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WeST People and Knowledge Networks
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Enrichment of ontological taxonomies using a neural network approach

Bachelorarbeit

zur Erlangung des Grades einer Bachelor of Science (B.Sc.)
im Studiengang Informatik

vorgelegt von
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1 Introduction

TODO: Motivation. Related work. Solution. Evaluation.

2 Foundations

2.1 Wikidata

Wikidata is an open, free, multilingual and collaborative knowledge base. It is a structured knowledge source for other Wikimedia projects. It tries to model the real world, meaning every concept, object, animal, person, etc. Wikidata is mostly edited and extended by humans, which in general improves the quality of entries compared to fully-automated systems, because different editors can validate and correct occurring errors. However, Wikidata, like most knowledge bases, is incomplete and therefore has to be operated under the *Open World Assumption* (OWA). OWA states that if a statement is not contained in a knowledge base, it is not necessarily false but rather unknown [12].

In Wikidata items and properties exist. Items are the aforementioned concepts, objects, etc. While properties are used to make claims about items, e.g. *photographic film (Q6293)* is a *subclass of (P279) data storage device (Q193395)* (see Figure 1). Each item and property has an unique identifier, which starts with the letter Q for items and the letter P for properties and is followed by a numeric code. The identifiers in Wikidata are essential to avoid ambiguity and to make items and properties multilingual.

Items consist of labels, aliases and descriptions in different languages. Sitelinks connect items to their corresponding pages of Wikimedia projects like Wikipedia articles. Most importantly item are described by statements. Statements are in their simplest form a pair of property and value, assigned to a specific item. A value is either a literal value or another item. It should be noted that an item can have multiple statements with the same property. The set of statements with the same property is called statement group. Statements can be annotated with qualifiers, which specify the context of the statement, e.g. population at a certain point of time. Additionally, references can be used for statements to include its source. See Figure 1 for an example of a Wikidata item.

Following, the terms of item and statement are defined in the context of Wikidata.

Definition 1 (Item). *An item is a tuple* $(id, label, aliases, description, sitelinks)$*:*

- $id \in \mathbb{N}$ *is the numerical item ID;*
- $label \in String$ *is the English label of the item;*
- $aliases \in \mathcal{P}(String)$ *is the set of English synonyms for the label;*

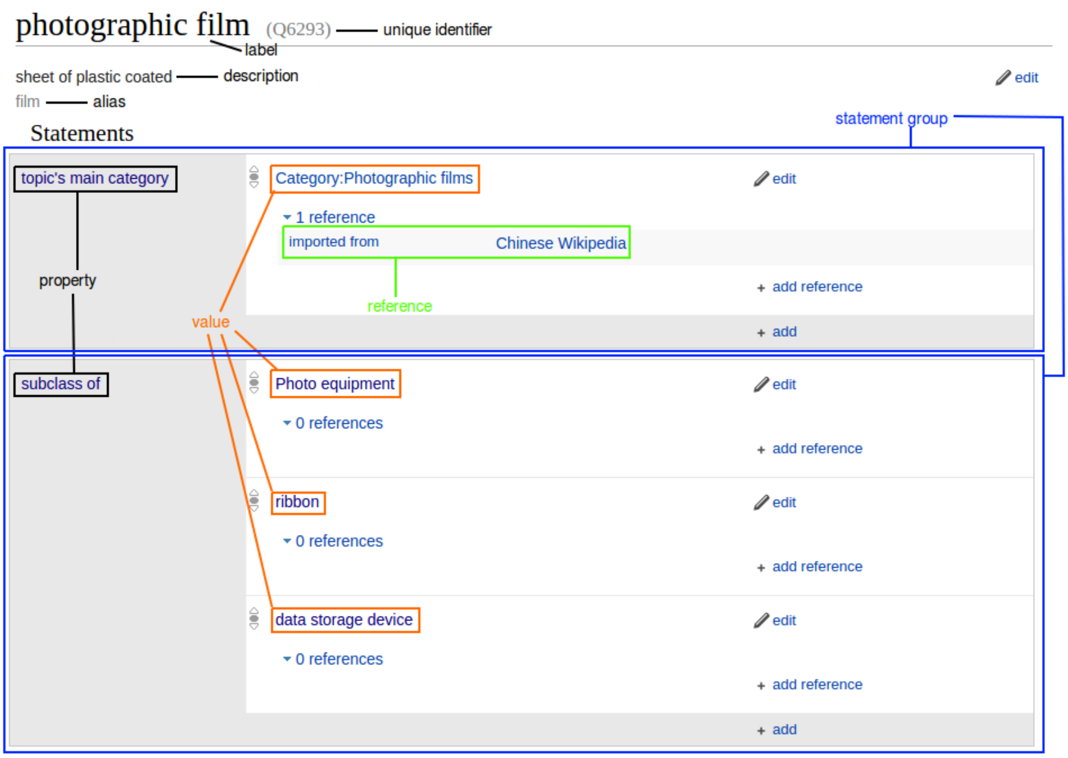

Figure 1: Example of Wikidata class: photographic film (Q6239)

- *$description \in String$ is a short sentence describing the item;*
- *$sitelinks \in String \times String$ is a set of tuples $(site, title)$, where $site$ refers to a specific site of the Wikimedia projects, e.g. enwiki, and $title$ is the corresponding article title of the item on this site.*

Definition 2 (Statement)**.** *A statement is a tuple $(itemid, pid, value, refs, qualifiers)$:*

- *$itemid \in \mathbb{N}$ is a numerical item ID, to which the statement belongs;*
- *$pid \in \mathbb{N}$ is a numerical property ID;*
- *$value$ is either a constant value like string, int, etc., or an item ID;*
- *$refs$ is a set of references, containing the source of information for the statement;*
- *$qualifiers$ is a set of qualifiers, which further specifies the statement.*

In Wikidata, there is no strict distinction between classes and instances. Both groups are represented as items. This leads to the issue, that recognizing, whether an item is a class or instance is not trivial. Based on which statements connect two items, a distinction can be made. A class is any item, which has instances, subclasses or is the subclass of another class. In Wikidata, the properties *instance of (P31)* and *subclass of (P279)* exist, which describe this relation between items. Therefore to identify whether an item is a class, it needs to be checked, whether the items fulfills any of the three above criteria.

Definition 3 (Class)**.** *Given a set of items I and a set of statements R. $c = (classid, \_, \_, \_, \_) \in I$ is a class, if at least one of the following assertions are true:*

$$\exists i = (instanceid, \_, \_, \_, \_) \in I \; \exists s = (itemid, pid, value, \_, \_) \in R : \quad instanceid = itemid \land pid = 31 \land value = classid \text{ (has instance)}$$

$$\exists s = (itemid, pid, \_, \_, \_) \in I : itemid = classid \land pid = 279 \text{ (is subclass)}$$

$$\exists i = (subclassid, \_, \_, \_, \_) \in I \; \exists s = (itemid, pid, value, \_, \_) \in R : \quad itemid = subclassid \land pid = 279 \land value = classid \text{ (has subclass)}$$

_ is used as an anonymous placeholder, for the purpose of not naming unused elements in tuples. For example, *photographic film (Q6293)* (Figure 1) is a class, because it is the subclass of three other classes.

2.2 Taxonomy

Ontologies are sets of concepts and relations, which formally define how knowledge can be related and ordered in a context. Additionally it is possible for ontologies to contain axioms used for validation and constraint enforcement. In comparison, a knowledge base like Wikidata can be seen as an instantiation of such an ontology,

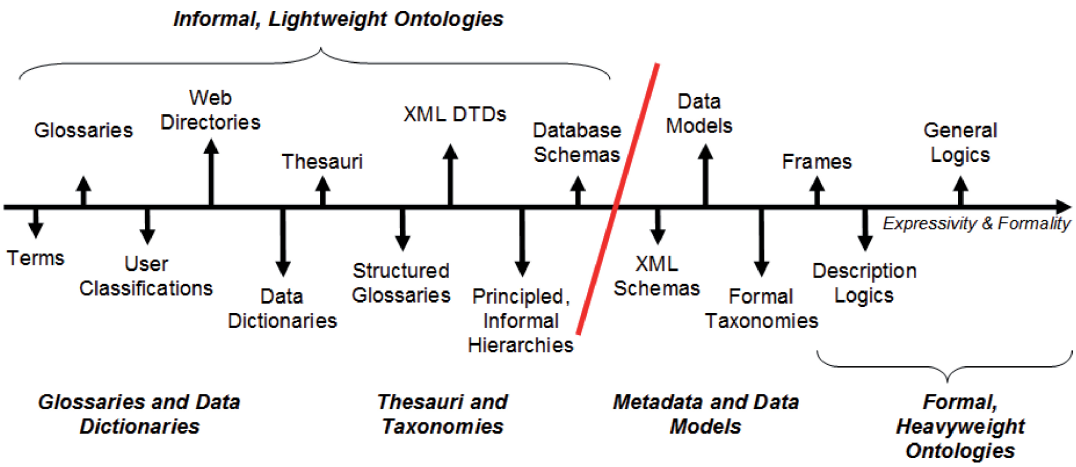

Figure 2: The spectrum of ontology kinds. [22]

since every knowledge base has to be conceptualized by an ontology [22]. Different types of ontologies can grouped by their level of formality and expressiveness. Wong et al. [22] differentiates ontologies as lightweight and heavyweight ontologies (see Figure 2). *Taxonomies* are concept or class hierarchies. They typically represent a parent-child structure, which can be formalized with a single relationship called for example *subclass-of* in the case of Wikidata. The observed taxonomy in Wikidata belongs to the category of lightweight ontologies, specifically *principled, informal hierarchies*, as the only enforced rule for the subclass-of relation is that it should connect two entities [2].

For the purpose of developing a formal definition of the thesis' problem statement the notion of taxonomy needs to be formalized. Cimiano [7] defines a heavyweight ontology, which includes a taxonomy, as follows:
"

Definition (Ontology). *An* ontology *is a structure*

$$\mathcal{O} := (C, \leq_C, R, \sigma_R, \leq_R, \mathcal{A}, \sigma_\mathcal{A}, \mathcal{T})$$

consisting of

- *four disjoint sets C, R, $\mathcal{A}$, and $\mathcal{T}$ whose elements are called* concept identifiers, relation identifiers, attribute identifiers *and* data types, *respectively,*
- *a semi-upper latice $\leq_C$ on C with top element $root_C$, called* concept hierarchy *or* taxonomy,
- *a function $\sigma_R : R \to C^+$ called* relation signature,
- *a partial order $\leq_R$ on R, called* relation hierarchy, *where $r_1 \leq_R r_2$ implies $|\sigma_R(r_1)| = |\sigma_R(r_2)|$ and $\pi_i(\sigma_R(r_1)) \leq_C \pi_i(\sigma_R(r_2))$, for each $1 \leq i \leq |\sigma_R(r_1)|$, and*

- *a function* $\sigma_{\mathcal{A}} : \mathcal{A} \rightarrow C \times \mathcal{T}$, *called* attribute signature,
- *a set* $\mathcal{T}$ *of datatypes such as strings, integers, etc.*

Hereby, $\pi_i(t)$ is the i-th component of tuple t. [...] Further, a semi-upper lattice $\leq$ fulfills the following conditions:

$\forall x(x \leq x)$ (reflexive)
$\forall x \forall y(x \leq y \wedge y \leq x \implies x = y)$ (anti-symmetric)
$\forall x \forall y \forall z(x \leq y \wedge y \leq z \implies x \leq z)$ (transitive)
$\forall x x \leq top$ (top element)
$\forall x \forall y \exists z(z \geq \wedge z \geq y \wedge \forall w(w \geq x \wedge w \geq y \implies w \geq z))$ (supremum)

So every two elements have a unique most specific supremum. "

A taxonomy can be modeled as a semi-upper lattice. This induces two important assumptions about the structure and to some degree completeness of the observed taxonomies. First, there is only one *root class*, top element of the lattice, of which every other class is (transitively) a subclass. Second, because of the supremum property, the taxonomy is fully connected, which means each class, but the root class, has a superclass. Wikidata's taxonomy does therefore not fulfill the definition by Cimiano [7], as it is not fully connected.
In the following, new definitions will presented, which attempt to model an incomplete taxonomy based on the already presented data model and structure of Wikidata. First, basic concepts of graphs will be introduced.

Definition 4 (Directed graph). *A* directed graph *G is an ordered pair* $G = (V, E)$*, where* V *is a set of vertices, and* $E = \{(v_1, v_2) \mid v_1, v_2 \in V\}$ *is a set of ordered pairs called directed edges, connecting the the vertices.*

Definition 5 (Predecessor). *Let* $G = (V, E)$ *be a directed graph.* $v_1 \in V$ *is a* predecessor *of* $v_2 \in V$*, if there exists an edge so that* $(v_1, v_2) \in E$*. Let* $v \in V$ *be a vertice of G, then* $pred_G(v) = \{w \mid (w, v) \in E\}$ *is the set of predecessors of* v*.*

Definition 6 (Successor). $v_1 \in V$ *is a* successor *of* $v_2 \in V$*, if there exists an edge so that* $(v_2, v_1) \in E$*. Let* $v \in V$ *be a vertice of G, then* $succ_G(v) = \{w \mid (v, w) \in E\}$ *is the set of successors of* v*.*

Definition 7 (Walk). *Let* $G = (V, E)$ *be a directed graph. A* walk W *of length* $n \in \mathbb{N}$ *is a sequence of vertices* $W = (v_1, \dots, v_n)$ *with* $v_1, \dots, v_n \in V$*, so that* $(v_i, v_{i+1}) \in E \; \forall i = 1, \dots, n-1$*.*

Definition 8 (Cycle). *A walk* $W = (v_1, \dots, v_n)$ *of length* n *is called a* cycle*, if* $v_1 = v_n$*.*

Definition 9 (Directed acyclic graph). *A directed graph G is called* directed acyclic graph*, if there are no cycles in G.*

In Wikidata, a class can have multiple superclasses, therefore a tree structure is not sufficient to model the taxonomy. However a directed acyclic graph, can model the taxonomy. The acyclic constraint is necessary to ensure that no class is transitively a subclass of itself. **TODO: define**

Definition 10 (Connectedness)**.**

Definition 11 (Component)**.**

Definition 12 (Taxonomy)**.** *A* taxonomy $T = (C, S)$ *is a directed acyclic graph, where* C *is a set of* class identifiers*, and* S *is the set of edges, which describe the* subclass-of relation *between two classes. such that* c_1 *is the subclass of* c_2*, if* $(c_1, c_2) \in S$*.*

Definition 13 (Subclass-of relation)**.** *The transitive binary relation* $\lhd_T$ *on the taxonomy* $T = (C, S)$ *represents the subclass relationship of two classes in* T*. Given* $c_1, c_2 \in C$*,* $c_1 \lhd_T c_2$*, if there is a walk* $W = (c_1, \ldots, c_2)$ *with length* $n \geq 1$*, which connects* c_1 *and* c_2*.* $\lhd_T$ *is transitive,* $\forall c_1, c_2, c_3 \in C : c_1 \lhd_T c_2 \land c_2 \lhd_T c_3 \implies c_1 \lhd_T c_3$*.*

If the taxonomy defined by Cimiano [7] is mapped on this graph-based taxonomy model, the following assumption is true, for $T = (C, S)$:

$$|\{c \in C \mid \neg \exists s \in C : c \lhd_T s\}| = 1$$

Only one class in this taxonomy has no superclasses. This class is called *root class*. However in the case of Wikidata, this assumption does not hold true. The following state is the case:

$$|\{c \in C \mid \neg \exists s \in C : c \lhd_T s\}| > 1$$

There are classes other than the root class, which also have no superclasses. These classes will be called *unlinked classes*.

Definition 14 (Root class)**.** *Given a taxonomy* $T = (C, S)$*, the* root class $root_T$ *is a specific, predefined class with no superclasses in* T*. For* $root_T$*,* $|succ_T(root_T)| = 0$ *applies.*

Definition 15 (Unlinked class)**.** *Given a taxonomy* $T = (C, S)$ *with a root class* $root_T$*, a class* $u \in C$ *is called* unlinked class*, if* $u \neq root_T \land |succ_T(u)| = 0$*.*

In Wikidata, the root class is *entity (Q35120)* [3]. All other classes, which are not subclasses of *entity (Q35120)*, are therefore either unlinked classes, or subclasses of unlinked classes. In Section 3, it will be shown that the Wikidata taxonomy graph is not fully connected. But the component, which contains root class *entity (Q35120)*, contains 97% of all classes. This component will be referred to as *root taxonomy* in later sections.

2.3 Similarity

- semantic similarity e.g. distributional similarity
  Lin [16]
  Rodríguez and Egenhofer [20]

- geometrical similarity e.g. distance based-similarity, cosine similarity

For the task of ontology learning [14] as well as classification, e.g. k-nearest-neighbors, the concept of similarity is of importance. A basic intuition of similarity is for example given by Lin [16]. Similarity is related to the commonalities and differences between two objects. More commonalities implies higher similarity. Vice versa, more differences implies lower similarity. Two identical objects should have the maximum similarity. In addition, only identical objects should be able to achieve maximum similarity. Typically, similarity can be defined as a binary function, which maps two objects to a value in the interval $[0, 1]$. A value of 1 represents identical input objects. For this thesis, semantic and vector similarity measures will be used.
TODO: example for Commonalities, Differences
Vector similarity.
Semantic similarity measures are needed when comparing structures, which cannot be sufficiently represented as vectors. These are for example words and classes in ontologies **citations needed**. Rodríguez and Egenhofer [20] develops a semantic similarity measure for comparing entity classes in ontologies. Entity

2.4 Problem statement

The task of this thesis is the classification of unlinked classes in Wikidata. In other words a function is needed, which given an unlinked class u of a taxonomy $T = (C, S)$ with a root class $root_T$, find an appropriate superclass for T. Doan et al. [10] suggests that for the task of placing a class into an appropriate position in T, either finding the most similar class, most specific superclass, or most general subclasses of u, are sensible approaches. This induces that the appropriate superclass for an unlinked class u is either the most similar class $c \in T$, or one of the superclasses of $succ_T(c)$. Therefore we can define the problem, as follows:

Definition 16 (Problem definition)**.** *Given a taxonomy $T = (C, S)$ with root class $root_T$ and a similarity function sim over T, find a function f, which, given an unlinked class $u \in C$, returns a class $s = f(u)$, fulfilling the following criteria:* ***TODO: define as the parents of the most similar class? for example german would be similar to english, therefore the superclass for german should be language and not english***

$$\neg(s \lhd_T u) \text{ no child} \tag{1}$$

$$s = \max_{c \in C}(sim(u, s)) \text{ most similar class} \tag{2}$$

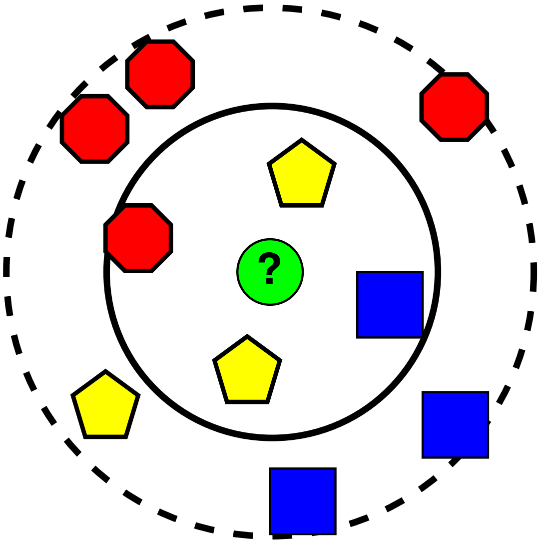

Figure 3: Example for k-nearest neighbors for 3 classes with k=4 and k=10.

2.5 k-nearest-neighbors classification

Chen et al. [5]
Zhang and Zhou [23]
Based on the characteristics of the classification problem, described by the problem statement, and the challenges attached to it, the k-nearest-neighbor algorithm seems like an appropriate tool for solving the task.

Explain how kNN works. Nearest-neighbors classification is a lazy method, as it does not require training before testing. This is useful for applications with high amounts of data, large numbers of classes, and changing data [23]. For the considered use case of classification in Wikidata, these are very important strengths, as the number of classes in the taxonomy is very high and Wikidata is being constantly edited.

3 Analysis of the Wikidata taxonomy

TODO: maybe separate this section into subsections For the task of developing an algorithm, which takes unlinked classes as input, it is necessary to know, what information the classes carry and if there are certain patterns among the classes. For this purpose an analysis of the taxonomy needs to be carried out, which may answer questions.

The taxonomy contained in the Wikidata dump of 2016/11/07 was analyzed. Classes were recognized as defined in Section 2.1. Unlinked classes were identified by checking whether a class does not have the *subclass of (P279)* property. The taxonomy contained a total of 1299501 classes at this time.

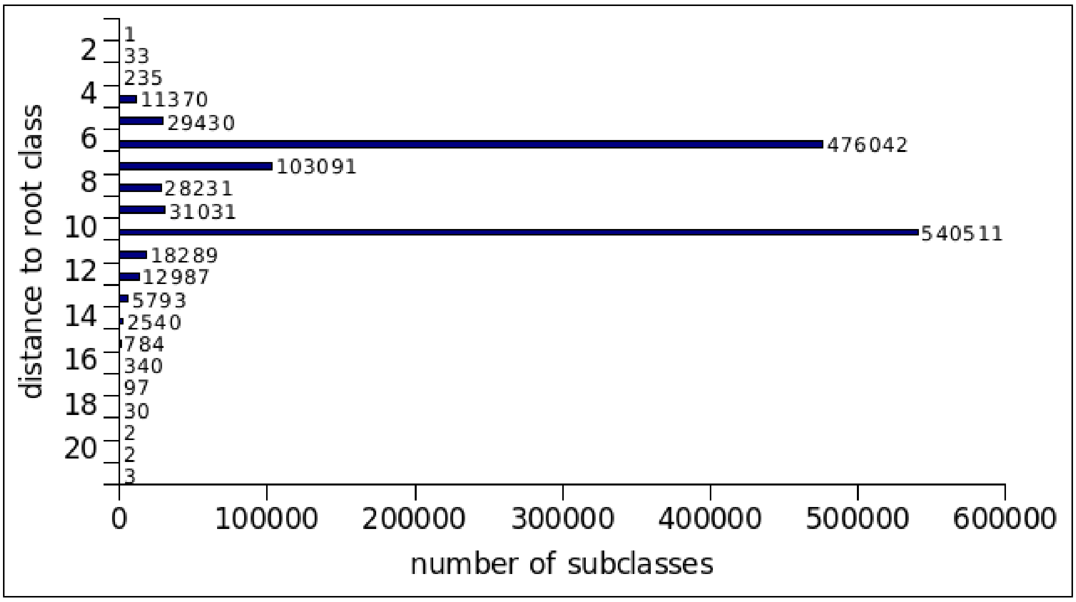

Figure 4: Distance of subclasses to root class *entity (Q35120)*. Wikidata (2016/11/07)

The state of the taxonomy was captured in regards to the root class *entity (Q35120)* (see Figure 4). 1260842 classes are currently subclasses of *entity (Q35120)*. 97% of all classes are therefore nodes in the root taxonomy. This implies a high agreement in the Wikidata community on which class is considered root, and thereby also supports the modeling decision made in Section 2.2, which assumes that a taxonomy only has one root, and this root is *entity (Q35120)* in Wikidata. **Last sentences of this paragraph are mostly interesting trivia, but have currently no further use.** The longest shortest distance between the root and a leaf class is 20. The classes *Q639064*, *Q15978631* and *Q151055* fulfill this characteristics. Each of them is subclass of *Homo (Q171283)*.

The characteristics of all unlinked classes and the root class were analyzed. This set contains a total of 16373 classes. 13807 classes have an English label and 11534 classes have a corresponding English Wikipedia page.

Regarding the number of unique properties (or statement groups) per class (see Figure 5) the median is 3 and the average is ≈ 4.8. Combined with the analyzed unique property frequency (see Figure 6), it can be seen that many unlinked classes are linked to other knowledge bases and taxonomies , e.g. Freebase or GND, using an identifier. Another observation is that 901 of the unlinked classes have properties related to taxons, which is a, to some degree, separate taxonomy in Wikidata, created with properties like *taxon name (P225)*, *parent taxon (P171)*, etc.

Most unlinked classes have only 0 to 1 instances, the median is 1 and the average is ≈ 4.65 instances per class (see Figure 7). There are however outliers with big numbers of instances, which skew the average number of instances per class. This may for example imply, that classes are created mainly for the purpose of grouping newly created instances.

The median and average for subclasses per class are 0 and ≈ 0.85 respectively (see Figure 8). This implies that the graph components of the unlinked classes are very small, and in most cases contain only the respective unlinked class.

The question has to be asked, whether an algorithm should try to handle the complete set of unlinked classes, or only a specific subset, which fulfills certain requirements. The answer depends on what information such an algorithm requires as input. The full set of unlinked classes is problematic for use in an algorithm as there are few shared characteristics over all classes. $\approx 16\%$ of classes are not labeled and $\approx 31.4\%$ of classes have no instances. Both labels and instances are useful characteristics for a class to have. The label allows the recognition of the class in natural text and ensures that the class fulfills a basic quality criteria, since the label is the first characteristic of a Wikidata item, which should be created by a user [1]. Instances represent classes and thereby describe them. For example, Rodríguez and Egenhofer [20] use instances to compute semantic similarity between classes. Therefore, I propose to only consider the set of classes, which have a label in the English language and at least 1 instance, as input for the algorithm. **TODO: Find a short name or acronym for this subset.**

Following this argument, the subset of labeled, instantiated and unlinked classes was analyzed. This set contains a total of 9157 classes. 7557 classes have an English Wikipedia page, which is $\approx 82.5\%$ of all analyzed classes in the subset, and an increase of $\approx 12\%$ in comparison to the full set of unlinked classes.

The average of unique properties per class increases from 4.8 to 5.5, while the median remains at 3 (see Figure 9). The frequency of different properties appearing in classes however is more distributed (see Figure 10). This implies that the classes of this subset are related to different topics, and share only few commonalities.

As expected the average of instances per class increased to ≈ 7.37 from ≈ 4.65. However the median is still 1 (see Figure 11). $\approx 59\%$ of classes have only 1 instance.

At the same time the average of subclasses per class halved to ≈ 0.4 (see Figure 12). **can i just do such an assumption? the data supports it a bit, but i am not searching for counterclaims. and the assumption is not directly relevant to the thesis.** Combined with the unchanged median of 1 instance per class, supports the assumption, that classes are mainly created for the purpose of grouping instances. While adding the newly created class to the main taxonomy is being neglected.

The classes of the subset have, on average, a better level of description, more unique properties and instances, than the full set of unlinked classes. Between these classes the number of commonalities is lower, because the same properties occur not as frequently for different classes. The lack of commonalties between unlinked classes is not very problematic, as the algorithm would not compare unlinked classes with each other but with classes in the root taxonomy.

After completing the analysis, it can be seen that *entity (Q35120)* is the root class

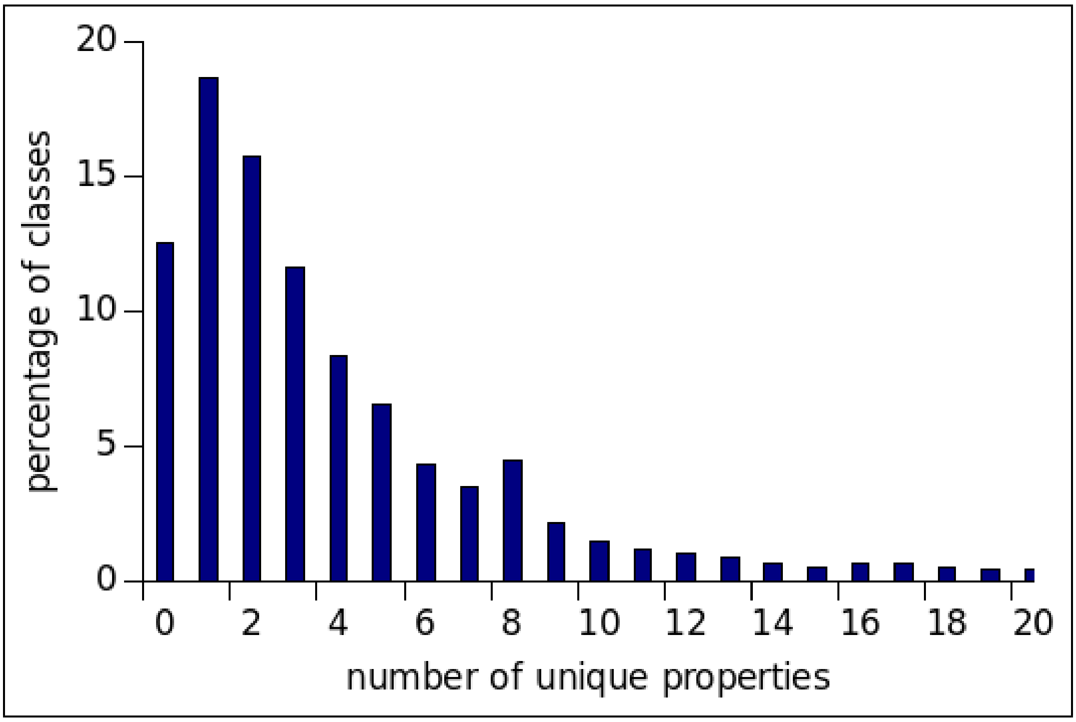

Figure 5: Percentage of unlinked classes with a specific amount of unique properties. Wikidata (2016/11/07)

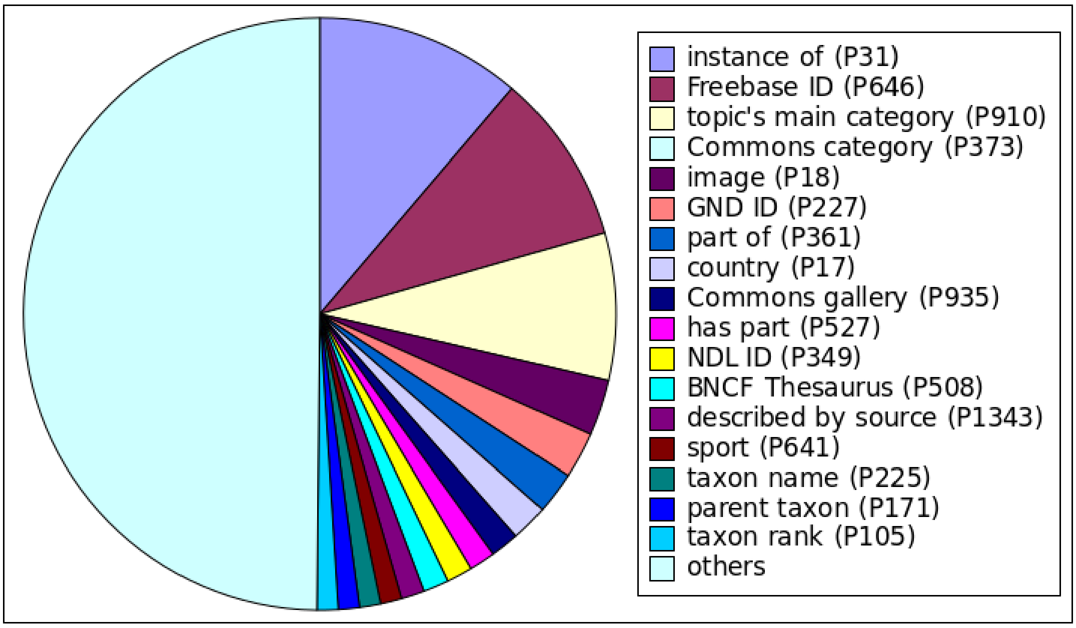

Figure 6: Frequency of properties in unlinked classes. Wikidata (2016/11/07)

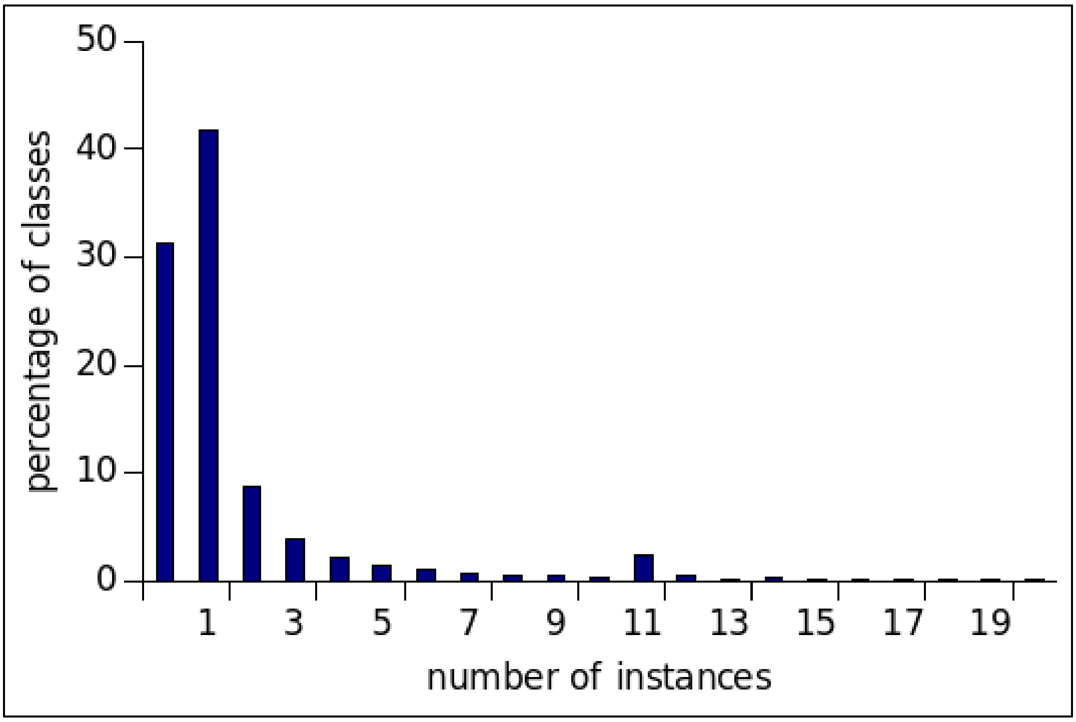

Figure 7: Percentage of unlinked classes with a specific amount of instances. Wikidata (2016/11/07)

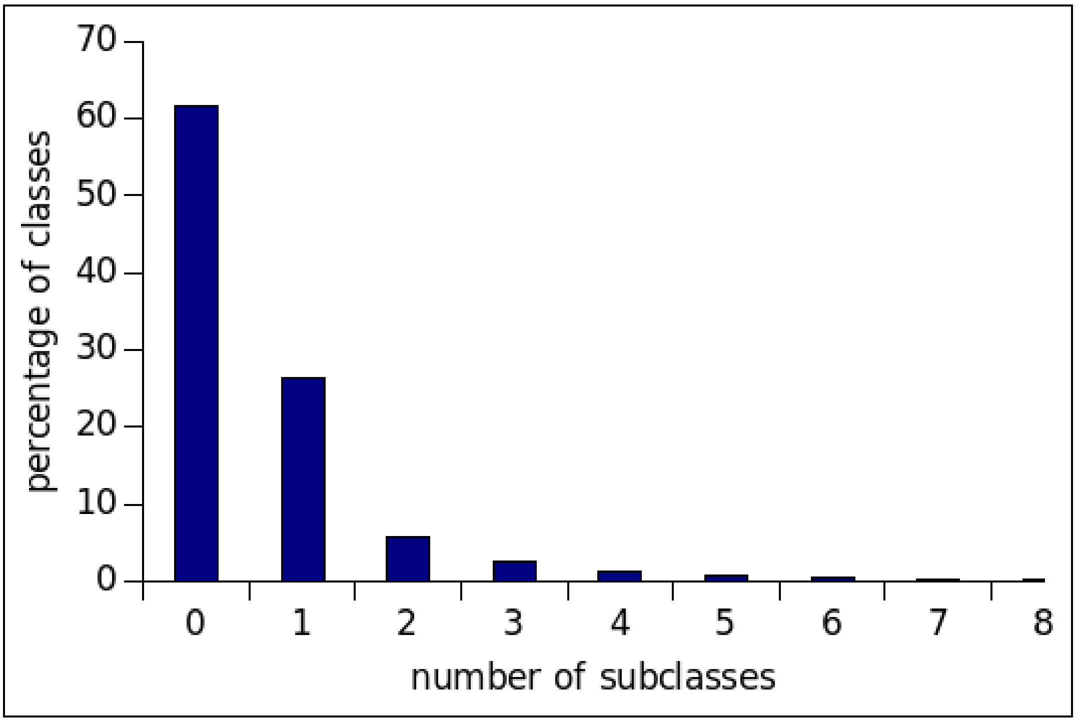

Figure 8: Percentage of unlinked classes with a specific amount of subclasses. Wikidata (2016/11/07)

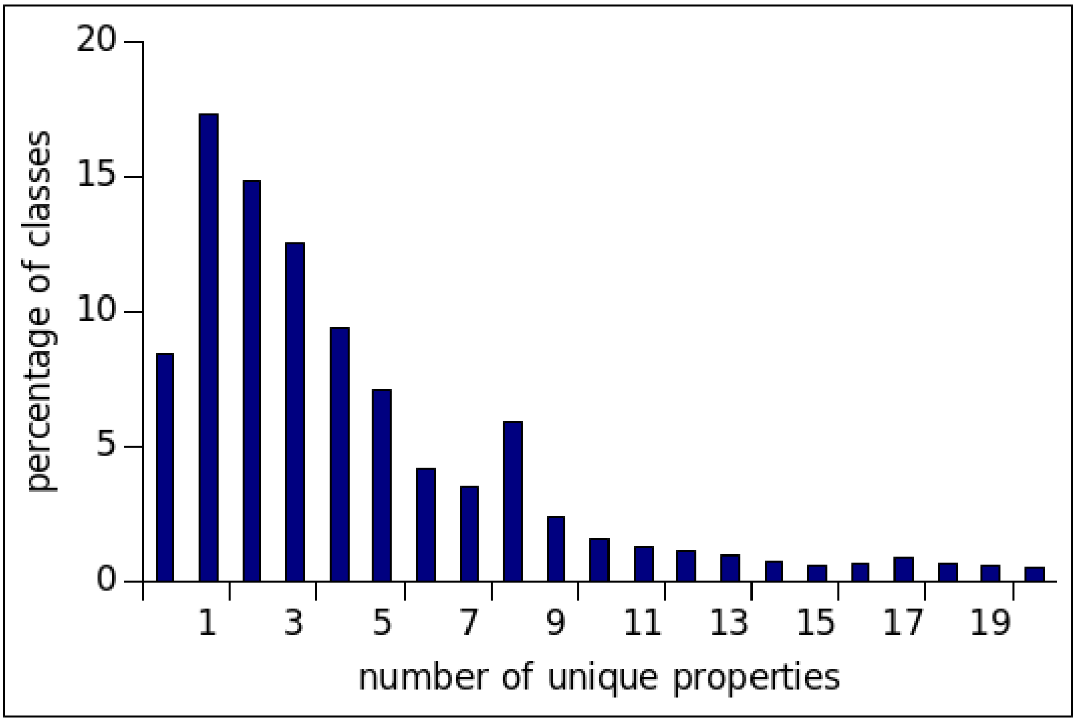

Figure 9: Percentage of unlinked, labeled, instantiated classes with a specific amount of unique properties. Wikidata (2016/11/07)

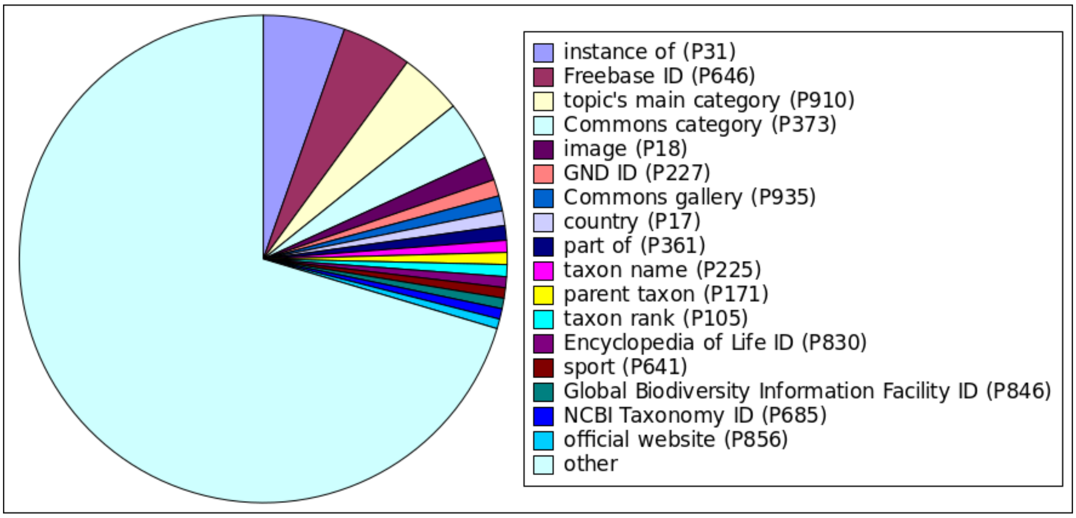

Figure 10: Frequency of properties in unlinked, labeled, instantiated classes. Wikidata (2016/11/07))

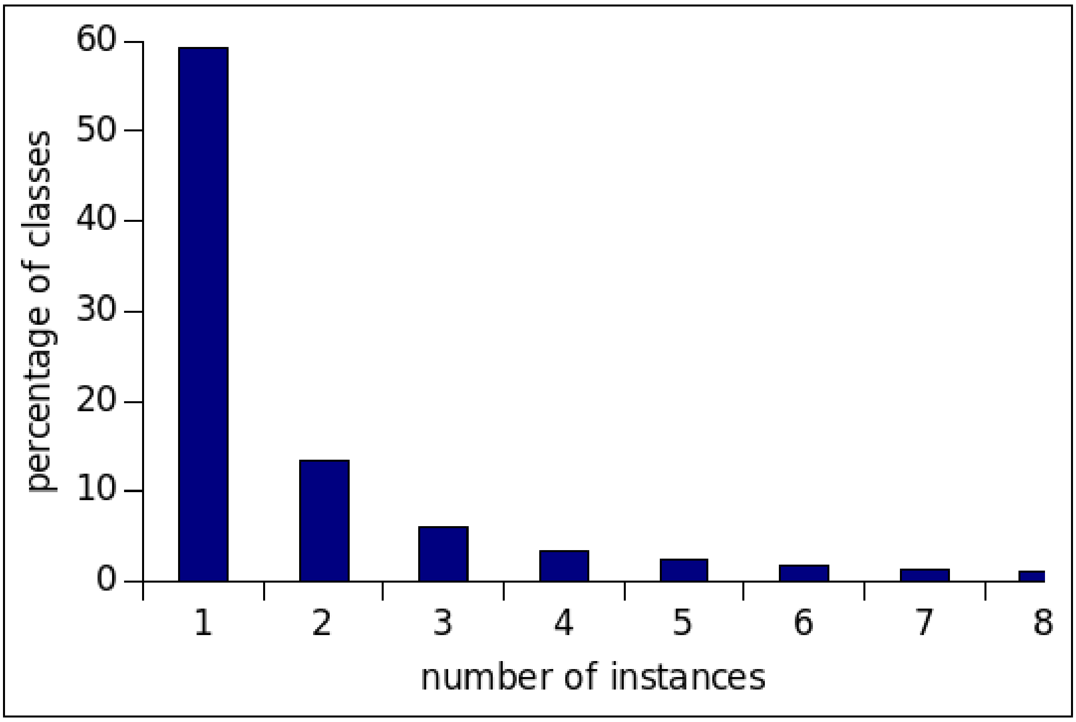

Figure 11: Percentage of unlinked, labeled, instantiated classes with a specific amount of instances. Wikidata (2016/11/07))

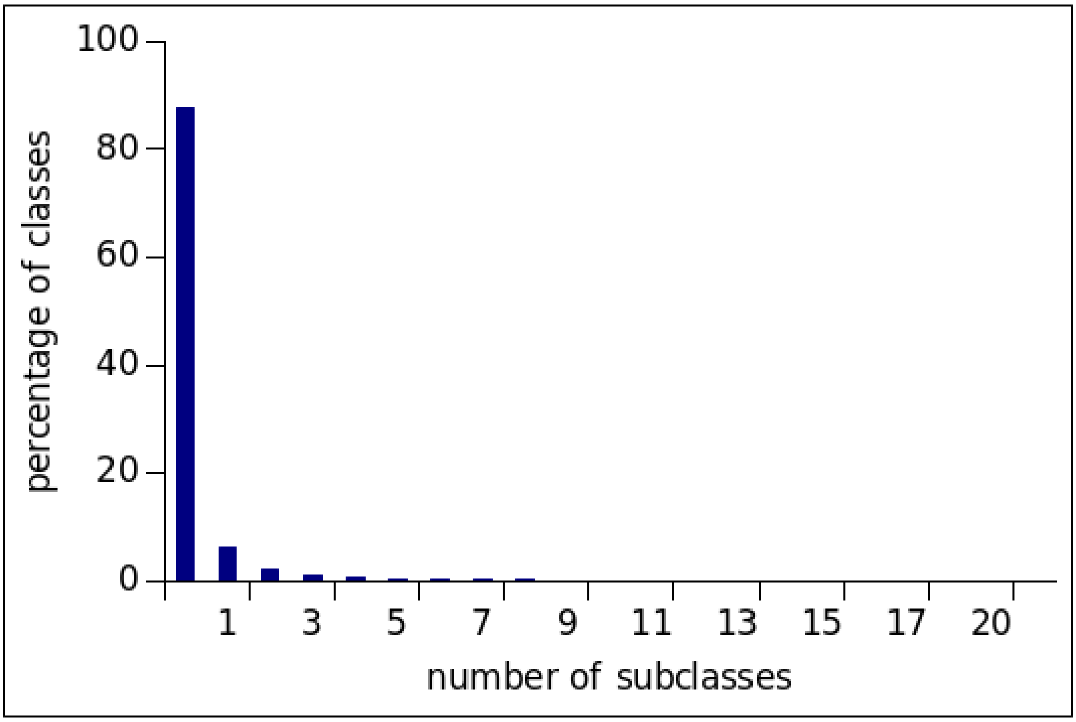

Figure 12: Percentage of unlinked, labeled, instantiated classes with a specific amount of subclasses. Wikidata (2016/11/07)

of the taxonomy, and Wikidata's taxonomy is in a good state, since 97% of classes are part of the root taxonomy. **TODO: not sure if i can just say that it is in a good state** Unlinked classes share few commonalities, and as shown above, a percentage of classes lack even basic information like a label. For developing an algorithm it is necessary to set a baseline, of what can be expected from the input. In this case, input is required to be labeled and have at least one instance. The benefit of this specific restriction is, that a basic level of descriptiveness can be assumed for every class. A label additionally allows supplementing the information, provided by Wikidata, to be supplemented with natural text sources, like Wikipedia, since it is now possible to recognize occurrences of the class in text.

4 Ontology learning

General concepts. Classification of considered problem in the task of ontology learning. Related work.
Cimiano et al. [6]
Wong et al. [22]
d'Amato et al. [8]
Petrucci et al. [18]
Fu et al. [11]

5 Neural networks

Notion of neural networks will be introduced.

5.1 Recursive neural networks for graph representation

Scarselli et al. [21]

5.2 Deep neural networks for graph representation

Cao et al. [4]
Raghu et al. [19]

5.3 Continuous Bag-of-Words

Mikolov et al. [17]

5.4 Skip-gram with negative sampling

Mikolov et al. [17]
Levy et al. [15]

Goldberg and Levy [13]
graph representations are not really relevant as there is only one big component and the input classes are not part of that component.

5.5 Comparison

6 Algorithm

6.1 Baseline

- Hyper parameters
- Training data

6.2 Supplementing with other resources

e.g. Wikipedia

7 Evaluation

7.1 Method

Dellschaft and Staab [9]

7.2 Generation of gold standard

7.3 Results

References

[1] Wikidata: Create a new item. https://www.wikidata.org/wiki/Special:NewItem, . Accessed: 2017-02-05.

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