Understanding and Improving Ontology Reasoning Efficiency through Learning and Ranking

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Abstract

Ontologies are the fundamental building blocks of the Semantic Web and Linked Data. Reasoning is critical to ensure the logical consistency of ontologies, and to compute inferred knowledge from an ontology. It has been shown both theoretically and empirically that, despite decades of intensive work on optimising ontology reasoning algorithms, performing core reasoning tasks on large and expressive ontologies is time-consuming and resource-intensive. In this paper, we present the meta-reasoning framework $R_2O_2^*$ to tackle the important problems of understanding the source of TBox reasoning hardness and predicting and optimising TBox reasoning efficiency by exploiting machine learning techniques. $R_2O_2^*$ combines state-of-the-art OWL 2 DL reasoners as well as an efficient OWL 2 EL reasoner as components, and predicts the most efficient one by using an ensemble of robust learning algorithms including XGBoost and Random Forests. A comprehensive evaluation on a large and carefully curated ontology corpus shows that $R_2O_2^*$ outperforms all six component reasoners as well as AutoFolio, a robust and strong algorithm selection system.

Keywords: OWL, Reasoning, Performance prediction, Ontology, Metrics, Learning, Meta-reasoning, Semantic Web

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1 1. Introduction

Ontologies are essential building blocks of the Semantic Web. Expressive ontology languages OWL DL and OWL 2 DL are widely used to represent many complex 3 phenomena in a number of application domains, including bioinformatics [1], software engineering [2] and data management [3-6]. In these domains, maintaining the logical 5 correctness of ontologies (i.e. consistency checking) and deducing implicit facts from ontologies (i.e. classification) are both important tasks that may need to be performed repeatedly. However, ontologies as expressed in common ontology languages such as 8 OWL [7] and OWL 2 [8] can be large, complex, or both. The high worst-case com-9 plexity of these ontology languages incurs high computational costs on the above core 10 reasoning problems. Checking the logical consistency of an ontology in $SHOIN(\mathbf{D})$, 11 the description logic (DL) underlying OWL DL, has NExpTIME-complete worst-case 12 complexity [7]. The complexity of the same problem for SROIQ(D), the DL underlying 13 OWL 2 DL, is even higher (2NEXPTIME-complete) [8]. 14

The past decade has seen the development of highly optimised inference algo-15 rithms for description logics, with (hyper) tableau algorithms [9] being a leading ex-16 emplar. A number of high-performance DL reasoners have been developed, including 17 FaCT++ [10], HermiT [11], Konclude [12], Pellet [13] and TrOWL [14]. Despite the 18 tremendous progress in both theoretical research and practical implementation, the high 19 theoretical worst-case complexity results for OWL DL and OWL 2 DL still imply that 20 core reasoning services may be computationally very expensive. It has been shown 2 empirically that reasoning on large and complex ontologies in OWL 2 DL and OWL 22 2 EL (a less expressive profile that enjoys a PTIME-complete complexity) can be very 23 time-consuming for state-of-the-art reasoners [15, 16]. Such high difficulty of reasoning 24 and the fundamental role inference plays in ontology-based applications make it highly 25 desirable to be able to accurately predict inference performance for ontologies and 26 reasoners. 27

It is well-known that worst-case complexity does not necessarily provide useful insights into hardness of individual instances [17, 18]. In this context, it is noteworthy that reasoner benchmarking has been conducted previously [15, 19–22]. Except the two ORE competitions, these works only compared inference performance on a small set of ontologies. Moreover, they did not attempt to correlate characteristics of ontologies with their inference performance. Hence, they do not provide insight into what makes inference difficult on a given ontology.

The *robustness* of ontology reasoners was recently investigated [23], with a particular focus on reasoning efficiency. It was observed that given a corpus of ontologies and a number of state-of-the-art reasoners, it is highly likely that one of the reasoners performs sufficiently well on any given ontology in the corpus. However, this *virtual best reasoner* is only found *a posteriori*, and the paper did not discuss how the best reasoner may be selected automatically. It only stated that this task is not straightforward.

In our previous work we studied the characterisation of ontology's design complexity 4 using metrics [24], the prediction of ontology classification efficiency [25, 26], and 42 proposed a meta-reasoner R₂O₂ [27]. A meta-reasoner is one that combines other 43 (component) reasoners. Given an ontology, a meta-reasoner predicts the most efficient 44 component reasoner and selects it to carry out reasoning on that ontology. In this 45 paper, we improve upon our existing work and present a learning- and ranking-based 46 framework for the understanding of sources of ontology reasoning hardness, prediction 47 of ontology reasoning time, and ultimately improving reasoning performance, under 48 a unifying meta-reasoning framework. The main contributions of this paper can be 49 summarised as follows: 50

• Accurate prediction models: A regression based prediction model is learned for each of a number of state-of-the-art OWL 2 DL reasoners. Evaluated with 10fold cross validation, all the models are highly accurate, with R^2 (*coefficient of determination*) values in [0.71, 0.95].

• A meta-reasoning framework: A novel meta-reasoning framework, $R_2O_2^*$, is developed. Building on our previous work, $R_2O_2^*$ ranks and selects OWL reasoners with the aim of determining the most efficient reasoner for an unknown ontology. Compared with R_2O_2 [27], $R_2O_2^*$ utilises a robust, state-of-the-art prediction model XGBoost [28] based on gradient boosting [29] and an emsemble learning method *stacking* that combines multiple learning algorithms to obtain better predictive performance. $R_2O_2^*$ integrates state-of-the-art, *sound* and *complete* reasoners that are both efficient and robust. Moreover, $R_2O_2^*$ also incorporates ELK [30], an efficient reasoner for OWL 2 EL ontologies, to further improve reasoning efficiency for a wider variety of ontologies.

Comprehensive evaluation: A comprehensive evaluation on reasoning time has • 65 been conducted on a modern, large, and carefully-curated ontology corpus from the 66 ORE 2015 reasoner competition [22]. Our evaluation shows that R₂O₂* outperforms 67 all of the six OWL 2 DL component reasoners in the evaluation. The complete 68 meta-reasoner variant, $R_2O_2*_{(all)}$, also outperforms our previous meta-reasoners PR 69 and R₂O₂ [27]. More importantly, R₂O₂* outperforms AutoFolio [31], a state-of-70 the-art portfolio-based algorithm selection model that has demonstrated excellent 71 performance in a number of domains. 72

Ontology metrics: Furthermore, we give full definitions of a large suite of 91 on-• 73 tology metrics that have been mentioned but not formally defined in our previous 74 work [24, 26]. The formal definitions provide a valuable insight into ontology en-75 gineering and maintenance. We also identify the most important metrics that affect 76 ontology reasoning efficiency, which further informs ontology engineering practices. 77 The R₂O₂* meta-reasoner, including components that calculate metrics and train 78 prediction models and rankers, has been made freely available for wider dissemination.¹ 79 The rest of the paper is organised as follows. A brief overview of background 80 knowledge of ontologies and reasoning is given in Section 2, followed by a discussion 81 of closely-related work in Section 3. The suite of all metrics that characterise the design 82 complexity of OWL ontologies are formally defined in Section 4. The four variants 83 of the meta-reasoner R₂O₂* are described in detail in Section 5. Section 6 presents 84 the evaluation framework for building prediction models and the meta-reasoner. Our 85 detailed evaluation results and analysis are presented in Section 7. Lastly, we conclude 86 the paper and discuss future work in Section 8. 87

¹https://github.com/liyuanfang/r2o2-star

88 2. Ontologies and Reasoning

Ontologies organise domain knowledge in a structured and logical way. Semantic 89 Web ontologies have been widely used in many different areas as a medium for knowl-90 edge representation and data integration. Common ontology languages such as OWL 9. 1 [7] and OWL 2 [8] have formal semantics defined by Description Logics (DL) [32], a 92 family of logics created specifically for the purpose of knowledge representation. In 93 simple terms, knowledge in DL is characterised by abstract concepts, which represent 94 sets of entities; properties or roles, which are binary relations between entities; and indi-95 viduals, which represent entities themselves. Hence, a concept semantically represents 96 a set of individuals. 97

The logical nature gives rise to reasoning support for ontologies. These, among others, include concept satisfiability checking, concept subsumption checking, and classification. Concept satisfiability checking ensures that a concept can contain at least one individual. Concept subsumption checks whether two concepts have a sub-class relationship. Classification computes the subsumption relationship between all pairs of (named) concepts in an ontology.

For example, the following axioms in the *DL syntax* describe some knowledge about pizzas. Axioms (1) and (2) state that *AmericanHot* is a *Pizza*, and that it has some *MozzarellaTopping*. Axiom (3) states that *MozzarellaTopping* is a *CheeseTopping*. Axiom (4) states that *CheeseyPizza* is exactly those *Pizza* that has some *CheeseTopping*. Through classification, the concept *AmericanHot* is found to be subclass of *CheeseyPizza*, as it is a Pizza, and that it also has some *MozzarellaTopping*, which is a type of *CheeseyTopping*.

AmericanHot \sqsubseteq Pizza	(1)
$AmericanHot \sqsubseteq \exists has Topping. Mozzarella Topping$	(2)
$MozzarellaTopping \sqsubseteq CheeseTopping$	(3)
$CheeseyPizza \equiv Pizza \sqcap \exists hasTopping.CheeseTopping$	(4)

A number of different DLs have been proposed over the years. These DLs include

different combinations of language constructs, hence they have different expressive power. As a result, they also have different worst-case complexity results for core reasoning tasks. A detailed introduction to the syntax, semantics and complexity of these ontology languages can be found in the literature [7, 8].

Optimisation of ontology reasoning algorithms has been aggressively pursued over 116 the past decades, and a number of highly optimised reasoners have been produced. 117 These include sound and complete reasoners such as FaCT++ [33], HermiT [34], Kon-118 clude [12], and Pellet [13]; as well as the sound but incomplete reasoner TrOWL [14]. 119 Despite tremendous progress in optimisation, there has been ample empirical evidence 120 of the actual hardness of real-world ontologies [15, 25, 35]. Therefore, efficient reason-121 ing over large and expressive ontologies remains a computationally challenging task. 122 On the other hand, efficient reasoners dedicated to less expressive profiles have also 123 been developed. ELK [30] is such a concurrent reasoner for ontologies in the OWL 2 124 EL profile. 125

126 **3. Related Work**

Our related work is divided into the three categories according to the focuses in this paper: ontology metrics, prediction models for OWL reasoners, and algorithm selection and meta-reasoners.

Ontology Metrics. There has been research on the development of a series of metrics for 130 analysing ontology complexity [36]. The pioneering work for identifying the proposed 131 metrics in this paper is found in [24] that introduced a suite of 8 metrics with the 132 aim of characterising different aspects of ontology design complexity. Further, we 133 identified an additional 19 metrics that can measure different aspects of the size and 134 structural characteristics of an ontology [25]. These 27 metrics were used for predicting 135 discretised reasoning performance of reasoners. These 27 metrics were combined with 136 another set of metrics that capture ontology complexity in [26]. In total, 91 metrics 137 were collected and used to build models for predicting absolute reasoning performance 138 of reasoners. In this work, we use these 91 metrics to build prediction models and the 139

meta-reasoner $R_2O_2^*$. We also give the full definitions of all the 91 metrics, which have not been previously defined formally.

Prediction of Reasoning Performance. Ontology reasoning tasks are hard decision problems that may go beyond NP-hard. For very expressive DLs, ontology reasoning has a very high worst-case complexity of 2NExpTIME-complete [8]. For ontolgy reasoning optimisation, the research community have been interested in benchmarking of reasoner performance. In [15, 16], a number of modern reasoners were compared, and it was observed that the reasoners exhibit significantly different performance characteristics, thereby choosing an efficient reasoner for an ontology is a non-trivial task.

In a previous work [25], we developed classifiers to predict ontology classification 149 performance categories for FaCT++, HermiT, Pellet and TrOWL, using ontology metrics 150 as predictors [25]. The raw reasoning time is discretised into 5 increasingly large 15 categories. High prediction accuracy of over 80% is achieved for all the 4 reasoners. 152 Although highly accurate, the limitation of this work is that only the hardness category 153 is predicted, not the actual reasoning time. To overcome this problem, we further 154 investigated regression-based prediction models [26] to predict actual (or absolute) 155 reasoning time of reasoners. In this approach, regression analysis was applied to 156 estimate a numeric response variable (i.e. predicted reasoning time) from some predictor 157 variables (i.e. 91 ontology metrics). These regression models were built on a small 158 number of ontologies (i.e. 451) for 6 reasoners (FaCT++, HermiT, JFact, MORe, Pellet, 159 TrOWL). These were implemented in R². In this work, we improve upon these models 160 by using a modern, carefully curated dataset of 1,920 ontologies from the ORE 2015 16 reasoner competition [22], an additional robust learning algorithm XGBoost [28], and 162 an updated list of reasoners that includes Konclude [12] and ELK [30] (for OWL 2 163 EL ontologies only) and excludes TrOWL [14] as it is an approximate thus incomplete 164 reasoner. 165

Sazonau et al. [37] proposed a *local* approach to predicting OWL reasoner effi ciency. Small subsets of a given ontology are repeatedly created, on which reasoning

²https://www.r-project.org/

is performed. Reasoning time data is then used to extrapolate a reasoner's discretised reasoning time on the whole ontology. Principal component analysis (PCA) was also employed to reduce the number of features (metrics). Evaluation conducted on 357 ontologies and 3 reasoners shows that the local prediction method performs as well as the *global* approach [25]. Moreover, they observed that the prediction model based on one feature (number of axioms) has comparable performance as that using a set of 57 features.

In a similar spirit, we investigated the prediction of reasoning time of ABox-intensive
 OWL 2 EL ontologies [38] and energy consumption of reasoning tasks on the Android
 platform [39].

Algorithm selection and meta-reasoner. Algorithm selection [40] is the problem of selecting a well-performing algorithm for a given problem instance. It has been successfully applied to machine learning, combinatorial optimisation and constraint satisfaction problems [41, 42]. SATzilla [43], for instance, a portfolio-based SAT solver, has demonstrated higher efficiency over single solvers. Compared to SAT, ontology languages are more expressive with the inclusion of many more language constructs. As a result, it is more challenging to accurately characterising ontology complexity.

AutoFolio [31] is a state-of-the-art, general-purpose algorithm selection system that performs automatic algorithm selection as well as hyper-parameter tuning. In this paper we use AutoFolio as a strong baseline to evaluate $R_2O_2^*$ in Section 7.2.3.

CHAINSAW [44] first proposed the notion of a metareasoner for OWL ontologies. 188 Given a query (i.e. reasoning task) on an ontology, CHAINSAW constructs the smallest 189 possible subset of the ontology while guaranteeing completeness of answering the query. 190 This is achieved through the extraction of *locality-based modules* [45] using atomic 191 decomposition [46]. The size of the extracted module is dependent on the reasoning 192 task. For certain tasks such as consistency checking, the entire ontology needs to 193 be extracted, hence not resulting in gains in efficiency. Also, given the potentially 194 substantial overhead of computing modules, CHAINSAW may not be competitive for 195 simpler ontologies. As a prototype reasoner, CHAINSAW uses FaCT++ version 1.5.3 as the 196 delegate (i.e. component) reasoner. In the ORE 2015 ontology reasoner competition [47], 197

¹⁹⁸ CHAINSAW, CHAINSAW did not perform competitively against state-of-the-art reasoners:
¹⁹⁹ it was ranked 10/10 for the task of OWL DL classification and 11/13 for OWL EL
²⁰⁰ classification.

WSReasoner [48] is a hybrid reasoner designed for large and complex ontologies 20 in the description logic ALCHOI. Given an ontology O, WSReasoner builds two 202 approximate ontologies: a weakened version O_{wk} and a strengthened version O_{str} , both 203 of which are in the less expressive (thus less complex) logic ALCH. WSReasoner 204 employs two component reasoners: a consequence-based reasoner that classifies both 205 O_{wk} and O_{str} . As reasoning over O_{str} may not be sound, WSReasoner also employs a 206 tableau-based reasoner to verify these results obtained on O_{str} . In its evaluation on a 207 number of well-known hard ontologies including DOLCE, FMA and variants of Galen, 208 WSReasoner outperforms tableau-based reasoners FaCT++, HermiT, Pellet and the 209 approiimate, consequence-based reasoner TrOWL. 210

In our preliminary work [27], we proposed a meta-reasoner, R₂O₂, that makes use of 211 regression-based prediction models of six OWL 2 DL reasoners (i.e. FaCT++, HermiT, 212 JFact, Konclude, MORe, TrOWL). R₂O₂ takes two steps in the training phase. First, 213 given training ontologies characterised by a set of metrics [26] and their reasoning 214 time by the reasoners, R_2O_2 constructs a regression-based prediction model for each 215 of the six reasoners. Second, given another set of training ontologies, a ranking matrix 216 is generated using the prediction models. In the ranking matrix, each row represents 217 the values of the ontology metrics and a ranking of the reasoners according to their 218 predicted reasoning time. Several rankers were trained on this ranking matrix to learn 219 how ontology metrics can be mapped to a relative ordering by the *predicted* performance 220 of the reasoners. In the actual reasoning (testing) phase, given an unknown ontology, 221 R_2O_2 makes performance predictions for the reasoners. It then ranks the reasoners 222 according to their predicted reasoning time. The rankings recommended by the trained 223 rankers are averaged to determine a unique rank of each reasoner. The highest ranked 224 reasoner is chosen to perform the reasoning task for the unknown ontology. The 225 evaluation on R₂O₂ [27] shows that R₂O₂ outperforms all of the six state-of-the-art 226 OWL 2 DL reasoners, including Konclude [12], the most efficient OWL 2 DL reasoner. 227 As a baseline model to evaluate R_2O_2 [27], we also constructed a portfolio-based 228

OWL reasoner PR, which always selects the most efficient reasoner for any given ontology according to predicted reasoning time of all component reasoners.

R₂O₂ is different from PR in the following way. Instead of choosing the best reasoner according to predicted reasoning time of reasoners, as in PR, R₂O₂ selects a best possible reasoner from an aggregation of the *rankings* of component reasoners.

Recently a multi-criteria meta-reasoner Multi-RakSOR [49, 50] has been proposed 234 for reasoning about OWL 2 DL and EL ontologies. Multi-RakSOR incorporates two 235 objectives in selecting the best reasoner: reasoning efficiency and robustness. Efficiency 236 is measured by execution time. The robustness of a reasoner is measured by four ordered 237 *termination states*: (1) success (\mathcal{B}_{S}); (2) unexpected (\mathcal{B}_{U}), where the reasoning result is 238 not expected; (3) timeout (\mathcal{B}_T), where the reasoner times out on an ontology; and (4) 239 halt (\mathcal{B}_H), where the reasoner crashes. The ordering on these states is then defined to be 240 $\mathcal{B}_S \prec \mathcal{B}_U \prec \mathcal{B}_T \prec \mathcal{B}_H.$ 24

Multi-RakSOR encompasses two main components: (1) a multi-label classifier that 242 predicts the termination state of a reasoner, and (2) a multi-target regression model that 243 predicts the ranking of the reasoners (with tie breaking) that respects the above ordering. 244 A comprehensive evaluation of Multi-RakSOR is performed on the ORE 2015 245 reasoner competition ontology dataset³, which we also use for evaluating $R_2O_2^*$, and a 246 set of 10 OWL 2 DL/EL reasoners. The paper also describes an "upgraded" version of 247 Multi-RakSOR, dubbed Meta-RakSOR, that is able to handle both OWL 2 DL (more 248 expressive) and OWL 2 EL (less expressive) ontologies. Meta-RakSOR is evaluated on 249 the task of ontology classification on two datasets: one for OWL 2 DL and for OWL 250 2 EL. The main evaluation results show that for both datasets, Meta-RakSOR has the 25 highest number of ontologies successfully reasoned over. In terms of efficiency, for 252 OWL 2 DL, Meta-RakSOR demonstrates competitive performance (but not better) than 253 the best single reasoner Konclude. For OWL 2 EL, it is shown that Meta-RakSOR ranks 254 6th of the eleven reasoners evaluated, in terms of average reasoning time. 255

The meta-reasoners/hybrid reasoners described so far are all focussed on TBox reasoning (consistency checking or classification). PAGOdA [51] is a hybrid system

³https://zenodo.org/record/50737

designed for the task of *query answering* over ABox data. Employing an approach similar to WSReasoner [48], PAGOdA uses an efficient reasoner, in this case a Datalog reasoner, to compute a lower bound answer (sound but possibly incomplete) and an upper bound answer (complete but possibly unsound). When the two answers do not completely coincide, PAGOdA extracts relevant subsets from the TBox and the ABox are extracted, which are used to verify the answers by a fully-fledged OWL 2 DL reasoner.

265 4. Ontology Metrics

Metrics have been proposed to quantitatively measure the quality, complexity, testa-266 bility, and maintainability of ontologies. Inspired by software metrics [52], we proposed 267 a set of 91 metrics [24–26] for characterising the design complexity of ontologies. How-268 ever, the definition of many of these metrics were not formally given. In this section, 269 we give a detailed account of this suite of 91 metrics that comprehensively characterise 270 ontologies in terms of their size and syntactic and structural complexity. These metrics 27 serve as distinctive features for learning ontology reasoning prediction models and 272 building the proposed meta-reasoning framework $R_2O_2^*$. 273

These metrics are organised by what they characterise: (1) *the ontology itself*, (2) *classes*, (3) *anonymous class expressions*, and (4) *properties*. These metrics are proposed with efficient computation as a key consideration. In the calculation of metrics, we adopt a graph-based view of ontologies [24] to capture the complexity of ontologies and generate a set of metrics.

The subsequent subsections present details of the metrics. Note that a metric name 279 without the percent sign (%) is a count, and one with it is a ratio. A count metric 280 shows how a component of an ontology has impact on the reasoning performance 28 by its occurrences. A ratio metric is used to explain the relationship between such a 282 component with respect to the overall structure of the ontology. Intuitively, a count/ratio 283 metric represents the absolute/relative value of a metric of an ontology, respectively. We 284 note that all metrics are computed on the *asserted* ontology hierarchy. In other words, 285 no reasoning is performed prior to computing these ontologies. 286

287 4.1. Ontology-level Metrics (ONT)

The 6 ONT metrics were previously defined [24]. Here, we define an additional 18 ONT metrics that have not been described previously. They measure the overall size and complexity of an ontology.

IND counts the number of (named or anonymous) *individuals* in an ontology. The
 remaining 17 metrics are collected by observing the structure (i.e. language constructs)
 of a given ontology.

GCI/HGCI: These metrics measure the number of general concept inclusion (GCI) 294 axioms and hidden GCI (HGCI) axioms, respectively. GCI counts the number of sub-295 sumption axioms whose subclass is a complex concept (anonymous class expression). 296 HGCI counts the number of (named) concepts that appear as a subclass in some sub-297 sumption axioms as well as in some equivalent classes axioms. In general, the presence 298 of GCI axioms may increase reasoning complexity as they may introduce nondetermin-299 ism [53]. A GCI axiom is hidden when a named class is the LHS of a subclass axiom as 300 well as an equivalent class axiom. 30

Either an equivalent class axiom or a subclass axiom where the left-hand side of the subclass axiom is a named class.

ESUB%/DSUB%/CSUB%: These metrics measure ratios of subclass axioms that contain (possibly nested) specific types of class expressions, including those that are nested, and all subclass axioms. For these metrics, the subclasses and super classes are *flattened*, and an axiom is considered to contain a specific type of expressions iff one of the flattened expressions is of that type.

Respectively, ESUB%, DSUB% and CSUB% calculate the ratio of subclass axioms 309 that contain existential restrictions $(\exists R._)$, disjunctions $(_ \sqcup _)$, and conjunctions 310 $(_ \sqcap _)$. Additionally CSUB% requires that at least one of the conjuncts in the 311 subclass is an anonymous class expression. Existential restrictions (ESUB%) and 312 disjunctions (DSUB%) could generate AND-branching and OR-branching, respectively, 313 during the reasoning process. AND- and OR-branching are major sources of complexity 314 for tableau-based algorithms [54], hence their presence may negatively correlate with 315 performance. For the CSUB% metric, anonymous conjuncts in the subclass can generate 316

more axioms during the normalization process, hence it may increase workload for a reasoner.

ELCLS%/ELAX%: These two metrics measure the ratios of (nested) class expressions (ELCLS%) and axioms (ELAX%), respectively, in the OWL 2 EL profile, a sublanguage of OWL that is based on \mathcal{EL} [55], a description logic with efficient PTIME-complete algorithms. Our intuition is that as reasoning in the EL profile is in general easier, a reasoner such as MORe [56] that is able to delegate EL reasoning to an efficient EL reasoner could be more efficient with ontologies with a large percentage of EL expressions and axioms.

HLC/HLC%: These metrics are the count (HLC) and ratio (HLC%) of *hard* language constructs, which include disjunctions, transitive properties, inverse properties and property chains, in superclass expressions. These language constructs can potentially negatively influence the performance of ontology reasoners.

SUBCECHN/SUPCECHN: These metrics are the count of top-level class expressions containing *chained* (a sequence of) existential restrictions (i.e., $\exists R.C$ in the DL syntax) as a subclass (SUBCECHN) or a superclass (SUPCECHN). These metrics measure the impact of $\exists R.C$ expressions on the performance of reasoning as they can potentially slow down the reasoning process by increasing the search space.

For example, suppose an ontology contains two subsumption axioms: (1) $\exists R.(A \sqcap \exists R.(B \sqcap \exists P.C)) \sqsubseteq E$, and (2) $\exists R.(D \sqcap \exists R.(F \sqcap \exists P.G)) \sqsubseteq H$, where *R*, *P* represent properties and *A*, ..., *H* represent classes. For this ontology, SUBCECHN = 2 because axiom (1)'s subclass is a chained class expression containing existential restriction $\exists R.(A \sqcap \exists R.(B \sqcap \exists P.C))$ and axiom (2)'s subclass is also a chained existential restriction $\exists R.(D \sqcap \exists R.(F \sqcap \exists P.G))$. On the other hand, there is no chained class expressions containing existential restrictions as the superclass hence SUPCECHN = 0.

DSUBCECHN/DSUPCECHN: These count metrics calculate, in a depth-first manner, the maximum depth of nested class expressions containing existential restrictions as a subclass (DSUBCECHN) or a superclass (DSUPCECHN), with the intuition that deeper subclass chains may increase reasoning time. For example, suppose an ontology contains $\exists R.(A \sqcap \exists R.(B \sqcap \exists P.C)) \sqsubseteq E, D \sqcap \exists R.(F \sqcap \exists P.G) \sqsubseteq H$, where *R*, *P* represent properties and *A*, *B*, *C*, *D*, *E*, *F*, *G*, *H* represent classes. DSUBCECHN is 3 because the depth of nested class expressions containing existential restrictions in the first axiom $\exists R.(A \sqcap \exists R.(B \sqcap \exists P.C)) \sqsubseteq E \text{ is } 3 \text{ and that of the second axiom } D \sqcap \exists R.(F \sqcap \exists P.G) \sqsubseteq H$ is 2. In addition, there is no nested class expression containing existential restrictions in the superclass, hence DSUPCECHN is 0.

SUBCCHN/SUPCCHN: These metrics represent the number of class expressions containing *chained* conjunction expression as a subclass/superclass. For tableau-based algorithms, conjunctions of complex concepts in a subclass may not be easily normalised for some reasoners. Hence a subclass expression containing many complex class expressions may slow down the reasoning process.

DSUBCCHN/DSUPDCHN: These metrics represent maximum depth of nesting
 of class expressions containing disjunction expressions as a subclass/superclass. The
 idea of these metrics is similar to the metrics DSUBCECHN/DSUPCECHN.

In total there are 24 ONT metrics, which are summarised in Table A.12 in the appendix.

362 4.2. Class-level Metrics (CLS)

The CLS metrics capture characteristics of classes, which are first-class citizens in OWL ontologies. Five functions, NOC (number of children), NOP (number of parents), 364 DIT (depth of inheritance tree), CID (class in-degree), and COD (class out-degree), 365 were defined previously [24]. Each of these functions returns, for a (named or possibly 366 nested anonymous) class expression in an ontology, a count value respectively. For a 367 given class C, NOC(C) and NOP(C) return the number of direct subclasses and super classes of C in the ontology, respectively. DIT(C) returns the longest path from C to \top , 369 the root class, in a depth-first manner. CID(C) and COD(C) calculate, respectively, the 370 number of incoming and outgoing edges of C. 37

For each of these five functions, we identify three metrics: the *total*, the *average*, and the *maximum* values across all classes for a given ontology. For example for NOC, the total NOC (tNOC) is calculated by summing the NOC value for all classes in an ontology, and the average NOC (aNOC) is tNOC divided by the total number of class expressions. Similarly, the maximum NOC (mNOC) is the maximum number of children among all classes. Thus, in total, 15 CLS metrics are identified, which are shown in Table A.13 in the appendix.

380 4.3. Anonymous Class Expression Metrics (ACE)

The ACE metrics are an important ingredient in building expressive classes. Dif-38 ferent types of anonymous class expressions can have different impact on reasoning 382 performance. The 9 ACE count metrics have been previously defined [25], one for 383 each different type of (possibly nested) anonymous class expressions (enumerations, 384 negations, conjunctions, disjunctions, universal restrictions, existential restrictions, and 385 min/max/exact cardinality restrictions). We further define two additional ACE count 386 metrics that represent the number of value restrictions (VALUE, for $\exists R.\{a\}$, where a 387 is an individual) and *self references* (SELF, for $\exists R.self$). We also propose their corre-388 sponding ratio metrics that measure the percentage of each count ACE metric over all 389 (possibly nested) anonymous class expressions. 390

Hence in total there are 22 ACE metrics, shown in Table A.14 in the appendix.

392 4.4. Property Metrics (PRO)

Additional pairs of count and ratio metrics are defined: ASYM/ASYM% (asymmetric properties), REFLE/REFLE% (reflective properties), IRREF/IRREF% (irreflective properties), and CHN/CHN% (property chains).

Similarly, the 6 of the 8 existing count PRO metrics [25] are augmented with 396 their corresponding ratio metrics. For example, the DTP metric counts the number of 397 datatype properties. The metric DTP% records the ratio between the number of datatype 398 properties and the total number of properties. These 6 are: OBP (object properties), 399 DTP (datatype properties), FUN (functional properties), SYM (symmetric properties), 400 TRN (transitive properties), and IFUN (inverse functional properties). Furthermore, 40 four count metrics are defined to record the number of some property axioms, including 402 SUBP (subproperties), DISP (disjoint properties), DOMN (domain), and RANG (range). 403 Finally, four additional metrics are defined to measure the usage of properties in an 404 ontology. 405

ELPROP%: This metric measures the ratio, of all property axioms, the number of
 property axioms allowed in the OWL 2 EL profile, which include subproperty axioms,
 equivalent property axioms, transitive axioms, reflexive axioms, domain/range axioms,
 and functional data property axioms. Intuitively, the higher the ELPROP% of an
 ontology is, the more efficient its reasoning may be.

- IHR, IIR, ITR: These metrics measure the count of class axioms (e.g., subclass axioms and class/property assertions) that make use of some property in some property hierarchy (IHR), inverse properties (IIR), and transitive properties (ITR). The intuition is that the more these types of properties are used in class axioms, the more difficult reasoning may be for this ontology.
- ⁴¹⁶ There are in total 30 PRO properties as summarised in Table A.15.

417 5. Meta-Reasoning Models

In this section, as our major contributions of this paper, we propose our metareasoning framework $R_2O_2^*$ and its four different *meta-reasoning models* (simply *meta-reasoners*). Each meta-reasoner recommends the most efficient reasoner for unknown ontologies using different machine learning techniques. We first introduce basic notations we use in the paper. Then, we present the details of the four metareasoners with their learning objectives in the training phase and their utilisation in the recommendation (or testing) phase.

425 5.1. Notation Definition

- ⁴²⁶ The following basic notations are used in the paper.
- Let $R = \{r_1, ..., r_n\}$ be a set of *n* reasoners, also called *component reasoners* in the paper.
- Let $\hat{R} = {\hat{r}_1, ..., \hat{r}_n}$ be a set of *n* prediction models such that \hat{r}_i predicts the reasoning time of r_i .
- Let $OM = \{om_1, ..., om_q\}$ be a set of q ontology metrics.
- Let $O = \{o_1, ..., o_h\}$ be a set of *h* ontologies that can be reasoned about by at least one reasoner in *R* without timing out or errors. Each ontology in *O* is represented using its values of ontology metrics *OM* in this paper.

- Given a reasoner r and an ontology o, let $\theta(r, o)$ represent the actual reasoning time
- of *r* for *o* for the task of ontology classification. Similarly, let $\theta(\hat{r}, o)$ represent the

reasoning time predicted by \hat{r} for o for the same task.

• Two partitioned subsets O_{tr} and O_{te} are drawn from O for training and testing the proposed meta-reasoners, respectively.

440 5.2. Details of the Meta-Reasoners

In the following, we present the details of each of our four meta-reasoners. For each reasoner, we describe its learning objective and how to build it in detail. All these meta-reasoners are built on the training dataset $O_{tr} \subset O$.

The first meta-reasoner, $R_2O_2^{*}(pt)$, directly trains prediction models \hat{R} of R on the 444 training data O_{tr} , and uses the predicted reasoning time that has been estimated by \hat{R} 445 to find the most efficient reasoners for unknown ontologies. The underlying idea is to 446 choose a reasoner r, whose predicted reasoning time estimated by \hat{r} is the most efficient 447 among \hat{R} , as the most efficient reasoner for an unknown ontology. The second meta-448 reasoner, $R_2O_2^*(rk)$, trains a ranking algorithm to learn the rankings of the reasoners 449 in R according to the actual reasoning time of the training data O_{tr} , and uses it to 450 predict the best ranked reasoners for unknown ontologies. The third meta-reasoner, 45 $R_2O_2^{*}(mc)$, trains a classifier that learns the most efficient reasoner on O_{tr} , and uses 452 it to directly predict the most efficient reasoners for unknown ontologies. The forth 453 meta-reasoner, R2O2*(all), is an ensemble classifier that uses the predictions of the above 454 three meta-reasoners. 455

456 5.2.1. Meta-reasoner based on the direct use of predicted reasoning time: $R_2O_2*_{(pt)}$

The meta-reasoner $R_2O_2^{*}_{(pt)}$ aims to recommend the most efficient reasoners for unknown ontologies based on the *direct use of the predicted reasoning time* of all reasoners in *R*. Therefore, for all reasoners in *R*, building their corresponding prediction models \hat{R} is essential prior to making use of $R_2O_2^{*}_{(pt)}$ for determining such most efficient reasoners. $R_2O_2^{*}_{(pt)}$ is similar to the non-ranking portfolio reasoner PR described in our preliminary work [27] in that it leverages predicted reasoning time of \hat{R} . The difference is that $R_2O_2^{*}_{(pt)}$ uses an ensemble regression model instead of using a random forest regression algorithm as PR [27]. Also, $R_2O_2^{*}_{(pt)}$ incorporates the average rankings of the reasoners on the training data when there are more than two reasoners that were chosen as the most efficient (i.e. their predicted reasoning time is the same), while PR chooses one in random. The details of resolving a tie-breaking method $R_2O_2^{*}_{(pt)}$ is explained below.

Consequently, the effectiveness of $R_2O_2^{*}(pt)$ relies mainly on the accuracy of the 469 prediction models in \hat{R} . In order to build such prediction models, we use *stacking* [57], 470 an ensemble learning technique to combine multiple classification (or regression) models 47 in which (1) base learners (or regression models) (or level-0 models) are trained on the 472 training data O_{tr} , and (2) the outputs of the base learners are combined using a *meta*-473 learner (or meta-regression models) (level-1 model), in our context. More specifically, 474 for each reasoner, each learner is trained to learn a mapping function from the values 475 of ontology metrics on the training data O_{tr} to their actual reasoning time. Then, a 476 meta-learner is trained to learn a mapping function from the predicted outputs of O_{tr} , 477 which have been estimated by the base learners, to actual reasoning time. 478

Here, our aim is to use the decisions of the individual base learners that employ
different learning criteria, and to combine their decisions to outperform each individual
base learner using a meta-learner.

More formally, to build each prediction model $\hat{r}_k \in \hat{R}$ for reasoner $r_k \in R$, we represent each ontology $o_i \in O_{tr}$ as follows:

$$o_{i} = \underbrace{om_{i,1}, \dots, om_{i,q}}_{\text{ontology metrics}}, \underbrace{\theta(r_{k}, o_{i})}_{\text{actual reasoning time}}$$
(5)

where $om_{i,j}$ is the value of the *j*-th ontology metric om_j of ontology o_i , and $\theta(r_k, o_i)$ denotes the actual reasoning time of r_k on ontology o_i .

Using the above representation scheme, for each reasoner, we train *k* base learners (level-0 models) on O_{tr} . Then, we generate level-1 data obtained from the predictions of the *k* base learner over the instances in O_{tr} . The level-1 data have *k* attributes whose values are the predictions (i.e. predicted time) of the *k* base learners for every instance in O_{tr} . Thus, each training example for a meta-learner (level-1 model) will be composed of *k* attributes (e.g. *k* predictions from the *k* base learners) and the target which is the actual reasoning time for every instance in O_{tr} . Once the level-1 data have been built from all instances in O_{tr} , any learning regression models can be used to generate the meta-learner. In this paper we choose k = 2.

In this paper, we use two robust base learners: (1) the *random forest regression algorithm* and (2) the *XGBoost (eXtreme Gradient Boosting)* algorithm [28]:

Random forest regression algorithm: As a base learner, we build a regression model using *random forest regression algorithm*, an efficient and robust learning model, which has produced good predictive performance in our previous work [26].
In our context, the random forest model combines a number of *decision trees*, each of which is trained using a subset of training ontologies, to build a prediction model for a given reasoner.

• XGBoost: As another base learner, we use the state-of-the-art learning algorithm, XGBoost [28], which has recently shown dominant performance on a number of Kaggle competitions for structured or tabular data. It is an implementation of gradient boosted decision trees designed for achieving better computational efficiency and prediction performance.

We again consider random forest and XGBoost as candidates of a meta-learner (level-1 model) due to their strong predictive performance. These level-1 candidates are denoted by meta-RF and meta-XGBoost in this paper. As can be seen in Section 7.1.1, we eventually choose meta-XGBoost as our meta-learner given its best overall performance.

Once we train the meta-regression model on O_{tr} , given an unknown ontology in the testing data O_{te} , the meta-reasoner $R_2O_2^*_{(pt)}$ will recommend a reasoner whose predicted reasoning time is the fastest among all of the predictions of the prediction models in \hat{R} as the most efficient reasoner.

If more than two reasoners are chosen as the most efficient, a tie-breaking method is also applied to select one of them. This method takes into consideration the *precision at 1* (P@1) of the reasoners in *R* that are measured on the training data O_{tr} . In this context, for each reasoner in *R*, its P@1 is measured by the proportion that the reasoner is the most efficient across all instances in O_{tr} . Our tie-breaking method chooses the reasoner with the highest P@1. This tie-breaking method is applied to all the other

⁵²¹ meta-reasoners in our $R_2O_2^*$.

522 5.2.2. Meta-reasoner based on ranking algorithm: $R_2O_2^*_{(rk)}$

⁵²³ $R_2O_2^{*}(rk)$ is a meta-reasoner that learns the rankings of the reasoners in *R*. During ⁵²⁴ the training phase, it trains a *ranking algorithm* (simply *ranker*) that learns the rankings ⁵²⁵ of the reasoners on O_{tr} in terms of their reasoning time. Once the ranker is trained, ⁵²⁶ given an unknown ontology in O_{te} , $R_2O_2^{*}(rk)$ ranks and recommends the most efficient ⁵²⁷ reasoner for that ontology.

⁵²⁸ $R_2O_2^*(rk)$ follows a similar spirit of R_2O_2 [27] in that $R_2O_2^*(rk)$ uses a *ranking* ⁵²⁹ *matrix* and uses a ranker. The difference is that $R_2O_2^*(rk)$ uses a single ranker, rather ⁵³⁰ than aggregating multiple rankers as R_2O_2 , to recommend the most efficient reasoner ⁵³¹ for an unknown ontology. Given a pool of rankers using different criteria for learning, ⁵³² we have chosen the one with the best ranking performance through our experiments ⁵³³ which will be further discussed in Section 7.1.1.

Given the training data O_{tr} , we generate a *ranking matrix*, where each row represents the values of ontology metrics and the rankings of reasoners *R* according to their actual reasoning time. Then, a ranker is trained on this matrix to learn how the characteristics of the ontologies in O_{tr} can be optimally mapped to the relative ordering of the reasoning performance of the reasoners in *R*. Initially, we build an $|O_{tr}| \times (q + n)$ data matrix $\mathbf{M}_{\mathbf{d}}$ (recall that q = |OM|, $n = |R| = |\hat{R}|$), where row *i* represents an ontology $o_i \in O_{tr}$ and the actual reasoning time of the reasoners in *R* for o_i :

$$o_i = \underbrace{om_{i,1}, \dots, om_{i,q}}_{\text{ontology metrics}}, \underbrace{\theta(r_1, o_i), \dots, \theta(r_n, o_i)}_{\text{actual reasoning time}},$$
(6)

where $om_{i,j}$ is the value of the *j*-th ontology metric om_j of o_i , and $\theta(r_s, o_i)$ denotes r_s 's actual reasoning time for o_i . From $\mathbf{M}_{\mathbf{d}}$, we build the corresponding $|O_{tr}| \times (q+n)$ ranking matrix $\mathbf{M}_{\mathbf{r}}$, where row *i* is represented as:

$$o_i = \underbrace{om_{i,1}, \dots, om_{i,q}}_{\text{ontology metrics}}, \underbrace{\pi(r_1, o_i), \dots, \pi(r_n, o_i)}_{\text{ranking of reasoners}},$$
(7)

where $\pi(r_s, o_i)$ denotes the *rank* of $r_{s_{[1,n]}} \in R$ for o_i determined by $\theta(r_s, o_i)$. On **M**_r, the more efficient a reasoner is, the higher ranked it is (the smaller the rank number). To illustrate this, suppose there are 3 reasoners $\{r_1, r_2, r_3\}$, and their actual reasoning time for an ontology o_i is 100s, 90s, and 10s, respectively, i.e., $(\theta(r_1, o_i), \theta(r_2, o_i), \theta(r_3, o_i))$ = (100s, 90s, 10s). Thus, the ranking is $(\pi(r_1, o_i), \pi(r_2, o_i), \pi(r_3, o_i)) = (3, 2, 1)$. If the reasoning time is (10s,10s,100s) instead, the ranking will be (1, 1, 3).

In summary, the goal is to learn rankings of all reasoners in *R* on the ranking matrix M_r , and to predict a ranking of the reasoners for an unseen ontology. The top-ranked reasoner will be chosen by the meta-reasoner $R_2O_2^*(_{rk})$ to be the most efficient reasoner to reason over the ontology. Comparing to $R_2O_2^*(_{pt})$, the main feature of $R_2O_2^*(_{rk})$ stems from that it is built on the ranking matrix that uses rankings of the reasoners in *R*, rather than the direct use of the predicted reasoning time estimated from \hat{R} .

546 5.2.3. Meta-reasoner based on multi-class classification: $R_2O_2^*(mc)$

 $R_2O_2*_{(mc)}$ formulates the learning problem into a multi-class classification problem, where its goal is to classify an ontology with one of the reasoners that is able to reason about the ontology the most efficiently. During the training phase, $R_2O_2*_{(mc)}$ learns the most efficient reasoner for each ontology on the training data O_{tr} . The most efficient reasoner is determined by means of the actual reasoning time of the reasoners in *R*, meaning that the fastest reasoner is chosen as the most efficient reasoner.

More formally, to build $R_2O_2^*(mc)$, we represent each ontology $o_i \in O_{tr}$ as follows:

$$o_i = \underbrace{om_{i,1}, \dots, om_{i,q}}_{\text{ontology metrics}}, \underbrace{\gamma_i}_{\text{the most efficient reasoner}}$$
(8)

where $om_{i,j}$ is the value of the *j*-th ontology metric om_j of o_i , and γ_i denotes the actually most efficient reasoner for o_i . If there is an ontology $o_i \in O_{tr}$ that has *k*-reasoners (where k > 1) that show the equivalently most efficient reasoning time, we generate *k* instances with *k* most efficient reasoners for o_i . For example, given on ontology o_i , suppose that there are two most efficient reasoners: Konclude and Pellet. We then generate two instances for o_i as follows: (1): " $om_{i,1}, \ldots, om_{i,q}$, Konclude", and (2) " $om_{i,1}, \ldots, om_{i,q}$, Pellet".

Using the above representation scheme, we train a classifier on the training data O_{tr} . In our experiments, we have considered two classifiers: (1) *random forest algorithm* and (2) *XGBoost*, because of their robust classification performance as in the case of the meta-reasoner $R_2O_2^{*}(pt)$. Based on our cross-validation on O_{tr} , we eventually choose

XGBoost which will be further discussed in Section 7.1.1.

In comparison with the meta-reasoner $R_2O_2^{*}_{(pt)}$, $R_2O_2^{*}_{(mc)}$ does not directly use the predicted reasoning time of the reasoners in *R*, that is, it does not rely on \hat{R} . Rather it learns which reasoners have been the most efficient reasoners for ontologies in the training data O_{tr} . The learning goal of $R_2O_2^{*}_{(mc)}$ is similar to the meta-reasoner $R_2O_2^{*}_{(rk)}$ in that its learning is based on the ranks of the reasoners in *R* on the training data O_{tr} . However, $R_2O_2^{*}_{(mc)}$ differs in that it learns the most efficient reasoner only, not the rankings of all reasoners in *R* as $R_2O_2^{*}_{(rk)}$.

572 5.2.4. Ensemble meta-reasoner: $R_2O_2^*$ (all)

⁵⁷³ $R_2O_2*_{(all)}$ is a stacking classifier that learns from the predictions of the above three ⁵⁷⁴ meta-reasoners: (1) $R_2O_2*_{(pt)}$ that directly uses the predicted reasoning time of reasoners ⁵⁷⁵ for the training set O_{tr} , (2) $R_2O_2*_{(rk)}$ that learns the rankings of reasoners by means ⁵⁷⁶ of their actual reasoning time for O_{tr} , and (3) $R_2O_2*_{(mc)}$ that learns the most efficient ⁵⁷⁷ reasoners for ontologies in O_{tr} . In other words, in $R_2O_2*_{(all)}$, those three meta-reasoners ⁵⁷⁸ can be seen as base classifiers (i.e. level-0 models), and $R_2O_2*_{(all)}$ learns a meta-classifier ⁵⁷⁹ (i.e. level-1 model) from the predictions of the base classifiers.

Thus, $R_2O_2^*_{(all)}$ trains a meta-classifier on the training data O_{tr} , where each ontology $o_i \in O_{tr}$ is represented as follows:

$$o_i = \underbrace{\mathbf{R}_2 \mathbf{O}_2^*(\mathbf{pt})(o_i), \mathbf{R}_2 \mathbf{O}_2^*(\mathbf{rk})(o_i), \mathbf{R}_2 \mathbf{O}_2^*(\mathbf{mc})(o_i)}_{\text{predicted reasoners of the meta-reasoners}}, \underbrace{\gamma_i}_{\text{the most efficient reasoner}}$$
(9)

where $R_2O_2^{*}(pt)(o_i)$, $R_2O_2^{*}(rk)(o_i)$ and $R_2O_2^{*}(mc)(o_i)$ are the predicted most efficient reasoners of $R_2O_2^{*}(pt)$, $R_2O_2^{*}(rk)$, $R_2O_2^{*}(mc)$, respectively, for o_i . As in Equation 8, γ_i denotes the actually most efficient reasoner for o_i .

As candidates for a meta-classifier, we also consider the same learning algorithms used to built the meta-reasoner $R_2O_2*_{(pt)}$ because of the same reason: their proven, robust predictive performance: (1) random forest algorithm and (2) XGBoost. The one with the better performance from these two candidates is chosen, where the performance is measured via cross-validation on the training data O_{tr} . Eventually, XGBoost is chosen as our meta-classifier which will be presented in Section 7.1.1. Thus, $R_2O_2^{*}(all)$ trains the meta-classifier that learns relationships between the predicted reasoners of the previous three meta-reasoners and the actually most efficient reasoners on the training data O_{tr} , and then make predictions about the most efficient reasoners for unknown reasoners for the testing ontologies O_{te} .

593 5.2.5. Meta-reasoners with ELK

In the previous sections, we have presented the four different meta-reasoners in $R_2O_2^*$. Note that all of these meta-reasoners utilise a number of high-performance DL reasoners. Here, an interesting question is whether incorporating an EL reasoner into the meta-reasoners, such as ELK [30], can further improve reasoning efficiency for the less complex OWL 2 EL ontologies.

To address this question, we augment our meta-reasoners to incorporate an EL reasoner, ELK, that is designed to support the less expressive OWL 2 EL profile. ELK does not support reasoning over non-EL ontologies. Thus, the meta-reasoners only incorporate ELK when predicting the most efficient reasoners for unknown OWL 2 EL ontologies.

First, we train a prediction model for ELK on the training data O_{tr} following the steps presented in Section 5.2.1. Then, given an ontology $o \in O_{te}$ whose reasoning time is unknown, each meta-reasoner (representatively denoted by $R_2O_2^*$) is extended by taking the following further steps to find the most efficient reasoner to reason about o:

- 1. Check whether *o* is an EL ontology or not.
 - If *o* is an EL ontology, compare the predicted reasoning time and the most efficient reasoner determined by R₂O₂*. Then, we choose the fastest one as the most efficient reasoner. Formally,

$$\hat{\gamma}(o) = \underset{\hat{r}_i \in \mathbb{R}_2 O_2 *, \hat{r}_{elk}}{\operatorname{argmin}} \theta(\hat{r}_i, o) \tag{10}$$

where $\hat{\gamma}(o)$ is the most efficient reasoner for o determined eventually; $\theta(\hat{r}_i, o)$ is the predicted reasoning time of the reasoner r_i for o; and \hat{r}_{elk} is the prediction model of ELK. ⁶¹² 3. If *o* is not an EL ontology, follow the recommendation of $R_2O_2^*$ not considering ⁶¹³ r_{elk} .

Thus, in our extension for EL ontologies, for each meta-reasoner, the main idea is to simply incorporate predicted reasoning time of ELK and the most efficient reasoner determined by the meta-reasoner, to compare their reasoning time, and finally to recommend the one with the most efficient predicted reasoning time.

Here we summarise the main differences between our meta-reasoning framework $R_2O_2^*$ and our preliminary meta-reasoner R_2O_2 and the portofolio-based meta-reasoner PR, which were described in detail in Section 3.

1. As a framework (but not individual meta-reasoners), $R_2O_2^*$ adapts and incorporates both R_2O_2 (as $R_2O_2^*(rk)$) and PR (as $R_2O_2^*(pt)$).

 ⁶²³ 2. R₂O₂* incorporates more advanced prediction models (Random Forests and XGBoost) through *ensembling*.

 $R_2O_2^*$ generates a ranking matrix using the actual reasoning time of the component reasoners. On the other hand, R_2O_2 built a ranking matrix using the predicted reasoning time of the reasoners, where such time was estimated by prediction models.

4. $R_2O_2^*$ incorporates a single best ranker instead of using an aggregation of multiple rankers as R_2O_2 . The single best ranker is determined empirically through crossvalidation on the training data.

 $_{632}$ 5. $R_2O_2^*$ invokes the efficient reasoner ELK [30] directly for OWL 2 EL ontologies.

6. R₂O₂* is built using a different mix of component reasoners that includes Pellet
 (which R₂O₂ does not include) but excludes TrOWL, as TrOWL is an approximate,
 therefore incomplete reasoner.

Finally, R₂O₂* is built and evaluated using a more modern set of ontologies and
 more recent versions of reasoners.

In the following sections, we discuss our evaluation framework and results that compare the performance of all the proposed meta-reasoners (with and without ELK) using the ORE 2015 competition corpus [22].

641 6. Evaluation Framework

In this section, we describe the evaluation framework used for evaluating the proposed prediction models and meta-reasoners, including details of the reasoners, ontologies and the evaluation environment. The notations used in this section follow those defined in Section 5.1.

Reasoners: Six state-of-the art OWL 2 DL reasoners that participated in ORE the 646 2015 reasoner competition [22] are used as component reasoners (simply reasoners)⁴: 647 FaCT++ [10], HermiT [34], JFact,⁵ Konclude [12], MORe [56] (with HermiT as the 648 underlying OWL 2 DL reasoner), and Pellet [13]. Besides these six OWL DL reasoners, 649 we also incorporate ELK [30], the efficient reasoner for the less expressive OWL EL 650 profile. The versions of the reasoners are the same as those in ORE 2015. As described 65 in Section 5, we build a prediction model for each reasoner, which is one of the key 652 components in the meta-reasoner framework R2O2*. 653

Target Reasoning Task: For the ontology reasoning task, we choose ontology *classification*. The actual reasoning time (wall-time) of each ontology in the dataset was measured on a high-performance server running CentOS Linux 7.4 (Core) and Java 1.8 on single-core Intel Gold 6140 each at 2.3 GHz, with a maximum of 10 GB memory allocated to the reasoner. A timeout of *30 minutes* of wall-time is imposed on each (reasoner, ontology) pair.

To ensure consistency of the evaluation across reasoners, the ORE 2015 competition framework⁶ is used to invoke all reasoners and record their reasoning time. For each ontology, the competition framework converts it into the OWL functional syntax (FSS),

⁴Chainsaw [44] and Racer [58] (two OWL 2 DL reasoners that participated in ORE 2015) are excluded due to reasoning errors in an excessive number of ontologies.

⁵http://jfact.sourceforge.net

 $^{^{6} \}tt https://github.com/andreas-steigmiller/ore-competition-framework$

invokes reasoners for classification using a Bash shell script, and records reasoning time
 using the GNU time command. We follow the framework and include ontology loading
 time as part of classification time.

Ontologies: We collected all 1,920 ontologies from the ORE 2015 reasoner competition [22] ⁷. Prior to building our proposed meta-reasoners, we performed the three preprocessing steps on the 1,920 ontologies, following the steps in [26, 27]. The aim of these steps is to remove duplicate ontologies that may exist in the given ontology collection, normalise their metric values to avoid the high skewness of values of ontology metrics *OM*, and remove ontology metrics that may influence learning a prediction model with lower prediction accuracy:

Cleansing: Since the given ontology collection has been obtained from multiple
 repositories, it may contain duplicates. All but one ontology is removed from
 each set of ontologies with duplicate metric values. After removing duplicates,
 1,760 ontologies remained.

Normalisation: In the given 1,760 ontology collection, values of some of the
 metrics span a large range and are very skewed as discussed in [26]. We apply a
 commonly-used log-transformation on the metric values of the ontologies that are
 greater than 10. The log-transformation is also performed on reasoning time.

3. Metric removal: It is a widely used practice to remove features that have near-zero 681 variance values and features that are highly correlated (with respect to the dataset). 682 In this paper we follow this practice. Following our previous work [26, 27], we 683 consider two metrics with correlation coefficients above 0.9 to be highly correlated. 684 To observe a better generalised distribution of these metrics, we measure their 685 correlation on a larger ontology collection, the one used in the ORE 2014 reasoner 686 competition [21]. It contains 16,555 ontologies, which are split into four groups 687 by percentiles of file size. Ontologies are randomly sampled from within these 688 groups. This is to ensure that files of different sizes are sufficiently represented. 689

⁷http://owl.cs.manchester.ac.uk/publications/supporting-material/ ore-2015-report/

Given correlation calculated from this ontology collection, we remove all but
29 metrics: 12 ONT metrics (SOV, ENR, EOG, CYC, RCH, IND, ESUB%,
ELCLS%, ELAX%, HLC, HLC%, SUPCECHN); 7 CLS metrics (tNOC, aNOC,
aCID, mCID, tCOD, aCOD, aNOP); 4 ACE metrics (CONJ%, UF%, EF, EF%);
and 6 PRO metrics (OBP%, DTP%, FUN%, CHN%, ELPROP%, IHR).

⁶⁹⁵ Finally, as our ontology collection (*O*), we used 1,760 ontologies, where each ⁶⁹⁶ ontology is represented by the 29 metrics and the metric values are log-scaled.

Table 1 shows, for each reasoner, the total number of ontologies it successfully 69 handled, that result in an error, and that time out, and brief statistics of reasoning time 698 (in seconds, and excluding those ontologies that time out). It can be observed that 699 the reasoning time spans a large range for all the reasoners, and that Konclude is the 700 most efficient as well as most robust reasoner (the least number of error and timeout 70' ontologies). In total, 1,269 ontologies (excluding timeout ontologies) were reasoned 702 about successfully (no error, no timeout) by all the six reasoners, and 1,390 ontologies 703 did not result in a runtime error (timeout ontologies are included in this case). Note that 704 timeout ontologies are used to evaluate our meta-reasoners in one set of experiments. 705 Figure 1 in Section 7 depicts the performance characteristics of the component reasoners 706 in more details in violin plots. Of the 1,760 ontologies, 761 are in the OWL 2 EL profile. 707 Hence, we performed classification on these ontologies using ELK. 708

Evaluation method: We evaluate our meta-reasoners with the state-of-the-art algorithm 709 selection framework AutoFolio [31] that is configured to minimise runtime. As discussed 710 earlier in Section 5, meta-reasoners PR and R2O2 described in our previous work [27] 71 are similar to R₂O₂*(pt) and R₂O₂*(rk), respectively. Hence this comparison also assesses 712 the performance of $R_2O_2^*$ (all) against our previous models. We also attempted to 713 evaluate our meta-reasoners against a recently proposed multi-criteria meta-reasoner 714 Meta-RakSOR [49, 50], which has dual optimisation objectives of reasoning correctness 715 as well as efficiency. However, we are unable to evaluate Meta-RakSOR due to two 716 reasons. Firstly, for the OWL 2 DL classification task, Meta-RakSOR incorporates 717 eight component reasoners but our meta-reasoners only incorporates six. Among the 718 two reasoners that are not considered by our meta-reasoners, TrOWL [14], which is 719

Reasoner	No. of	gies	Reasoning time (s)					
Reasoner	Successful	Error	Timout	М	in	Max	Median	Mean
FaCT++	1,461	109	190	0.	53	1,638.6	1.4	72.4
HermiT	1,658	51	51	0.	70	1,622.4	3.6	35.8
JFact	1,292	161	307	1.	03	1,788.6	3.4	72.8
Konclude	1,737	8	15	0.	03	1,087.2	0.3	3.7
MORe	1,706	18	36	2.	00	1,684.5	4.5	87.1
Pellet	1,477	114	169	1.	01	1,773.9	3.5	39.5

Table 1: A summary of statistics of the deduplicated ORE 2015 competition dataset containing a total of 1,760 unique ontologies. Note the reasoning time is measured in seconds and without considering timeout ontologies.

an approximate hence incomplete reasoner, and RACER [59], which did not execute 720 properly on our evaluation hardware. Secondly, even though Meta-RakSOR has released 72' source for running the meta-reasoner⁸, it however does not include the source code 722 of Meta-RakSOR itself. Therefore we are unable to modify it and compare with it. 723 However, as can be seen from Table 1 of Meta-RakSOR [50], Meta-RakSOR does 724 not outperform Konclude on average reasoning time, it is thus not unreasonable to 725 hypothesise that our meta-reasoners would outperform Meta-RakSOR, as our meta-726 reasoners outperform Konclude. 727

In our evaluation we retain timeout ontologies to realistically assess performance of all reasoners. We assess the impact of those ontologies that result in a runtime error in two different experiments. In the first experiment (hereinafter referred as **ErrorsRemoved**), the error ontologies for each reasoner are removed. In the second experiment (hereinafter referred as **ErrorsReplaced**), the error ontologies for each reasoner are treated as they timeout. Note that in ErrorsRemoved, it may be the case that a reasoner that strictly conforms to OWL semantics may throw many runtime errors

⁸https://github.com/Alaya2016/Multi-RakSORDemo

on a corpus of ontologies as it may reject non-conformant constructs (e.g. imaginary
 numbers). As such, such a reasoner may turn out to be efficient in the experiment
 ErrorsRemoved than in ErrorsReplaced.

In each experiment, standard 10-fold cross validation is performed to adequately assess the performance of the meta-reasoners. That is, we take the following steps: (1) shuffle the ontologies *O* randomly; (2) split *O* into 10 subsets; (3) for each subset, take the subset (i.e 10%) as test set (O_{te}), and take the remaining subsets (i.e. 90%) as a training set (i.e. O_{tr}); (4) fit a model on the training set and evaluate it on the test set; and (5) average the evaluation scores of the model across 10-times.

As evaluation metrics, average runtime (i.e. reasoning time) is used as the main 744 evaluation metric for the meta-reasoner. To evaluate our runtime prediction (regression) 745 models, we used the standard 'coefficient of determination' (R^2) as used in [26]. R^2 746 denotes the proportion of the variation in the target variable (i.e. reasoning time) that 747 can be explained by each prediction model $\hat{r} \in \hat{R}$. The higher the R^2 value is, the more 748 accurate the model is. Moreover, we evaluate our meta-reasoners using the standard 749 metric precision at 1 (P@1), as the meta-reasoners require the predicted best reasoner. 750 The performance number reported in the rest of the section is the average on the test set 75 over the 10 folds for each experiment. 752

In the experiment **ErrorsReplaced**, in each fold of the cross-validation, 90% of 1,760 ontologies (\approx 1,584) are used for training, and the rest 10% (\approx 176) are used for testing. In the experiment **ErrorsRemoved**, the 1,389 ontologies are randomly divided into the training set (\approx 1,250) and the test set (\approx 139) in each fold.

757 7. Evaluation Results and Analysis

In this section we present the evaluation results and their detailed analysis. The evaluation is conducted in two parts. In Section 7.1, we present the performance evaluation of the prediction models used in $R_2O_2^*$ on the training set O_{tr} . In Section 7.2, we present the overall evaluation results, obtained on the test set O_{te} , comparing $R_2O_2^*$ with component reasoners and AutoFolio.

763 7.1. Performance Evaluation of the Key Learning Components in $R_2O_2^*$

Here, we present the performance evaluation of the prediction models (regression models, classifiers and rankers) used in our meta-reasoning framework $R_2O_2^*$, obtained through 10-fold cross-validation on the training set O_{tr} .

767 7.1.1. Performance of regression models in $R_2O_2^{*}(pt)$

Here, our goal is to assess the generalizability of the prediction models \hat{r}_i of reasoner $r_i \in R$. As described in Section 5.2.1, these prediction models are central to $R_2O_2^*(pt)$. Performance (i.e. generalizability) was measured in terms of the coefficient of determination (R^2), as introduced in Section 6.

As presented in Section 5.2.1, we use a stacking approach to build a prediction model with two base regression models (level-0 models): random forest regression algorithm and XGBoost [28]. As a meta-regression model (level-1 model), we also used these two algorithms.

We employed the widely-used Weka framework ⁹ as our evaluation environment.
For ease of experimentation we chose Weka's version of the random forest algorithm.
For XGboost, we used Weka-XGBoost ¹⁰ that can easily interface with Weka.

For the random forest algorithm, we use the default configuration in Weka. For 779 XGBoost, we set the following parameters keeping all the others fixed as default 780 throughout this paper: num_round = 50 (the number of rounds for boosting), eta = 78' 0.1 (learning (or shrinkage) parameter that controls how much information from a new 782 tree will be used in the Boosting), max_depth = 10 (controls the maximum depth of 783 the trees: deeper trees have more terminal nodes and fit more data), sub sample = 784 0.5 (determines if we are estimating a Boosting or a Stochastic Boosting. A value 1 785 represents the regular boosting, and a value between 0 and 1 is for the stochastic case. 786 The stochastic Boosting uses only a fraction of the data to grow each tree. For example, 787 if we use 0.5 each tree will sample 50% of the data to grow). Note that these parameter 788 values were chosen empirically. XGBoost uses multiple parameters and determining 789

⁹https://www.cs.waikato.ac.nz/ml/weka/.

¹⁰https://github.com/SigDelta/weka-xgboost.

⁷⁹⁰ optimal parameter values is beyond the scope of this paper.

Tables 2 and 3 show the R^2 values of the 7 prediction models obtained from cross-79' validation on the training data O_{tr} in the two experiments: ErrorsRemoved and Er-792 rorsReplaced. Note that we have compared the prediction performance of 4 regression 793 models as candidates as a prediction model for each reasoner: (1) random forest regres-794 sion algorithm (denoted by RF), (2) XGBoost, (3) a stacking meta-regression model 795 using random forest regression algorithm (denoted by meta-RF), and (4) a stacking 796 meta-regression model using XGBoost (denoted by meta-XGBoost). R^2 denotes the pro-797 portion of the variation in the target variable (i.e. reasoning time) that can be explained 798 by the model. For example, 0.853 in the model \hat{r}_{FaCT++} , implemented by meta-XGBoost, 799 indicates that 85.3% of the variation in the reasoning time can be accounted for by 800 meta-XGBoost. In Table 2, both RF and meta-XGBoost show the best prediction perfor-80 mance whereas in Table 3, meta-XGBoost has the highest R^2 value. Thus, we choose 802 meta-XGBoost to implement the meta-reasoner $R_2O_2^{*}(pt)$. 803

Model	RF	XGBoost	meta-RF	meta-XGBoost
$\hat{r}_{\mathrm{FaCT}++}$	0.852	0.852	0.852	0.853
$\hat{r}_{\mathrm{HermiT}}$	0.825	0.824	0.831	0.833
\hat{r}_{JFact}	0.904	0.903	0.906	0.907
$\hat{r}_{\mathrm{Konclude}}$	0.910	0.905	0.909	0.909
\hat{r}_{MORe}	0.723	0.705	0.707	0.708
$\hat{r}_{\mathrm{Pellet}}$	0.770	0.763	0.765	0.766
\hat{r}_{Elk}	0.948	0.947	0.949	0.950
Mean	0.847	0.843	0.846	0.847

Table 2: A summary of prediction model performance as measured by R^2 on the dataset **ErrorsRemoved**.

The above observations provide insight into how well the 7 prediction models can fit the given data. The similar values of R^2 with the ones in [26] (i.e. averaged $R^2 = 0.869$) suggest a good generalizability of the models.

Model	RF	XGBoost	meta-RF	meta-XGBoost
$\hat{r}_{\mathrm{FaCT}++}$	0.835	0.832	0.834	0.835
$\hat{r}_{\mathrm{HermiT}}$	0.807	0.807	0.812	0.814
\hat{r}_{JFact}	0.843	0.833	0.839	0.840
$\hat{r}_{\mathrm{Konclude}}$	0.909	0.909	0.912	0.913
\hat{r}_{MORe}	0.757	0.744	0.750	0.756
$\hat{r}_{\mathrm{Pellet}}$	0.727	0.724	0.719	0.723
\hat{r}_{Elk}	0.939	0.936	0.939	0.940
Mean	0.831	0.826	0.829	0.832

Table 3: A summary of prediction model performance as measured by R^2 on the dataset **ErrorsReplaced**.

7.1.2. Performance of rankers in $R_2O_2^*(rk)$ 807

As explained in Section 5.2.2, our meta-reasoner, $R_2O_2^{*}(r_k)$, incorporates a single 808 ranker which differs from our previous approach in R₂O₂ [27] that uses an aggregation of 809 multiple rankers. To implement $R_2O_2^*(rk)$, we initially considered the 5 rankers¹¹ that are 810 used in R_2O_2 [27] on the ranking matrix M_r : (1) KNNRanker that aggregates rankings 81 using the nearest neighbors, (2) PCTRanker that is based on predictive clustering tree for 812 ranking, (3) RPCRanker that is based on a multiple binary pairwise classifier to construct 813 a ranking model, (4) RegRanker where the ranking problem is cast to a multi-target 814 regression problem, where the rank position values of each reasoner are the targets in 815 the multi-target regression setting, and (5) ARFRanker that is based on using random 816 forests for ensembling multiple binary approximated ranking trees. Then, we choose 817 the one showing the best performance in 10-fold cross-validation on the training data 818 O_{tr} . For each ranker, its performance was measured by precision at 1 (denoted by P@1) 819 that measures the proportion of the reasoners that are correctly recommended by the 820 ranker as most efficient reasoner. 82

822

Table 4 shows the performance of the 5 rankers in terms of P@1 on both datasets,

¹¹These rankers are available in http://www.quansun.com, Readers interested in the details of the rankers are referred to [60].

ErrorsRemoved and **ErrorsReplaced**. For each ranker, P@1 was measured using 10-fold cross-validation from the ranking matrix generated from the training data O_{tr} . The ranking matrix formation was presented in Equation 7 in Section 5.2.2. As seen in the table, all 5 rankers showed high performance, achieving more than 90% of the P@1 values. ARFRanker shows the best performance (denoted in bold): 0.978 and 0.955 on **ErrorsRemoved** and **ErrorsReplaced**, respectively. Consequently, to implement our meta-reasoner $R_2O_2^*_{(tk)}$, we use ARFRanker.

Table 4: A summary of performance assessment of the 5 rankers in terms of P@1.

Ranker	ErrorsRemoved	ErrorsReplaced
KNNRanker	0.973	0.952
PCTRanker	0.974	0.944
RPCRanker	0.970	0.947
RegRanker	0.967	0.947
ARFRanker	0.978	0.955

7.1.3. Performance of the classifiers in $R_2O_2^{*}(mc)$

As presented in Section 5.2.3, the meta-reasoner: $R_2O_2^{*}(mc)$ learns the most efficient reasoner on the training data, and predicts the most likely efficient reasoner for an unknown ontology. Using the ontology representation scheme in Equation 5, we considered two classifiers: random forest algorithm and XGBoost.

Table 5 shows the prediction performance in terms of classification accuracy on both datasets, **ErrorsRemoved** and **ErrorsReplaced**. As can be seen, the prediction performance is very similar between RF and XGBoost where the best one on each dataset is denoted in bold. In our evaluation, we use XGBoost as it shows the better performance than RF overall.

In the following subsection, we present and analyse the evaluation results of our proposed four meta-reasoners on the testing data O_{te} .

Table 5: A summary of performance of the two prediction models for meta-reasoner $R_2O_2*_{(mc)}$ in terms of accuracy.

Model	ErrorsRemoved	ErrorsReplaced
RF	0.984	0.944
XGBoost	0.984	0.945

⁸⁴² 7.2. Performance Evaluation of $R_2O_2^*$ on Reasoning Efficiency

In this subsection we discuss the evaluation results comparing our meta-reasoners with the various component reasoners as well as AutoFolio [31], a state-of-the-art algorithm selection framework as a strong and robust baseline, following the evaluation framework presented in Section 6.



Figure 1: A summary of reasoning time characteristics, in seconds and log-scale, of various reasoners in violin plots.

To summarise the performance characteristics of the various component and metareasoners, Figure 1 shows a violin plot of the reasoning time of the reasoners on log scale, for the experiment **ErrorsReplaced**. A violin plot is a combination of a boxplot and a mirrored kernel density plot. As a result, a violin plot visualises the underlying

- distribution that boxplot does not show. Each shape in Figure 1 contains the following
- 852 components.
- The (mirrored) violin itself shows the distribution of reasoning time.
- The cross (\times) in the middle shows the mean reasoning time of the reasoner.
- The plus symbol (+) in the middle shows the median reasoning time of the reasoner.
- The three horizontal lines within each shape shows the 25%, 50%, and 75% of data, respectively.
- The grey dots represent the actual reasoning time of all ontologies.

As can be seen from the figure, the dominance of Konclude over the other five component reasoners is evident. $R_2O_2^*_{(all)}$ shares similar performance characteristics with AutoFolio and VBR, but with a lower mean reasoning time than AutoFolio. The term VBR stands for the virtual best reasoner, which exhibits the optimal efficiency. Even VBR times out on a number of ontologies (grey dots on 1800.0 at the top of the plot), showing the challenging nature of ontology reasoning. The remainder of the section will present more details and discussions on these performance comparisons.

866 7.2.1. Meta-reasoner time overhead

The four different variants of $R_2O_2^*$ all require some additional tasks at both training time and test time. At training time, overall across the 10-fold cross validation, $R_2O_2^*_{(pt)}$ needs to learn regression models (Section 5.2.1); $R_2O_2^*_{(rk)}$ needs to learn rankers (Section 5.2.2), $R_2O_2^*_{(mc)}$ needs to learn a multi-class classifier (Section 5.2.3); and $R_2O_2^*_{(all)}$ ensembles all the above (Section 5.2.4), hence needing to learn all those models. At testing time, each of the meta-reasoners will need to apply these models.

⁸⁷³ We have calculated the time overhead of learning and applying these models. At ⁸⁷⁴ training time, building a regression model for a reasoner takes 1–2.5 sec (stacking ⁸⁷⁵ model that combines RF and XGBoost), building a ranker takes 0.3–0.6 sec, building a ⁸⁷⁶ multi-class classifier takes 0.3–0.5 sec, and building a final stacking model ($R_2O_2^*$ (all)) ⁸⁷⁷ takes an additional 0.1 sec. At testing time, making prediction for a given ontology by ⁸⁷⁸ $R_2O_2^*$ (all) takes a negligible < 0.5 millisecond.

We note that the time overhead at training time does not affect $R_2O_2^*$'s performance as an OWL reasoner. It is only the overhead at testing time that does, as for a new ontology, predictions need to be made for the various models. In all the experiments below in the rest of this section, $R_2O_2^*$'s reported reasoning time already includes the

testing-time time overhead.

⁸⁸⁴ 7.2.2. Comparison with our meta-reasoners and component reasoners

We now evaluate our meta-reasoners against the six component reasoners, Autofolio 885 and VBR in detail. The evaluation is conducted for the two experiments described 886 in the previous section, ErrorsRemoved, in which error ontologies are removed, and 887 ErrorsReplaced, in which error ontologies are treated as they time out. Furthermore, 888 for each experiment, we experiment with the inclusion/exclusion of ELK in our meta-889 reasoners, as described in Section 5. By incorporating ELK, our meta-reasoners can 890 handle the simpler OWL 2 EL ontologies more efficiently, which will improve the 89' overall performance. 892

The reasoners are evaluated on two metrics: (1) average precision at 1 (P@1), which 893 measures whether a reasoner is the most efficient on a given test collection O_{te} across 10-894 fold cross validation, and (2) average runtime (Avg. runtime), which measures the mean 895 reasoning time on a given test collection O_{tr} in seconds across 10-fold cross-validation. 896 The results presented in the rest of this subsection are the average of those obtained 897 on the test set in each of the 10 folds. Note that in each fold, the test collection O_{te} is 898 differently chosen from the total ontology collection O. A more detailed description 899 about our evaluation framework is found in Section 6. 900

Table 6 and Table 7 show evaluation results for the two experiments, ErrorsRe-90' moved and ErrorsReplaced, respectively. We note that in the case where ELK is 902 included in our meta-reasoners, the P@1 and Avg. runtime values for ELK are not 903 recorded over the entire test set, but only the subset of OWL 2 EL ontologies. Hence a 904 comparison between ELK and the other reasoners is not meaningful. Note that as we 905 discussed in Section 5.2, R₂O₂*(pt) follows a similar spirit of the non-ranking portfolio 906 reasoner PR [27], and $R_2O_2^*_{(rk)}$ follows a similar spirit of R_2O_2 [27]. A number of 907 important observations can be made from these tables. 908

• In the experiment **ErrorsRemoved**, in all but one case, the best variant of our metareasoners outperforms all component reasoners in terms of P@1. Konclude has

Reasoner	Witl	nout ELK	W	ith ELK
	P@1	Avg. runtime	P@1	Avg. runtime
FaCT++	0.36%	201.62	0.36%	201.62
Hermit	0.14%	54.17	0.14%	54.17
JFact	0.07%	308.47	0.07%	308.47
Konclude	98.78%	<u>8.58</u>	97.26%	8.58
MORe	0.79%	89.93	0.58%	89.93
Pellet	0.22%	164.30	0.22%	164.30
ELK	-	-	1.73%	0.69
R ₂ O ₂ *(pt)	<u>98.56%</u>	8.60	98.20%	8.53
$R_2O_2*_{(rk)}$	98.78%	<u>8.58</u>	<u>98.42%</u>	<u>8.51</u>
$R_2O_2*_{(mc)}$	98.78%	7.48	98.49%	7.40
$R_2O_2*_{(all)}$	98.78%	7.48	98.49%	7.40
VBR	100%	4.50	100%	4.43

Table 6: Performance evaluation in the experiment **ErrorsRemoved**, in which error ontologies are removed. Our meta-reasoners are compared with component reasoners and the virtual best reasoner (VBR). In each column, the best results are **bolded** and the second best results are <u>underlined</u>.

the same performance (98.78%) as our meta-reasoners ($R_2O_2^*(rk)$, $R_2O_2^*(mc)$, and

 $_{912}$ R₂O₂*_(all)) when ELK is not considered.

In both experiments ErrorsRemoved and ErrorsReplaced, in all cases, the best
 variant of our meta-reasoners outperforms all component reasoners in terms of average
 runtime, including the highly efficient, parallelising reasoner Konclude.

• Out of all the variants of our meta-reasoners, $R_2O_2^*_{(all)}$ exhibits overall best efficiency. Of all the four experimental setups, $R_2O_2^*_{(all)}$ exhibits the best performance of three, and second best in the other one. $R_2O_2^*_{(all)}$ achieves a speedup of at least 1.10x (over Konclude in experiment **ErrorsReplaced**) and at most 41.69x (over JFact in experiment **ErrorsRemoved**). Its best efficiency is the result of the stacking technique employed in $R_2O_2^*_{(all)}$.

Reasoner	With	nout ELK	Wi	ith ELK
	P@1	Avg. runtime	P@1	Avg. runtime
FaCT++	1.31%	365.92	1.25%	365.92
Hermit	0.68%	138.06	0.68%	138.06
JFact	0.57%	532.11	0.57%	532.11
Konclude	97.22%	27.15	94.55%	27.15
MORe	2.16%	139.68	1.48%	139.68
Pellet	0.91%	322.59	0.85%	322.58
ELK	-	-	3.47%	0.97
$R_2O_2*_{(pt)}$	97.10%	24.50	96.82%	<u>23.89</u>
$R_2O_2*_{(rk)}$	97.73%	25.72	<u>97.05%</u>	24.45
$R_2O_2*_{(mc)}$	97.39%	26.93	96.82%	25.66
$R_2O_2*_{(all)}$	<u>97.56%</u>	24.67	97.16%	23.39
VBR	100%	16.65	100%	16.22

Table 7: Performance evaluation of the experiment **ErrorsReplaced**, in which error ontologies are replaced by timeouts (30 minutes). Our meta-reasoners is compared with component reasoners and the virtual best reasoner (VBR). In each column, the best results are **bolded** and the second best results are <u>underlined</u>.

• The inclusion of ELK in our meta-reasoners indeed improves reasoning efficiency. 922 Even though ELK is only able to handle the less expressive OWL 2 EL profile, our 923 meta-reasoners are able to take advantage of its efficiency in handling such ontologies. 924 Table 1 in Section 7 shows the vast efficiency dominance of Konclude over the other 925 component reasoners. To better understand the reasoners' performance, we divide the 926 ORE 2015 dataset into four bins of discretised reasoning time. The discretisation is 927 performed on the best reasoning time (in seconds) of the virtual best reasoner (VBR), 928 into four bins: 'A' (0, 1), 'B' [1, 10), 'C' [10, 100), and 'D' [100, 1,800], which represent 929 ontologies with increasing difficulty. 930

Tables 8 and 9 below summarise, in each bin and the entire ontology collection O, the percentage of each component reasoner being the most efficient. The component

Rank	Ove	rall	А		В		С		D	
	%	Rea	%	Rea	%	Rea	%	Rea	%	Rea
1	96.92	Κ	100	K	88.62	Κ	80.56	Κ	27.27	F,K
2	1.72	Е	0	E,F,H,J,M,P	8.94	E	11.11	М	18.18	М
3	0.57	М	_	-	0.81	M,P	5.56	Е	9.09	H,J,P
4	0.36	F	_	-	0.41	F,H	2.78	F	0	Е
5	0.22	Р	_	-	0	J	0	H,J,P	_	_
6	0.14	Н	_	-	_	-		-	_	_
7	0.07	J	_	_	-	-		-		-

Table 8: Comparison of percentage of each component reasoner being the most efficient in each bin and overall in experiment **ErrorsRemoved** (Rea: Reasoner, E: ELK, F: FaCT++, H: HermiT, J: JFact, K: Konclude, M: MORe, P: Pellet).

Table 9: Comparison of percentage of each component reasoner being the most efficient in each bin and overall in experiment **ErrorsReplaced** (Rea: Reasoner, E: ELK, F: FaCT++, H: HermiT, J: JFact, K: Konclude, M: MORe, P: Pellet).

Rank	Ove	rall	А		В		С		D	
	%	Rea	%	Rea	%	Rea	%	Rea	%	Rea
1	91.93	K	100	K	84.41	K	67.31	K	20.83	М
2	3.37	Е	0	E,F,H,J,M,P	11.18	Е	22.12	Е	18.06	F,K
3	1.44	М	-	-	2.35	F	7.69	М	15.28	Н
4	1.22	F	-	-	0.88	M,P	1.92	Р	13.89	J,P
5	0.83	Р	_	-	0.29	Н	0.96	F	0	Е
6	0.66	Н	-	-	0	J	0	H,J	_	_
7	0.55	J	_	_	-	-		_		-

reasoners are ordered by their percentages of being the most efficient, from highest to
lowest. Note ELK only performs reasoning on the subset of OWL 2 EL ontologies.
Note that the % values in the tables are averaged from the test sets of 10-fold cross
validation in the above two experimental setups. Also note that the % values in Tables 8

and 9 are different from the P@1 values in Table 6 and Table 7. The % values show the percentage being the most efficient across all the component reasoners. Thus, the sum of the % values in each of the columns - 'Overall', 'A', 'B', 'C' and 'D' is 1. From these tables, we note a number of interesting observations:

- Konclude's dominance is again evident, as it is the most efficient reasoner for all
 bins except only in bin D, experiment ErrorsReplaced, where MORe is the most
 efficient.
- Despite its dominance, Konclude does not dominate the most challenging category,
 bin D. In experiment ErrorsRemoved both FaCT++ and Konclude are the most
 efficient, and in experiment ErrorsReplaced MORe is the most efficient.
- For the most difficult category, bin D, many component reasoners are the most efficient
 for a considerable percentage. In other words, the dominance of any component
 reasoner is much less pronounced. This shows the challenging nature of algorithm
 selection in the ontology reasoning context, where for the most challenging instances,
 a large number of choices are possible. This observation also indicates considerable
 room for further investigation.

953 7.2.3. Comparison with AutoFolio

In this section, we evaluate R2O2*(all) against AutoFolio for the ontology classifica-954 tion problem¹². We have chosen $R_2O_2*_{(all)}$ for comparison with AutoFolio as it shows 955 the best performance overall in our evaluation as discussed in the previous section. 956 AutoFolio and R2O2*(all) use the same set of metrics, and are trained and tested on the 957 same data splits and the same set of six reasoners. Hence, the comparison is fair. Note 958 that AutoFolio makes use of functionally equivalent components hence it cannot take 959 advantage of ELK. As described in Section 6, 10-fold cross validation is carried out for 960 both experiments. In each fold, an AutoFolio model is trained on the training set, and 961 then evaluated on the test set. 962

Table 10 summarises the mean reasoning time for the two experiments. As can be observed in the table, $R_2O_2^*(all)$ outperforms AutoFolio in both experiments. The

¹²AutoFolio is available at https://github.com/mlindauer/AutoFolio.

best performance is achieved when ELK is incorporated in $R_2O_2*_{(all)}$, where $R_2O_2*_{(all)}$ 965 outperforms AutoFolio by 15.95% and 16.08% respectively. However, even without 966 ELK, R₂O_{2*(all)} also outperforms AutoFolio, by 14.71% and 10.05% respectively. These 967 results demonstrate the effectiveness of $R_2O_2^*$ _(all) as AutoFolio represents the state-of-968 the-art method in automated algorithm selection. 969

Table 10: Summary of mean reasoning performance (in seconds) comparison between AutoFolio and $R_2O_2^{*}(all)$ ($R_2O_2^{*}(all)$, both with and without ELK). In each row, best performance in the test set is highlighted in **bold**, and second best performance in the test set is underlined.

Experiment	AutoFolio	$R_2O_2*_{(all)}$ (without ELK)	$R_2O_2*_{(all)}$ (with ELK)
ErrorsRemoved	8.58	<u>7.48</u>	7.40
ErrorsReplaced	27.15	24.67	23.39

We further analysed the component reasoners selected by AutoFolio and R2O2*(all) 970 in both experiments. In ErrorsRemoved, AutoFolio exclusively selects Konclude for 971 all 1,389 instances. In ErrorsReplaced, AutoFolio selects MORe in 11 (0.625%) of

972

the 1,760 instances, and Konclude 1,749 (99.375%) instances. 973

On the other hand, $R_2O_2^*_{(all)}$ is able to select a more diverse set of efficient reasoners. 974 Table 11 shows, with ELK included, the number and percentage of times each compo-975 nent reasoner is selected by $R_2O_2*_{(all)}$ for each bin as well as the entire dataset. These 976 results provide additional evidence that always selecting the most-efficient-on-average 977 reasoner(s) is not the most optimal approach. For example, Table 1 shows that the 978 mean reasoning time of MORe is more than 20x slower than Konclude. However, in 979 experiments ErrorsReplaced, MORe is selected almost 30% among the most diffi-980 cult ontologies (bin D). Thus, this analysis further validates the effectiveness of the 98 sophisticated meta-reasoning framework R₂O₂*_(all). 982

7.3. Key Metrics Identification 983

Lastly, we investigate the identification of each of the 29 metrics' influence on the 984 performance of our meta-reasoners. This will provide insight into the contribution of 985 individual metrics we have chosen (i.e. 29 metrics) on their performance. We measure 986

	Overall (%)	A (%)	B (%)	C (%)	D (%)
ErrorsRemoved					
Konclude	1,354 (97.48)	1,101 (100)	219 (88.66)	28 (82.35)	6 (85.71)
MORe	1 (0.07)	0	0	0	1 (14.29)
ELK	34 (2.45)	0	28 (11.34)	6 (17.65)	0
ErrorsReplaced					
FaCT++	6 (0.34)	0	6 (1.80)	0	0
Konclude	1,682 (95.57)	1,294 (100)	291 (87.12)	79 (75.24)	18 (66.67)
MORe	13 (0.74)	0	0	5 (4.76)	8 (29.63)
Pellet	2 (0.11)	0	0	1 (0.95)	1 (3.70)
ELK	57 (3.24)	0	37 (11.08)	20 (19.05)	0

Table 11: The number and percentage of each component reasoner being selected by $R_2O_2^*{}_{(all)}$ in both experiments, with ELK included. Percentages are calculated column-wise.

the relative metric importance by using the feature importance values provided by the XGBoost classifier used in $R_2O_2*_{(mc)}$. Figure 2 shows the most important metrics for the prediction task of $R_2O_2*_{(mc)}$, which is to predict the most efficient reasoner, in both experiments. The weights are estimated by calculating the average of importance of the metrics through 10-fold cross validation and normalised into [0, 1]. The weight of each metric is measured based on the number of times it is used to split the data across all trees in XGBoost.

As can be seen from the figure, different metrics are important for each experiment. However, there are some common important metrics. Two metrics, SOV and mCID, are common to both experiments' top 5 metrics. Six metrics, IND, SOV, mCID, aCID, RHLC, and EOG, are common to both experiments' top 10 metrics. For both experiments, OBP% is the least important among the 29 metrics. Curiously, DTP% is the most important for experiment **ErrorsRemoved**, while it is the second least important for **ErrorsReplaced**.



Figure 2: Importance of ontology metrics for $R_2O_2*_{(mc)}$ in both experiments. For each experiment the metrics are ordered in descending order by their importance values.

1001 8. Conclusion

Reasoning support for OWL ontologies is essential for ensuring the correctness of ontologies, and for inferring implicit knowledge from them. For an expressive ontology language such as $SHOIN(\mathbf{D})$ and $SROIQ(\mathbf{D})$, worst-case complexity is very high. Moreover, ample empirical evaluation has also confirmed the hardness of actual, realworld ontologies, even on state-of-the-art ontology reasoners such as Konclude and HermiT.

This paper presented $R_2O_2^*$, a novel, robust meta-reasoning framework that automatically ranks component reasoners by efficiency and selects the one that is most likely the most efficient for any given ontology. The $R_2O_2^*$ framework comprises a number of novel contributions: (1) we learn regression models that accurately predict reasoning time for a number of state-of-the-art ontology reasoners; and (2) we propose a learning- and ranking-based meta-reasoner that ensembles base prediction models and thus combines component reasoners based on their predicted reasoning efficiency, and (3) we formally define a large suite of syntactic and structural metrics that describe ontologies.

We performed a comprehensive evaluation on six state-of-the-art OWL 2 DL reasoners and a large corpus of carefully curated ontologies. Our evaluation shows that $R_2O_2^*$ significantly outperforms all six component reasoners as well as AutoFolio, a strong, general-purpose, and state-of-the-art algorithm selection system. Compared to component reasoners, $R_2O_2^*$ achieves a speedup of at least 1.10x (over Konclude) and up to 41.69x (over JFact).

Extending our R2O2* meta-reasoning framework to a multi-criteria setting as done 1023 in Multi-RakSOR [49, 50] is a natural next step. We plan to extend our methodology 1024 to support ABox reasoning, and investigate support of other non-standard reasoning 1025 problems. Continuing on our work on ABox-intensive EL ontologies [38] and reasoning 1026 on the Android platform [39], we will further investigate sources of ABox reasoning 1027 hardness by studying structural and syntactic properties of ABoxes. Performance pre-1028 diction and optimisation utilising machine learning techniques is particularly interesting 1029 and relevant in the context of ontology-based data access (OBDA) [5], where a large 1030 database is enhanced by an ontology, and (conjunctive) query answering on the database 103 requires ontology reasoning [61]. We will also investigate the generation of synthetic, 1032 yet realistic benchmark ontologies (TBoxes) and instances (ABoxes) to assist in the eval-1033 uation and optimisation of reasoners. Finally, investigating the correlation of efficiency 1034 between different reasoning tasks by a same reasoner is also an interesting problem 1035 worthy of investigation. 1036

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1257 Appendix A. Metric Definitions

Table A.12: Definitions of the 24 ontology-level (ONT) metrics. Note that "___" represents "don't cares".

Metric	Definition
SOV	No. of named entities (classes, properties & individuals)
ENR	Ratio between number of (named and anonymous) entities
	and number of edges
TIP	Difference between number of subclass axioms and number
	of (named or anonymous) classes
EOG	The <i>entropy</i> of the ontology graph, measuring the diversity of
	the edge distribution
CYC	The cyclomatic complexity of the ontology, measuring the
	number of linearly independent paths
RCH	The ratio of (possibly nested) anonymous class expressions
	and all (named or anonymous) class expressions
IND	No. of (named or anonymous) individuals
GCI	No. of GCI axioms
HGCI	No. of hidden GCI axioms
ESUB%	Ratio of subclass axioms that contain (nested) existential
	restrictions $(\exists R._)$
DSUB%	Ratio of subclass axioms that contain (nested) class unions
	()
CSUB%	Ratio of subclass axioms that contain (nested) class intersec-
	tions ($_ \sqcap _$) and the subclass is anonymous
ELCLS%	Ratio of (nested) class expressions that are in OWL 2 EL
	profile
ELAX%	Ratio of subclass or equivalent class axioms that only contain
	expressions in the OWL 2 EL profile

Table A.12: Definitions of the 24 ontology-level (ONT) metrics. Note that "___" represents "don't cares".

Metric	Definition
HLC	Count hard language constructs containing in superclass ex-
	pressions
HLC%	Ratio of HLC and subclass axioms
SUBCECHN	No. of top-level subclass expressions that contain chained
	existential restrictions
SUPCECHN	No. of top-level superclass expressions that contain chained
	existential restrictions
DSUBCECHN	Max depth of chained existential restrictions in a subclass
	expression
DSUPCECHN	Max depth of chained existential restrictions in a superclass
	expression
SUBCCHN	No. of top-level subclass expressions that contain chains of
	conjunctions
SUPCCHN	No. of top-level superclass expressions that contain chains of
	conjunctions
DSUBCCHN	Max depth of nested conjunctions in a subclass expression
DSUPCCHN	Max depth of nested conjunctions in a superclass expression

Metric	Definition
tNOC	$\sum_{C} NOC(C)$
aNOC	$\frac{tNOC}{N_C}$
mNOC	$\max_C NOC(C)$
tNOP	$\sum_{C} NOP(C)$
aNOP	$\frac{tNOP}{N_C}$
mNOP	$\max_C NOP(C)$
tCID/tCOD	\sum_{C} incoming/outgoing edges of C
aCID/aCOD	$aCID = \frac{tCID}{N_C}, aCOD = \frac{tCOD}{N_C}$
mCID/mCOD	$mCID = \max_{C} CID(C), mCOD = \max_{C} COD(C)$
tDIT	\sum_{C} distance of C from owl: Thing in a depth-first manner
aDIT	$\frac{tDIT}{N_C}$
mDIT	$\max_C DIT(C)$

Table A.13: Definitions of the 15 class-level (CLS) metrics. Note that C represents a (named or possibly nested) class expression in an antology, and N_C denotes the total number of (named or possibly nested) class expressions in a given ontology.

Metric	Definition
ENUM[%]	For enumerations/nominals ($\{a, b, c\}$, where a, b, c are in-
	dividuals)
NEG[%]	For class negations $(\neg C)$
CONJ[%]	For class intersections (conjunctions, $C_1 \sqcap C_2$)
DISJ[%]	For class unions (disjunctions, $C_1 \sqcup C_2$)
UF[%]	For universal restrictions $(\forall R.C)$
EF[%]	For existential restrictions $(\exists R.C)$
VALUE[%]	For value restrictions $(\exists R.\{a\})$, where <i>a</i> is an individual
SELF[%]	For self references
MNCAR[%]	For min cardinality restrictions ($\geq n R.C$)
MXCAR[%]	For max cardinality restrictions ($\leq n R.C$)
CAR[%]	For (exact) cardinality restrictions $(= n R.C)$

Table A.14: Definition of the 22 (possibly nested) anonymous class expression (ACE) metrics. Note that each row represents a count metric and a ratio metric (represented by [%]) for the same type of class expressions.

Metric	Definition
OBP[%]	Count and ratio of object-properties
DTP[%]	Count and ratio of datatype-properties
FUN[%]	Count and ratio of functional properties
SYM[%]	Count and ratio of symmetric properties
TRN[%]	Count and ratio of transitive properties
IFUN[%]	Count and ratio of inverse functional properties
ASYM[%]	Count and ratio of asymmetric properties
REFLE[%]	Count and ratio of reflexive properties
IRREF[%]	Count and ratio of irreflexive properties
CHN[%]	Count and ratio of property chain axioms
SUBP	Count of subproperty axioms
EQVP	Count of equivalent property axioms
DISP	Count of disjoint property axioms
INV	Count of inverse property axioms
DOMN	Count of domain axioms
RANG	Count of range axioms
ELPROP%	Ratio of property axioms that are in the OWL 2 EL profile
IHR	Count of class axioms that involve property hierarchies
IIR	Count of class axioms that involve inverse properties
ITR	Count of class axioms that involve transitive properties

Table A.15: Definitions of the 30 property-level (PRO) metrics.