)*, given by a truth-value in the interval [0, 1], that stems from the extensions of the predicates that make a program, inclusive in dynamic environments, is set (Lucas, 2004). The goal is to build a quantification process of the *QoI* and the *Degree of Confidence (DoC)*, being the latter a measure of one's confidence that the argument values or attributes of the terms that make the extension of a given predicate, with relation to their domains, fit into a given interval. The *DoC* is evaluated as it is illustrated in Fig. 1, and computed using $DoC = (1-\Delta l^2)^{1/2}$, where Δl stands for the argument interval length, which was set in the interval [0, 1]. Thus, the universe of discourse is engendered according to the information presented in the extensions of such predicates, according to productions of the type:

$$predicate_i - \bigcup_{1 \le i \le m} clause_j\left(\left(QoI_{x_1}, DoC_{x_1}\right), \cdots, \left(QoI_{x_m}, DoC_{x_m}\right)\right) :: QoI_i :: DoC_i \tag{1}$$

where $\cup$ and m stand, respectively, for *set union* and the *cardinality* of the extension of $predicate_i$ (Fernandes, *et al.*, 2015).

2.2. Artificial Neural Networks

Artificial Neural Networks (*ANNs*) denote a set of connectionist models inspired in the behavior of the human brain. In particular, the *Multilayer Perceptron* (*MLP*) is the most popular *ANN* architecture, where neurons are grouped in layers and only forward connections exist (Haykin, 2009). This provides a powerful base-learner, with advantages such as nonlinear mapping and noise tolerance, increasingly used in *Data Mining* due to its good behavior in terms of predictive knowledge (Mitra, Pal, & Mitra, 2002). The interest in *MLPs* was stimulated by the advent of the *Backpropagation* algorithm in 1986 and since then several fast gradient based variants have been proposed (e.g., *RPROP*) (Riedmiller, 1994). Yet, these training algorithms minimize an error function by tuning the modifiable parameters of a fixed architecture, which needs to be set a priori. The *MLP* performance will be sensitive to this choice, i.e., a small network will provide limited learning capabilities, while a large one will induce generalization loss (i.e., over fitting). The correct design of the *MLP* topology is a complex and crucial task, commonly addressed by trial-and-error procedures (e.g., exploring different number of hidden nodes), in a blind search strategy, which only goes through a small set of possible configurations. More elaborated methods have also been proposed, such as pruning (Thimm & Fiesler, 1995) and constructive (Kwok & Yeung, 1997) algorithms, although these perform hill-climbing and are thus prone to local minima (Cortez *et al.*, 2004). On the other hand, the number of nodes in the input layer set the number of independent variables, while those in the output layer denote one and all the dependent ones (Haykin, 2009).

3. Methods

In order to collect data an instrument was designed specifically for this study. The questions included in the questionnaire were organized into three sections. The former section includes the questions related with the opinion of students about the subject *GC* (see *General Chemistry Related Factors* Table in Fig. 2). The second one comprises the questions related with the opinion of students about the importance of *GC* in course plan context and for future professional performance (see *Importance of General Chemistry* Table in Fig. 2). The latest section aims to know the opinion of students about the role of *GC* learning in higher education. The answers were given in a scale ranging between 1 (one) and 5 (five), where 1 (one) stands for *Strongly Negative Opinion* and 5 (five) denotes a *Strongly Positive Opinion*.

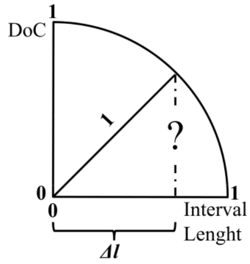

Fig. 1. Degree of Confidence's evaluation.

4. Case Study

4.1. Sample Characterization

A total of 122 *GC* students were enrolled in this study, with an age average of 20.8 years, ranging from 19 to 23 years old. The gender distribution was 32% and 68% for male and female, respectively, while course distribution was 39.1%, 41.2% and 19.7%, respectively for agronomy, biology and human biology.

4.2. A Logic Programming Data Assessment

Once one has the data it is possible to build up a knowledge database given in terms of the extensions of the relations (or tables) depicted in Fig. 2, which stands for a situation where one has to manage information related with the evaluation of the role of *GC*. Besides the information collected with the questionnaire, the number of *ECTS* (i.e., the *E(*uropean) *C(*redit) *T(*ransfer) and accumulation *S(*ystem), a standard for comparing the study attainment and performance of students of higher education) in *GC*, present in the study plans, was also included. The knowledge base yields also items with *incomplete*, *unknown*, and even *contradictory* values. For instance, for case 1 the information regarding *Importance to other Subjects* is *unknown*, being represented by the symbol ⊥, while the *Importance to Professional Performance* ranges in the interval [1, 2].

General Chemistry Related Factors						
#	*Adequacy Syllabus/ /Previous Knowledge*	*Objectives Adequacy*	*Syllabus Adequacy*	*Coherence Syllabus/Objectives*	*Adequacy of Theoretical Training Duration*	*Adequacy of Practical Training Duration*
1	2	3	[3, 4]	3	⊥	4
2	4	4	5	[4, 5]	4	4
…	…	…	…	…	…	…
122	3	3	4	4	3	4

General Chemistry Role					
#	*General Chemistry Related Factors*	*Importance to other Subjects*	*Importance to Professional Performance*	*Compulsory Component*	*Elective Component*
1	[15, 21]	⊥	[1, 2]	12	[0, 6]
2	[25, 26]	5	[4, 5]	12	[0, 8]
…	…	…	…	…	…
122	21	3	3	27	[0, 21]

Importance of General Chemistry		
#	*to other Subjects in Course Study Plan*	*to Professional Performance*
1	⊥	[1, 2]
2	5	[4, 5]
…	…	…
122	3	3

ECTS in Chemistry Area		
#	*Compulsory Component*	*Elective Component*
1	12	[0, 6]
2	12	[0, 8]
…	…	…
122	27	[0, 21]

Fig. 2. A fragment of the knowledge base for General Chemistry Role Assessment.

The values presented in the *General Chemistry Related Factors* column of *General Chemistry Role* table are the sum of the correspondent table, ranging between [0, 30]. The domains of *Importance to other Subjects* and *Importance to Professional Performance* are [0, 5], while the domains of *Compulsory* and *Elective Component* columns are [6, 27] and [0, 21] respectively.

Applying the algorithm presented in Fernandes *et al*. (2015) to all the fields that make the knowledge base for *GC Role Assessment* (Fig. 2) and looking to the DoC_s values obtained, it is possible to set the arguments of the predicate ***role**-of-**gen**eral-**chem**istry* ($role_{gen\_chem}$) referred to below, which extensions denote the objective function with respect to the problem under analyze:

$$role_{gen\_chem} : G_{eneral} C_{hemistry} R_{elated} F_{actors},\ I_{mportance\ to}\, o_{ther} S_{ubjects},\ I_{mportance\ to}\, P_{rofissional} P_{erformance},\ C_{ompulsory} C_{omponent},\ E_{lective} C_{omponent} \rightarrow \{0, 1\}$$

where 0 (zero) and 1 (one) denote, respectively, the truth values *false* and *true*.

Exemplifying the application of the algorithm presented in Fernandes *et al*. (2015) to a term that presents feature vector ($G_{eneral}\ C_{hemistry}\ R_{elated}\ F_{actors} = 23$, $I_{mportance\ to}\ o_{ther}\ S_{ubjects} = [3, 4]$, $I_{mportance\ to}\ P_{rofessional}\ P_{erformance} = \perp$, $C_{ompulsory}\ C_{omponent} = 12$, $E_{lective}\ C_{omponent} = [0, 8]$), one may have:

Begin %DoCs evaluation%

%The predicate's extension that sets the Universe-of-Discourse for the term under observation is fixed%

$$\{\ \neg\ role_{gen\_chem}\left(\left(QoI_{GCRF}, DoC_{GCRF}\right), \left(QoI_{IoS}, DoC_{IoS}\right), \left(QoI_{IPP}, DoC_{IPP}\right), \left(QoI_{CC}, DoC_{CC}\right), \left(QoI_{EC}, DoC_{EC}\right)\right)$$
$$\leftarrow not\ role_{gen\_chem}\left(\left(QoI_{GCRF}, DoC_{GCRF}\right), \left(QoI_{IoS}, DoC_{IoS}\right), \left(QoI_{IPP}, DoC_{IPP}\right), \left(QoI_{CC}, DoC_{CC}\right), \left(QoI_{EC}, DoC_{EC}\right)\right)$$
$$role_{gen\_chem}\underbrace{\left(\left(1_{23}, DoC_{23}\right), \left(1_{[3,4]}, DoC_{[3,4]}\right), \left(1_{\perp}, DoC_{\perp}\right), \left(1_{12}, DoC_{12}\right), \left(1_{[0,8]}, DoC_{[0,8]}\right)\right)}_{attribute's\ values} :: 1 :: DoC$$
$$\underbrace{[0, 30]\ \_\ \_\ \_\ [0, 5]\ \_\ \_\ \_\ [0, 5]\ \_\ \_\ [6, 27]\ \_\ \_\ \_\ [0, 21]}_{attribute's\ domains}$$
$$\}\ ::\ 1$$

%The attribute's values ranges are rewritten%

$$\{\ \neg\ role_{gen\_chem}\left(\left(QoI_{GCRF}, DoC_{GCRF}\right), \left(QoI_{IoS}, DoC_{IoS}\right), \left(QoI_{IPP}, DoC_{IPP}\right), \left(QoI_{CC}, DoC_{CC}\right), \left(QoI_{EC}, DoC_{EC}\right)\right)$$
$$\leftarrow not\ role_{gen\_chem}\left(\left(QoI_{GCRF}, DoC_{GCRF}\right), \left(QoI_{IoS}, DoC_{IoS}\right), \left(QoI_{IPP}, DoC_{IPP}\right), \left(QoI_{CC}, DoC_{CC}\right), \left(QoI_{EC}, DoC_{EC}\right)\right)$$
$$role_{gen\_chem}\underbrace{\left(\left(1_{[23,23]}, DoC_{[23,23]}\right), \left(1_{[3,4]}, DoC_{[3,4]}\right), \left(1_{[0,5]}, DoC_{[0,5]}\right), \left(1_{[12,12]}, DoC_{[12,12]}\right), \left(1_{[0,8]}, DoC_{[0,8]}\right)\right)}_{attribute's\ values\ ranges} :: 1 :: DoC$$
$$\underbrace{[0, 30]\ \_\ \_\ \_\ [0, 5]\ \_\ \_\ \_\ [0, 5]\ \_\ \_\ \_\ [6, 27]\ \_\ \_\ \_\ [0, 21]}_{attribute's\ domains}$$
$$\}\ ::\ 1$$

%The attribute's boundaries are set to the interval [0, 1]%

$$\{\ \neg\ role_{gen\_chem}\left((QoI_{GCRF}, DoC_{GCRF}), (QoI_{IoS}, DoC_{IoS}), (QoI_{IPP}, DoC_{IPP}), (QoI_{CC}, DoC_{CC}), (QoI_{EC}, DoC_{EC})\right)$$

$$\leftarrow\ not\ role_{gen\_chem}\left((QoI_{GCRF}, DoC_{GCRF}), (QoI_{IoS}, DoC_{IoS}), (QoI_{IPP}, DoC_{IPP}), (QoI_{CC}, DoC_{CC}), (QoI_{EC}, DoC_{EC})\right)$$

$$role_{gen\_chem}\underbrace{\left((1_{[0.77,\,0.77]}, DoC_{[0.77,\,0.77]}), (1_{[0.6,\,0.8]}, DoC_{[0.6,\,0.8]}), (1_{[0,\,1]}, DoC_{[0,\,1]}), (1_{[0.28,\,0.28]}, DoC_{[0.28,\,0.28]}), (1_{[0,\,0.38]}, DoC_{[0,\,0.38]})\right)}_{attribute's\ values\ ranges\ once\ normalized} :: 1 :: DoC$$

$$\underbrace{[0, 1]\qquad [0, 1]\qquad [0, 1]\qquad [0, 1]\qquad [0, 1]}_{attribute's\ domains\ once\ normalized}$$

$$\}\ ::\ 1$$

%The DoC's values are evaluated%

$$\{\ \neg\ role_{gen\_chem}\left((QoI_{GCRF}, DoC_{GCRF}), (QoI_{IoS}, DoC_{IoS}), (QoI_{IPP}, DoC_{IPP}), (QoI_{CC}, DoC_{CC}), (QoI_{EC}, DoC_{EC})\right)$$

$$\leftarrow\ not\ role_{gen\_chem}\left((QoI_{GCRF}, DoC_{GCRF}), (QoI_{IoS}, DoC_{IoS}), (QoI_{IPP}, DoC_{IPP}), (QoI_{CC}, DoC_{CC}), (QoI_{EC}, DoC_{EC})\right)$$

$$role_{gen\_chem}\underbrace{\left((1, 1), (1, 0.98), (1, 0), (1, 1), (1, 0.92)\right)}_{attribute's\ quality-of-information\ and\ respective\ confidence\ values} :: 1 :: 0.78$$

$$\underbrace{[0.77, 0.77]\ [0.6, 0.8]\ [0, 1]\ [0.28, 0.28]\ [0, 0.38]}_{attribute's\ values\ ranges\ once\ normalized}$$

$$\underbrace{[0, 1]\qquad [0, 1]\qquad [0, 1]\qquad [0, 1]\qquad [0, 1]}_{attribute's\ domains\ once\ normalized}$$

$$\}\ ::\ 1$$

4.3. Hybrid Computing Model

The previous section establishes how the information comes together and how it is processed. Now, a data mining approach to deal with the processed information is considered. A hybrid computing method was set to model the universe of discourse, based on *LP* and *ANNs* (*MLP* in this case), which are used, respectively, to structure data and capture complex relationships between inputs and outputs (Vicente *et al*., 2012). Besides to a computational model that enables the assessment of the role of *GC*, the proposed approach intends also obtain the *DoC* associated to this evaluation. Thus, is necessary apply an algorithm that allows more than one output variable. The choice fell on *MLP* due to their dynamics characteristics like adaptability, robustness and flexibility. Considering the case given above, where one may have a situation in which the evaluation of the role of *GC* in higher education is desired, Fig. 3 shows how the values of the attributes' intervals boundaries, their *DoCs* and *QoIs* values work as inputs to the *MLP*. The output depicts the evaluation of the role of *GC* and the confidence that one has on such a happening.

To implement the evaluation mechanisms and to test the model, 10 folds cross validation were applied (Haykin, 2009). The back propagation algorithm was used in the learning process of the *MLP*. As the output function in the pre-processing layer it was used the identity one, while in the other layers we considered the sigmoid. The *MLP* has a 5-4-2 topology, i.e. an input layer with five nodes (corresponding to the independent variables, i.e., *General Chemistry Related Factors (GCRF)*, *Importance to Other Subjects (IoS)*, *Importance to Professional Performance (IPP)*, *Compulsory Component (CC)* and *Elective Component (EC)*), one hidden layer with four nodes and a two nodes output layer, denoting the dependent variables (i.e., the assessment of the role of *GC* and the *DoC* associated to such evaluation). The accuracy model presents a value of 95.9% (117 instances correctly classified in 122).

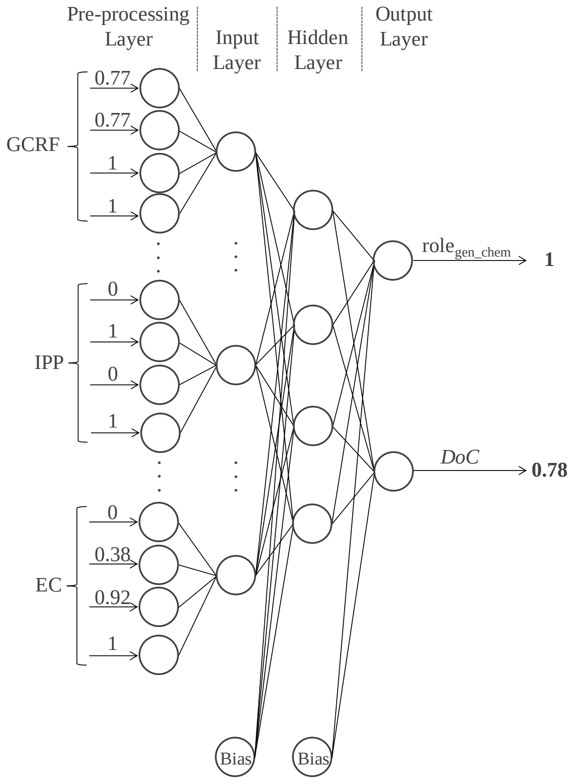

Fig. 3. The Artificial Neural Network Topology.

5. Conclusions

The assessment of the role of *GC* in *Higher Education* courses stands for an inestimable achievement. In order to have a true discussion about quality, accounting and accountability of the role of training on educational practice, these assets must be intertwined with an evaluation of the impact on the students' courses, as well as on future deliveries like career enactment. The involvement of students in evaluation of the educational process, aiming at to assess the role of *GC* in it, is a critical factor that has to be associated with the creation of added value to the higher education schools. Once the parameters to assess the role of *GC* in higher education are not fully represented by objective data (i.e., could be of types unknown, taken from a set or from an interval, or even contradictory), the problem was put into the area of those that must be tackled by Artificial Intelligence based methodologies and techniques for problem solving. In fact, the computational framework presented above uses powerful knowledge representation and reasoning methods to set the structure of the information and the associate inference mechanisms. This approach not only allows for the assessment of the role of *GC* in higher education, but it also permits the estimation of a measure of confidence (in terms of *DoC*) associated to such an evaluation. In fact, this is one of the added values of this method that arises from the complementarity between Logic Programming (for knowledge representation and reasoning) and the computing process based on *ANNs*. The computational model offered in this study revealed a good performance, once its overall accuracy unveiled values higher than 95%.

Acknowledgements

This work has been supported by COMPETE: POCI-01-0145-FEDER-007043 and FCT – Fundação para a Ciência e Tecnologia within the Project Scope: UID/CEC/00319/2013.

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