

Machine Learning for the Semantic Web: Lessons Learnt and Next Research Directions

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Abstract. Machine Learning methods have been introduced in the Semantic Web for solving problems such as link and type prediction, ontology enrichment and completion (both at terminological and assertional level). Whilst initially mainly focussing on symbol-based solutions, recently numeric-based approaches have received major attention, motivated by the need to scale on the very large Web of Data. In this paper, the most representative proposals, belonging to the aforementioned categories are surveyed, jointly with the analysis of their main peculiarities and drawbacks. Afterwards the main envisioned research directions for further developing Machine Learning solutions for the Semantic Web are presented.

1. Introduction

The Semantic Web (SW) vision has been introduced with the goal of making the Web machine readable [1], by enriching resources with metadata whose formal semantics is defined in OWL¹ ontologies acting as shared vocabularies to be reused. Ontologies are also empowered with deductive reasoning capabilities which allow to derive knowledge that is implicitly encoded. While developing this vision, some limitations [2, 3] arose: ontology construction resulted in a time consuming task; being strongly decoupled, ontologies and assertions can be out-of-sync, thus resulting incomplete, noisy and sometimes inconsistent with regard to the actual usage of the conceptual vocabulary in the assertions. These limitations became even more evident when pushing on Linked Data [4, 5] for enabling the actual creation of the Web of Data. As a consequence, multiple necessities emerged: reasoning at large scale; managing noise, inconsistencies and incompleteness in the Web of Data; (semi-)automatizing tasks such as ontology completion, enrichment (both at

schema and assertional level), link prediction; exploiting alternative forms of reasoning complementing the deductive approach.

In order to fill some of these gaps, machine learning (ML) methods have been proposed [6]. Problems such as query answering, instance retrieval and link prediction have been regarded as classification problems. Suitable machine learning methods, often inspired by symbol-based solutions in the *Inductive Logic Programming* (ILP) field (aiming at inducing an hypothesised logic program from a background knowledge and a collection of examples), have been proposed [7–11]. Most of them are able to cope with the expressive SW representations and the *Open World Assumption* (OWA) typically adopted, differently from the *Closed World Assumption* (CWA) that is usually assumed in the traditional ML settings. Problems such as ontology refinement and enrichment at terminology level, e.g. assessing disjointness axioms or complex descriptions for a given concept name, have been regarded as concept learning problems to be solved via supervised/unsupervised inductive learning methods for Description Logics [12] (DLs) representations [13–18].

¹<https://www.w3.org/OWL/>

Nowadays, the adoption of ML methods represents a major trend in several research fields such as computer vision, bioinformatics, image recognition, natural language processing and artificial intelligence. This is mostly due to the impressive scalability that recent methods, mainly grounded on numeric approaches (also called sub-symbolic), such as *embeddings* and *deep learning* [19], have shown. This trend is also occurred in SW. Indeed, motivated by the need for scaling, many of the recent ML-based solutions, e.g. for performing link/type predictions, as well as data-intensive tasks by exploiting the Web of Data and the emerging Knowledge Graphs (KGs) as background knowledge, are mainly grounded on *embeddings* [20–22] that are methods for translating high-dimensional vectors into relatively low-dimensional spaces. Nevertheless, the important gain in terms of scalability, that ML methods for the SW are obtaining is penalizing: a) having interpretable models as a result of a learning process; b) the ability to exploit deductive (and complementary forms of) reasoning capabilities; c) the expressiveness of the SW representations and the compliance with the OWA.

In the following, the main problems and ML methods that have been developed in the SW are surveyed along with the two categories: symbol-based (Sect. 2) and numeric-based (Sect. 3), hence the fundamental peculiarities and issues are discussed. The main envisioned research directions that need to be pursued for developing ML methods for the SW are illustrated in Sect. 4. Conclusions are drawn in Sect. 5.

2. Symbol-based Methods for the Semantic Web

The first efforts in developing ML methods for the SW have been devoted to solve deductive reasoning tasks over ontologies under an inductive perspective. This was motivated by the necessity of offering an alternative way to perform some forms of reasoning when deductive reasoning was not applicable, for instance because of inconsistencies within ontologies, but also for supplying a solution for reasoning in presence of incompleteness (that is when missing information with respect to a certain domain of reference is registered), and/or in presence of noise (that is when ontologies are consistent but the information therein is somehow wrong with respect to a reference domain, e.g. missing disjointness axioms, missing and/or wrong assertions). Particularly, the incompleteness of knowledge bases, both at assertional and

schema level, drove the development of ML methods trying to specifically tackle this problem. The overall idea consisted in exploiting the evidence coming from assertional knowledge for drawing plausible conclusions to be possibly represented with intensional models. In the following, the tasks that received major attention are reported jointly with the analysis of the main solutions for them.

2.1. Instance Retrieval

One of the first problems that has been investigated is the *instance retrieval* problem, which amounts at assessing if an individual is an instance of a given concept. It has been regarded as a classification problem aiming at assessing the class-membership of an individual with respect to a query concept. Similarity-based methods, such as *K-Nearest Neighbor* and *Support Vector Machine*, have been developed since they are well known to be noise tolerant [7, 23, 24]. This required to cope with: 1) the OWA rather than the CWA generally adopted in ML; 2) the non-disjointness of the classes (since an individual can be instance of more than one concept at the same time) while, in the usual ML setting, classes are assumed to be disjoint; 3) the definition of new *similarity measures* and *kernel functions* for exploiting the expressiveness of SW representations. Additionally, because of the OWA, new metrics for the evaluation of the classification results have been defined [7]. This is because, by using standard metrics as precision, recall and F-measure, new inductive results were deemed as mistakes whilst they could turn out to be correct inferences when judged by a knowledge engineer. The proposed solutions experimentally proved their ability to perform inductive instance retrieval when compared to a standard deductive reasoner. They also proved their ability to induce new knowledge that was not logically derivable, but they did not result fully able to work at large scale.

Methods characterized by more interpretable models have been also defined [15, 25]. Inspired by the ILP literature concerning the induction of decision trees in clausal representation [26], a solution for inducing a *Terminological Decision Tree* (TDT) has been formalized [15]. A TDT is a tree structure, naturally compliant with the OWA, employing: a DL language for representing nodes and inference services as corresponding tests on the nodes. The tree-induction algorithm adopts a classical top-down divide-and-conquer strategy with the use of refinement operators for DL concept descriptions. Once a TDT is induced, similarly to

1 logical decision trees, a definition for the target concept
2 (namely the concept with respect to perform clas-
3 sification) can be drawn, by exploiting the nodes in
4 the tree structure. This solution showed the interesting
5 ability to provide an interpretable model, but it turned
6 out slightly less effective than similarity-based classi-
7 fication methods.

8 2.2. Concept Learning for Ontology Enrichment

10 With the purpose of enriching ontologies at termi-
11 nological level, methods for learning concept descrip-
12 tions for a concept name have been proposed. The
13 problem has been regarded as a supervised concept
14 learning problem aiming at approximating an inten-
15 sional DLs definition, given a set of individuals of an
16 ontology acting as positive/negative training examples.

17 Various solutions, e.g. DL-FOIL [13] and CELOE [16]
18 (part of the DL-LEARNER suite²), have been formal-
19 ized. They are mostly grounded on a *separate-and-*
20 *conquer* (sequential covering) strategy: a new con-
21 cept description is built by specializing, via suitable
22 *refinement operators*, a partial solution to correctly
23 cover (i.e. decide a consistent classification for) as
24 many training instances as possible. Whilst DL-FOIL
25 works under OWA, CELOE works under CWA. Both
26 of them may suffer of ending up in sub-optimal solu-
27 tions. In order to overcome such issue, DL-FOCL [27],
28 PARCEL [28] and SPACEL [29] have been proposed.
29 DL-FOCL is an optimized version of DL-FOIL, im-
30 plementing a base greedy covering learner. PARCEL
31 combines top-down and bottom-up refinements in the
32 search space. The learning problem is split into vari-
33 ous sub-problems, according to a divide-and-conquer
34 strategy, that are solved by running CELOE. Once the
35 partial solutions are obtained, they are combined in a
36 bottom-up fashion. SPACEL extends PARCEL with a
37 symmetrical specialization of a concept description.

38 These solutions proved their ability to learn approx-
39 imated concept descriptions for a target concept name
40 but relatively small ontological knowledge bases have
41 been considered for the experiments.

42 2.3. Knowledge Completion

43 Knowledge completion consists in finding new in-
44 formation at assertional level, that is facts that are
45 missing in a considered knowledge base. This task has
46 become very popular with the development of KGs,
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1 that are well known to be incomplete, and it is also
2 strongly related to the link prediction task (see Sect. 3).

3 One of the most well known system for knowledge
4 completion of RDF knowledge bases is AMIE [10]. In-
5 spired by the literature in *association rule mining* [30]
6 and ILP methods for learning Horn clauses, AMIE
7 aims to mine logic rules from RDF knowledge bases
8 with the final goal of predicting new assertions. AMIE
9 (and its optimized version AMIE+ [31]) currently rep-
10 represents the most scalable rule mining system for learn-
11 ing Horn rules on large RDF data collections and is
12 also explicitly tailored to support the OWA. However,
13 it does not exploit any form of deductive reasoning.
14 A related rule mining system, similarly based on a
15 level-wise generate and test strategy has been proposed
16 in [32]. It aims to learn SWRL rules [33] from OWL
17 ontologies while exploiting schema level information
18 and deductive reasoning during the rule learning pro-
19 cess. Both AMIE and the solution presented in [32]
20 showed the ability to mine useful rules and to pre-
21 dict new assertional knowledge. the solution proposed
22 in [32] showed reduced scalability due to the exploita-
23 tion of the reasoning capabilities.

24 2.4. Learning Disjointness Axioms

25 Disjointness axioms are essential for making ex-
26 plicit the negative knowledge about a domain, yet they
27 are often overlooked during the modeling process (thus
28 affecting the efficacy of reasoning services). To tackle
29 this problem, automated methods for discovering these
30 axioms from the data distribution have been devised.

31 A solution grounded on *association rule mining* [30]
32 has been proposed in [17, 34]. It is based on studying
33 the correlation between classes comparatively, namely
34 *association rules*, *negative association rules* and *cor-*
35 *relation coefficient*. Background knowledge and rea-
36 soning capabilities are used to a limited extent.

37 A different solution has been proposed in [18]
38 where, moving from the assumption that two or more
39 concepts may be mutually disjoint when the sets of
40 their (known) instances do not *overlap*, the problem
41 has been regarded as a clustering problem, aiming at
42 finding partitions of similar individuals of the knowl-
43 edge base, according to a *cohesion* criterion quantify-
44 ing the degree of homogeneity of the individuals in an
45 element of the partition. Specifically, the problem has
46 been cast as a *conceptual clustering* problem, where
47 the goal is both to find the best possible partitioning
48 of the individuals and also to induce intensional def-
49 initions of the corresponding classes expressed in the
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51 ²<https://dl-learner.org/>.

standard representation languages. Emerging disjointness axioms are captured by the employment of *terminological cluster trees* (TCTs) and by minimizing the risk of mutual overlap between concepts. Once the TCT is grown, groups of (disjoint) clusters located at sibling nodes identify concepts involved in candidate disjointness axioms to be derived. Unlike [17, 34], based on the statistical correlation between instances, the empirical evaluation of [18] showed its ability to discover disjointness axioms also involving complex concept descriptions, thanks to the exploitation of the underlying ontology as background knowledge.

3. Numeric-based Methods for the Semantic Web

Whilst symbolic methods adopt symbols for representing entities and relationships of a domain and infer generalizations that provide new insights into the data and are ideally readily interpretable, numeric-based methods typically adopt feature vector (propositional) representations and cannot provide interpretable models but they usually result rather scalable [35].

The problem that has been mainly investigated in the SW context by adopting numeric solutions is *link prediction* which amounts to predict the existence (or the probability of correctness) of triples in (a portion of) the Web of Data. Data are considered in their graph representation, mostly RDF representation language has been targeted and almost no reasoning is exploited; most expressive SW languages are basically discarded. The attention towards this problem is also grown due to the increasing of KGs, that are known to be often missing facts [36]. In the KG context, link prediction is also referred to as *knowledge graph completion*. Methods borrowed from the Statistical Relational Learning (SRL) [37] (having as main goal the creation of statistical models for relational/graph-based data) have been mostly developed. In the following the main classes of methods and solutions targeting link prediction in the SW are analyzed.

3.1. Probabilistic Latent Variable Models

Probabilistic Latent Variable Models explains relations between entities by associating each resource to a set of intrinsic latent attributes (i.e. attributes not directly observable in the data) and conditions the probability distribution of the relations between two resources on their latent attributes. All relations are considered conditionally independent given the latent

attributes. This allows the information to propagate through the network of interconnected latent variables.

One of the first numeric-based link prediction solution belonging to this category is the *Infinite Hidden Semantic Model* (IHSM) [38]. It formalizes a probabilistic latent variable that associates a latent class variable with each resource/node and makes use of constraints expressed in First Order Logic during the learning process. IHSM showed promising results but resulted limited in scaling on large SW data collection because of the complexity of the probabilistic inference and learning, which is intractable in general [39].

3.2. Embedding Models

With the goal of scaling on very large SW data collections, *embedding models* have been investigated. Similarly to probabilistic latent variable models, in embedding models each resource/node is represented with a continuous embedding vector encoding its intrinsic latent features within the data collection. Models in this class do not necessarily rely on probabilistic inference for learning the optimal embedding vectors and this allows to avoid the issues related to the normalization of probability distributions, that may lead to intractable problems.

One of the first solution belonging to this category is RESCAL [20], which implements graph embedding by computing a three-way factorization of an adjacency tensor that represents the multi-graph structure of the data collection. RESCAL resulted a powerful model also was able to capture complex relational patterns over multiple hops in a graph, however, even if improving the scalability of IHSM, it did not result to be able to scale on very large graph-based data collection (e.g. the whole YAGO or DBPedia). The main limitation was represented by the parameter learning phase, which may take rather long for converging to optimal solutions.

Nevertheless, since embedding models proved interesting ability to scale while maintaining comparative performance to probabilistic latent variable models in terms of predictive accuracy [40], with the goal of improving the model training phase employed by RESCAL, a solution exploiting adaptive learning rates during training has been proposed [21]. Specifically, an energy-based embedding model has been formalized, where entities and relations are embedded in continuous vector spaces and the probability of an RDF triple to encode a true statement is expressed in terms of energy of the triple, which is an unnormalized

score that is inversely proportional to such a probability value. It is computed as a function of the embedding vectors of the subject, the predicate and the object of the triple. This solution experimentally showed improvements in terms of efficiency of the parameter learning process and more accurate results in a significantly lower number of iterations.

An aspect that needs to be highlighted is that, due to tackling RDF representation, most of the considered data collections only contain positive (training) examples, since usually false facts are not encoded. As training a learning model in all-positive examples could be tricky because the model might easily overgeneralize, for obtaining negative examples two different approaches are generally adopted: either *perturbing* true/observed triples with the goal of generating plausible negative examples or making a *local-closed world assumption* (LCWA) in which the data collection is assumed as *locally* complete [41].

3.3. Vector Space Embeddings for Propositionalization

A complementary research direction focused on the exploitation of vector space embeddings for obtaining a propositional feature vector representation of RDF data collections. Specifically, inspired by the data mining (DM) literature on propositionalization [42], that is a collection of methods for transforming a relational data representation into a (numeric) propositional feature vector representation so that scalable propositional DM/ML methods can be applied, RDF2Vec [43] has been proposed. It formalizes a solution for learning latent numeric representations of entities in RDF graphs by adapting language modeling approaches. A two-steps approach is adopted: first the RDF graph is converted into a set of sequences of entities (for the purpose two different approaches using local information, that are graph walks and Weisfeiler-Lehman Subtree RDF graph kernels, are exploited); in the second step, the obtained sequences are used to train a neural language model estimating the likelihood of a sequence of entities appearing in a graph. The outcome of the the training process provides each entity in the graph represented as a vector of latent numerical features. DBpedia and Wikidata have been processed. In order to show that the obtained vector representation is independent from task and algorithm, an experimental evaluation involving a number of classification and regression tasks has been performed.

An upgrade of RDF2Vec has been presented in [22]. The proposed solution is grounded on the exploitation of global patterns, differently from RDF2Vec which exploits local patterns. None of the two solutions can cope with literals.

4. Machine Learning for the Semantic Web: Next Research Directions

In this section the envisioned most challenging research problems are illustrated. Hence additional ML settings and methods that could be usefully adopted for SW related issues are briefly discussed.

4.1. Research Problems

The need to cope with the fast growing of the Web of Data and the emerging very large KGs required the SW community to show its ability to manage such tremendous amount of data and knowledge.

This mostly motivated the right attention towards numeric ML methods, particularly for providing scalable solutions to manage the inherent incompleteness of the Web of Data. Indeed, current symbolic methods are not actually comparable, in terms of scalability, to numeric-based solutions. This gain is not for free. It is obtained by giving up the expressive representation languages, such as OWL, that the SW community contributed to standardize with the goal of formalizing rich and expressive knowledge, but also by forgetting one of the most powerful characteristic of these languages, that is being empowered with deductive reasoning capabilities that allow to derive new knowledge. This means to loose knowledge that is already available. Indeed, as illustrated in Sect. 3, almost all numeric methods focus on RDF as a representation language and nearly no reasoning capabilities are exploited. Furthermore, differently from symbolic methods, numeric-based solutions lack of the ability to provide interpretable models (see Sect. 3), thus limiting the possibility to interpret and understand the motivations for the returned results. Additionally, tasks such as learning concept or disjointness axioms cannot be performed without symbol-based methods which can certainly benefit of very large amount of information to provide potentially more accurate results.

Integration of symbolic and numeric approaches: Research efforts need to be devoted towards ML solutions that, while keeping scalability, are able to target

1 most expressive representations as well as to provide
2 interpretable models. As a first step, the integration of
3 numeric and symbolic approaches should be focused.

4 Some discussions in this direction have been de-
5 veloped by the Neural-Symbolic Learning and Reasoning
6 community [44, 45], which seeks to integrate
7 principles from neural networks learning and logical
8 reasoning. The main conclusion has been that neural-
9 symbolic integration appears particularly suitable for
10 applications characterized by the joint availability of
11 large amounts of (heterogeneous) data and knowledge
12 descriptions, which is actually the case of the Web of
13 Data. A set of key challenges and opportunities have
14 been outlined [44], such as: how to represent expres-
15 sive logics within neural networks, how neural net-
16 works should reason with variables, or how to extract
17 symbolic representation from trained neural networks.

18 Some preliminary results for some these challenges
19 have been recently provided. For instance Simple [46]
20 has been proposed. It is a scalable tensor-based factor-
21 ization model that is able to learn interpretable embed-
22 dings incorporating logical rules through weight tying.
23 Ideas for extracting propositional rules from trained
24 neural networks under a SW background knowledge
25 have been also illustrated [47], showing that the ex-
26 ploitation of a background knowledge allows: to re-
27 duce the extracted rule set; to reproduce the input-
28 output function of the trained neural network. A con-
29 ceptual sketch for explaining artificial neural networks
30 classification behavior in a non-propositional setting
31 while using SW background knowledge bases has been
32 proposed in [48]. These initial results, show the fea-
33 sibility of this research direction while remarking the
34 importance of pursuing this goal.

35
36 **Providing Explanations:** The problem of explain-
37 ing artificial neural networks classification behav-
38 ior [48] sheds the light on another important issue,
39 that is the necessity to provide explanations for results
40 supplied by ML methods [49], particularly when they
41 come from very large sources of knowledge, e.g. re-
42 sults for a link prediction problem. The solution de-
43 picted in [48] is in agreement with the idea of exploit-
44 ing symbol-based interpretable models to explain con-
45 clusions [35, 50]. Nevertheless, interpretable models
46 describe *how* solutions are obtained but not *why* they
47 are obtained. As argued in [44, 51], providing an ex-
48 planation means to supply a line of reasoning, illus-
49 trating the decision making process of a model whilst
50 using human understandable features. Following this
51 direction, a solution providing human-centric transfer

1 learning explanation has been proposed [52]. It takes
2 advantage of ontologies (DBpedia is used) and rea-
3 soning capabilities to infer different kinds of human
4 understandable explanatory evidence.

5 Hence, providing an explanation means to open the
6 box of the reasoning process and make it understand-
7 able. In a complex setting such as the Web of Data,
8 where knowledge may result from an automatic infor-
9 mation acquisition and integration process from differ-
10 ent sources, thus potentially noisy and with conflicting
11 information, multiple reasoning paradigms may be re-
12 quired e.g. deduction (when rules and theory are avail-
13 able), induction (for building models from the avail-
14 able knowledge), abduction (for filling in partial mod-
15 els coping with incomplete theory), commonsense rea-
16 soning etc. Large research efforts have been devoted to
17 study each paradigm, however in the considered com-
18 plex scenario, multiple paradigms could be needed at
19 the same time. This may require the formalization of a
20 unifying reasoning framework.

21
22 **Capturing Context and Evolution:** Some acquired
23 knowledge may also evolve over the time, that is it can
24 be valid only for a certain time period, or it may be
25 context dependent [53]. Capturing these phenomenon
26 may be fundamental and unsupervised as well as pat-
27 tern mining methods would be useful for the purpose.
28 Some preliminary research on capturing knowledge
29 evolution by conceptual clustering methods has been
30 presented [54] showing the feasibility of the approach
31 but highlighting an existing limitation given by the
32 lack of gold standards for validating the results.

33 34 4.2. Additional Machine Learning Settings

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36 As for the settings to be exploited, multiple research
37 directions still need to be investigated. Several prob-
38 lems such as instance retrieval but also link predic-
39 tion and assertional knowledge completion have been
40 solved by casting them as classification tasks. How-
41 ever, as discussed in Sect. 2, when assessing the con-
42 cept membership for an individual, it may result in-
43 stance of more than one concept at the same time. As
44 such a more suitable way to regard the problem is as
45 *multi-label classification* task [55], where multiple la-
46 bels (concepts in the specific case) may be assigned
47 to each instance. Some preliminary research has been
48 presented in [56], focussing on type prediction in RDF
49 data collections where limited information from the
50 available background knowledge is considered.

Multiple-instance learning (MIL) [57] is also a setting that would need investigation. It deals with the problem of incomplete knowledge concerning labels in training sets, as it happens in SW knowledge bases due to OWA. MIL is a type of supervised learning where training instances are not individually labeled, they are collected in sets of labeled bags. From a collection of labeled bags, the learner tries to either (i) induce a concept that will label individual instances correctly or (ii) learn how to label bags without inducing the concept. It may be fruitfully exploited for discovering correlations among resources and/or emerging concepts.

Other settings that would be useful for coping with the large number of unlabelled instances are *semi-supervised learning* (SSL) [58] and *learning from imbalanced data*. SSL makes use of both labeled and unlabeled instances, during the learning process, for surpassing the classification performance that could be obtained by discarding the unlabeled data (as it would happen in a supervised learning setting). Very few research efforts have been made in this direction. Some initial results have been presented in [59], where a link prediction problem is solved in a transductive learning framework. In learning from unbalanced data [60, 61], that is data collections where the labels distribution is not uniform, sampling techniques are usually adopted in order to create a balanced dataset to be successively used for the learning task. *Ensemble methods*, consisting in using multiple learning algorithms to obtain better predictive performance, could be fruitfully adopted, as illustrated in [25, 62] where respectively a *boosting* [62] and *bagging* technique is employed.

As a last point, considering the increasing volume of the Web of Data, *online* and *incremental learning*, which input data is continuously used to further train and extend the learned model, would be naturally investigated. For the best of knowledge, no research efforts have been made in this direction.

5. Conclusions

In this paper, the progresses that have been made in SW by exploiting ML methods have been surveyed. Specifically symbol-based and numeric-based solutions have been analyzed highlighting their main peculiarities and drawbacks. Hence the main envisioned research directions have been drawn.

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