
Exploring the Properties and Structure of Real Knowledge Graphs across Scientific Disciplines

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Abstract

1 Despite the recent popularity of knowledge graph (KG) related tasks and bench-
2 marks such as KG embeddings, link prediction, entity alignment and their use in
3 many domains, the structure and properties of real KGs are not well studied. In
4 this paper, we perform a large scale comparative study of 29 real KG datasets from
5 diverse domains such as the natural sciences, medicine, and NLP to analyze their
6 properties and structural patterns. Based on our findings we make recommenda-
7 tions regarding KG-based model development and evaluation. We believe that the
8 rich structural information contained in KGs can benefit the development of better
9 KG models across fields and we hope this study will contribute to breaking down
10 the existing data silos between different scientific disciplines (e.g., biomedicine,
11 ML/NLP, 'AI for Sciences').

12 **1 Introduction**

13 Recent years have been marked by an increased use of multimodal and structured datasets in the form
14 of knowledge graphs (KGs) to enhance applications in diverse scientific and technical disciplines
15 such as natural language processing (NLP), natural sciences and medicine, manufacturing and process
16 automation to name a few (Zou, 2020; Peng et al., 2023). The wide applicability of KGs is not
17 surprising: they are scalable data objects that store factual (i.e., with high degree of certainty)
18 information in the form of triples and allow for encoding both topological and semantic information.

19 The growing interest in using KG across various domains has led to a surge in the release of new KG
20 datasets: for example, 43% the 37 datasets available in the PyKEEN v1.10¹ KG embedding library
21 have been published since 2020 (Ali et al., 2021b). Many other libraries – e.g., OGB (Hu et al., 2020,
22 2021), LibKGE (Ruffinelli et al., 2020; Broscheit et al., 2020) and PyTorch Geometric (Fey and
23 Lenssen, 2019) – consolidate multiple KG models in a central repository or provide tools for task-
24 specific benchmarking. Lastly, several recent studies focus on scalable benchmarking of KG related
25 tasks: for example Ali et al. (2021a) compare the performance of 21 KG link prediction models, Sun
26 et al. (2020) evaluate 12 embedding-based EA approaches on dedicated benchmark datasets, while
27 AlKhamissi et al. (2022) propose a KG-based framework for assessing the performance of pretrained
28 language models (PLMs) with the goal of achieving parity between PLMs and KGs.

29 Even with the abundance of KG datasets, benchmarking tools, and extensive large-scale model
30 comparisons across various KG tasks, to the best of our knowledge, there are no studies that address a
31 much more fundamental question, namely: *what properties and structure do real KGs have and how*
32 *do they compare to each other in terms of these properties?* We argue that a systematic approach of
33 analyzing KG properties (the goal of this paper) has the potential to inform algorithmic development

¹Permalink: <https://ezproxy.library.und.edu/login?url=https://github.com/pykeen/pykeen>

Table 1: Datasets that were analyzed in this study. #E, #R, and #T denote the number of entities, relations and triples, respectively. deg denotes the average degree of all the KG entities. d denotes the KG density, shown in log scale (a lower column value implies a denser KG).

#	dataset	# E	# R	# T	category	deg	$-\log(d)$
1	AristoV4	42,016	1,593	279,425	biomed	7	3.80
2	BioKG	105,524	17	2,067,997	biomed	20	3.73
3	CoDExLarge	77,951	69	612,437	semantic	8	4.00
4	CoDExMedium	17,050	51	206,205	semantic	12	3.15
5	CoDExSmall	2,034	42	36,543	semantic	18	2.05
6	ConceptNet	28,370,083	50	34,074,917	semantic	1	7.37
7	Countries	271	2	1,158	society	4	1.80
8	CSKG	2,087,833	58	4,598,728	semantic	3	5.98
9	DB100K	99,604	470	697,479	semantic	7	4.15
10	DBpedia50	24,624	351	34,421	semantic	1	4.25
11	DRKG	97,238	107	5,874,257	biomed	60	3.21
12	FB15k	14,951	1,345	592,213	semantic	40	2.58
13	FB15k-237	14,505	237	310,079	semantic	21	2.83
14	Globi	404,207	39	1,966,385	biomed	5	4.92
15	Hetionet	45,158	24	2,250,197	biomed	50	2.96
16	Kinships	104	25	10,686	society	103	0.01
17	Nations	14	55	1,992	society	143	-1.01
18	OGBWikiKG2	2,500,604	535	17,137,181	semantic	7	5.56
19	OpenBioLink	180,992	28	4,563,407	biomed	25	3.86
20	OpenEA	15,000	248	38,265	semantic	3	3.77
21	PharmKG	188,296	39	1,093,236	biomed	6	4.51
22	PharmKG8k	7,247	28	485,787	biomed	67	2.03
23	PrimeKG	129,375	30	8,100,498	biomed	63	3.32
24	UMLS	135	46	6,529	biomed	48	0.45
25	WD50K	40,107	473	232,344	semantic	6	3.84
26	Wikidata5M	4,594,149	822	20,624,239	semantic	4	6.01
27	WN18	40,943	18	151,442	semantic	4	4.04
28	WN18RR	40,559	11	92,583	semantic	2	4.25
29	YAGO3-10	123,143	37	1,089,000	semantic	9	4.14

34 across disciplines and empower the next generation of KG-based applications in NLP, biomedicine
35 and other areas where KGs are used.

36 **Contribution and Scope.** In order to begin addressing the above question, we analyze the structure
37 of KGs in terms of their network statistics, topology and relation types. Our large scale comparative
38 study is based on 29 real KG datasets from diverse domains such as biology, medicine, and NLP.
39 Towards our goal, we: (1) measure various KG properties (e.g., KG density, degree distribution);
40 (2) analyze the KG structure in terms of the relational types and the KG topology; and (3) describe
41 common/distinct structural patterns we observe KG datasets derived from fundamentally different
42 underlying domains. Based on our findings, we make several recommendations for future model
43 development and evaluation. Lastly, our primary goal is to analyze KG datasets and their properties
44 along different dimensions, rather than benchmark downstream task-specific models on said datasets.

45 2 Application of Knowledge Graphs in Different Disciplines

46 **Notation.** For a given set of entities E and a set of relations R , a knowledge graph $\mathcal{K} \subseteq \mathcal{K} = E \times R \times E$
47 is a directed multi-relational graph that contains triples of the form $(h, r, t) \in \mathcal{K}$ in which $h, t \in E$
48 represent the head and tail entities and $r \in R$ is the relation between them. KG embedding models
49 (e.g. TransE (Wang et al., 2014), DistMult (Yang et al., 2014)) learn latent vector representations of
50 the entities $e \in E$ and relations $r \in R$ that best preserve the KG’s structural properties.

51 **Natural Sciences and Medicine.** KGs are used in various biomedical applications (Nicholson and
52 Greene, 2020; Ektefaie et al., 2023) and have recently found use in precision medicine (Chandak
53 et al., 2023). In biology and medicine KGs typically describe the relationships between biomedical
54 entities such as diseases, drugs, phenotypes, and regulatory pathways. They are a convenient tool
55 for aggregating knowledge fragmented across publications, repositories, ontologies and databses
56 (Chandak et al., 2023). KGs embeddings and link prediction find application in pharmaceutical
57 applications (e.g. discovery and drug repurposing), clinical applications (e.g., disease diagnosis and
58 treatment) and genomics (e.g., the study of phenotyping) (Morselli Gysi et al., 2021; Chandak et al.,
59 2023; Wang et al., 2023). Natural science disciplines such as physics (Zou, 2020) and geology (Zhu
60 et al., 2017) make use of multimodal data such as scientific literature and other natural language
61 datasets to construct domain-specific KGs.

62 **ML and NLP.** In ML and NLP PLMs have gained immense popularity in recent years due to their
63 impressive ability to process and generate human-like text. PLMs, such as GPT-4 (OpenAI, 2023)
64 or Llama (Touvron et al., 2023) are able to generate answers to complex user queries on a variety
65 of technical topics. However, these models are known to suffer from a lack of grounding of their
66 outputs (in factual, common sense and domain specific knowledge) and from having difficulties in
67 properly dealing with the meaning of inter-related concepts (Carta et al., 2023). Some approaches
68 use factuality, common sense, physical and domain specific knowledge to mitigate the weaknesses of
69 PLMs (Wei et al., 2021; Zamini et al., 2022; Hu et al., 2023); see (Yang et al., 2023) for a review.
70 Many ‘LMs as KBs’ works, reviewed in (AlKhamissi et al., 2022), also use KGs for fine-grained
71 evaluation of different aspects of PLMs such as their ability to recover factual knowledge or their
72 consistency (Heinzerling and Inui, 2021). However, in none of those approaches the properties of the
73 KGs at hand are considered.

74 **Other Areas of Science.** Many other domains such as cybersecurity, finance, education, factory
75 monitoring and process automation, geopolitics and combating human trafficking benefit from KGs
76 and apply KG tasks such as EA and link prediction – Li et al. (2020); Zou (2020) provide a review of
77 domain-specific KGs and their downstream use in these areas.

78 2.1 Knowledge Graph Datasets Analyzed

79 Among all the datasets in the various domains described above, we used a set of 29 KGs, which we
80 list in Tab. 1 together with their summary statistics. We categorize them into three distinct groups:

- 81 1. **biomedical KGs** (count=9) which store facts related to biology and medicine such as relationships
82 between genes, proteins or cellular pathways. Datasets in this group are typically derived from
83 high quality public databases such as DrugBank (Wishart et al., 2018) and PubChem (Kim et al.,
84 2016) – for construction details see (Zheng et al., 2021).
- 85 2. **semantic web KGs** (count=17) which incorporate knowledge extracted using the tools of the
86 semantic web or analogous mechanism such RDF (Fensel, 2005).² Many datasets in this category
87 are derived from each other or share common sources – for example ConceptNet (Speer et al.,
88 2017) is based, in part, on DBpedia (Auer et al., 2007), while CSKG (Ilievski et al., 2021) makes
89 use of ConceptNet and Wikidata.
- 90 3. **societal KGs** (count=3) are a set of manually curated datasets that contain factual information
91 about different domains such as geography and international relations We note that these KGs
92 are conceptually similar to the ones in the biomedical domain in the sense that they are based on
93 relationships between physical objects.

94 We use the datasets through the PyKEEN v1.10 software package (see details in the Appx.)

95 3 The Properties and Structure of Knowledge Graphs

96 The structural characteristics of KGs play an important role in the applicability and the performance
97 of various tasks such as KG embeddings, link prediction and reasoning. For example, KG properties
98 such as relation type (e.g., inverse, symmetric), cardinality and statistics affect the KG connectivity

²https://www.wikidata.org/wiki/Wikidata:Database_download

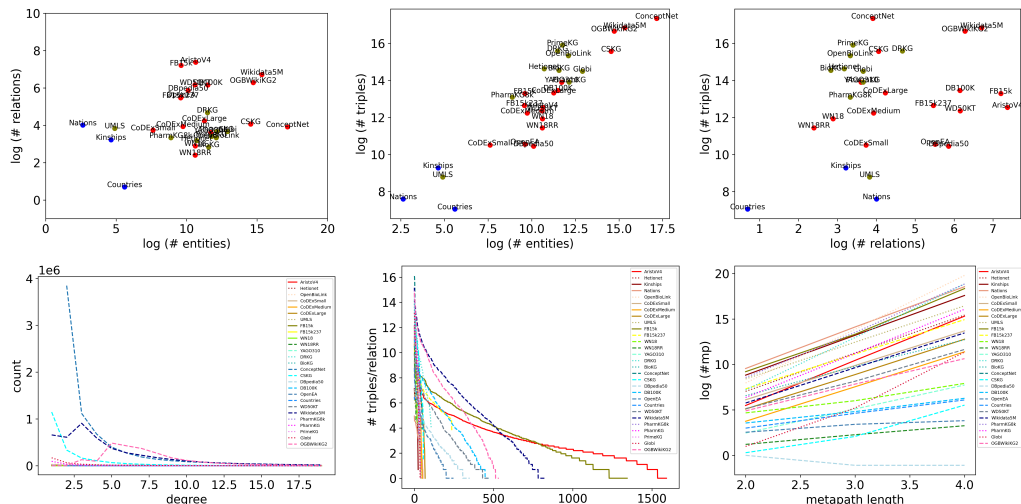


Figure 1: **(Top)** Relations between (left) number of entities vs. number of relations; (center) number of entities vs. number of triples; (right) number of relations vs. number of triples in different KGs. Biomedical, semantic web and societal datasets are colored in resp. olive, red, and blue. All axes are *log*-scale. **(Bottom)** (left) Degree distribution; (center) number of triples per KG relation, *log* scale; (right) metapath (mp) length distribution on the *y*-axis, *log* scale.

99 patterns which get encoded in the KG node and relation embeddings and used in downstream models.
 100 The effect relation types have was demonstrated by Toutanova and Chen (2015) who first described
 101 the ‘inverse relation problem’ in KG link prediction: essentially, an information leakage between
 102 the train and test splits due to the presence of *inverse* relations in the training dataset splits. They
 103 identified the issue in the FB15k dataset and released its updated version FB15k-237, both commonly
 104 used in NLP benchmarks. Moreover, the inference abilities of KG embedding algorithms vary by
 105 relation type and cardinality. For example, TransE cannot model symmetric and one-to-many relations
 106 well due to its scoring function $f(r, h, t) = -||h+r-t||$. Similarly, the distance functions for DistMult
 107 and ComplEx cannot model composite relations. Cao et al. (2022) provide a detailed review.

108 In the ML and NLP literature semantic web datasets are prevalent and the performance of KG
 109 embeddings, EA models and link prediction (both embedding-based and Graph Neural Network
 110 (GNN)-based (Cucala et al., 2021) approaches) is often demonstrated only on a small set of semantic
 111 web datasets such as FB15k, WN18 and Wikidata5M. On the other hand, in the biomedical domain it
 112 has been widely accepted that semantic web datasets do not reflect the domain specific properties
 113 of biomedical KGs due to a variety of factors (Zheng et al., 2021; Breit et al., 2020). One such
 114 factor are the interaction effects in KGs: biomedical KGs have been found to be sparse, incomplete
 115 and containing richly structured ontological hierarchies with large interaction networks instead of
 116 capturing knowledge networks (e.g., FB15k) or hierarchical taxonomies (e.g., WN18)(Zheng et al.,
 117 2021; Breit et al., 2020). Another distinguishing characteristic of biomedical KGs is the nature of the
 118 entities stored in them – for example automatically created datasets such as OpenBiolink (Breit et al.,
 119 2020) contain large number of meta data entities and trivial biomedical entities which can interfere
 120 with KG embeddings and link prediction models as reported by Zheng et al. (2021).

121 **KG vs. Graph Structure.** KGs remain relatively unexplored as topological objects, partially because
 122 KG datasets were not readily available in libraries or benchmarks, such as PyKEEN or PyTorch
 123 Geometric until recent years. In contrast, as network analysis gained momentum in the 1990s,
 124 thanks to the growing availability of web, social and other real networks, the topology and numerical
 125 characteristics of directed and undirected graphs (the homogeneous counterparts of KGs) have been
 126 extensively studied. Multiple libraries and benchmarks have been established for the analysis of
 127 graph/network properties – examples include the general purpose network and graph mining library
 128 SNAP (Leskovec and Sosič, 2016) and the SuiteSparse matrix collection (Davis and Hu, 2011;

129 Kolodziej et al., 2019) which systematizes graphs together with their numerical characteristics and
130 finds application in scientific computing research.

131 **Graph Structure in Existing Benchmarks.** Many KG benchmarks (Ali et al., 2021a; Widjaja
132 et al., 2022) focus on standardizing model training, hyper parameter tuning or task-specific model
133 evaluation. However, only a few benchmarks provide support for evaluation of KG tasks with respect
134 to the underlying KG structural properties. One example is the KGxBoard framework for KG link
135 prediction evaluation (Widjaja et al., 2022). KG link prediction performance is often measured using
136 metrics (e.g., precision) averaged over a held-out set, however, as noted by Widjaja et al. (2022),
137 single-score summary metrics cannot reveal exactly what the model has learned or failed to learn. To
138 remedy this, the KGxBoard framework implements a fine-grained performance reporting per relation
139 type. While in principle the KGxBoard framework offers support for multiple relation types, the
140 authors did not perform a systematic evaluation of link prediction performance for multiple relation
141 types or KG properties. In another benchmark, Ali et al. (2021a) evaluate 21 KG link prediction
142 models with respect to four relational patterns on 4 datasets (mix of semantic web and societal),
143 however, they do not analyze the link prediction performance in the context of the KG relational
144 distributions and properties. Lastly, Sun et al. (2020); Leone et al. (2022) benchmark KG heterogeneity
145 and its effect on EA performance.

146 4 Methodology and Results

147 **Methodology.** We perform a series of data analysis steps to measure various KG properties and
148 structural dimensions across all datasets. Below we provide details on each KG dimension we
149 considered, describe the experiments we conducted along each dimension and summarize empirical
150 observations and findings. Unless otherwise noted, we used the datasets in their entirety (incl. train,
151 test, and validation splits). The code from our experiments will be made available in the final version.

152 **Entities, relations and triples.** In Fig. 1 we show the relations between the total number of entities,
153 relations and triples in each dataset. When plotting the number of entities vs. number of relations in
154 Fig. 1 (top, left), we notice that on average semantic web KGs have more diversity in terms of the
155 entity/relation count, while most biomedical KGs cluster at similar entity/relation count. This implies
156 that regardless of the fact that many of the semantic web datasets are derivatives of each other, as
157 mentioned in Sec. 2.1, they exhibit some diversity along these two dimensions. Notably, Fig. 1 (top,
158 center) – plotting the number of entities vs. number of triples – shows the biomedical KGs cluster
159 together with the exception of the PharmKG8K and UMLS datasets. In the same panel (top right
160 corner) we also observe that the largest KG datasets in our study are predominantly semantic web
161 ones. Finally, Fig. 1 (top, right) shows that biomedical datasets exhibit less diversity in terms of the
162 relation vs. triples count, in comparison to the semantic web datasets.

163 **Average degree and degree distribution** KG entities are connected to each other by directed edges
164 (corresponding to the relations), hence an entity can have outgoing edges (or an out-degree) when
165 it is the head entity in a triple and incoming edges (or an in-degree) when it is the tail entity in a
166 triple. We sum the in-degrees and out-degrees to obtain the entity degrees analogously to the way
167 node degrees are computed in undirected graphs. A smaller average degree indicates that the KG is
168 sparser. Fig. 1 (btm, left) shows the degree distribution (over all entities). The average degree for each
169 KG is also shown in Tab. 1. From this table we notice that the semantic datasets have some of the
170 lowest average degrees across all datasets (e.g., ConceptNet with an average degree of 2). Among the
171 semantic datasets FB15k has the singularly highest average degree, while its derivative FB15k-237
172 has a value that aligns with the rest of the semantic datasets. On the other hand, the average degrees
173 of biomedical datasets are split into two groups: 5 of the biomedical datasets have average degrees in
174 the low 100's while PharKG, Globi, OpenBioLink, and BioKG have average degrees that are closer
175 to the values of the semantic datasets. The two societal datasets Kinship and Nations demonstrate
176 a significantly higher average degree than the rest of the KGs (see the Appx.) In Fig. 1 (btm.,
177 left) several datasets show a distinct degree distribution in the lower degrees. ConceptNet, CSKG
178 have the highest number of low-degree nodes, while the degree distributions of Wikidata5M and
179 OGBWikiKG2 are not as smooth, with oscillations at degrees 3 and 5, respectively.

180 **KG Density.** The KG density is computed as the ratio $|E|/|R|^2$ and like in homogeneous graphs
 181 higher density implies more sparsity (see Tab. 1, last column). The degree trends we described in
 182 the previous paragraph can also be traced along this dimension. Related to the KG density, we also
 183 quantify the KG connectivity by plotting the triples per KG relation in Fig. 1 (btm., center). The thick
 184 tails in the plot show that AristoV4, followed by FB15k, have a high number of relations with a low
 185 number triples per relation. Several other semantic datasets follow the same pattern, while none of
 186 the biomedical datasets do, with the exception of DRKG.

187 **Relation cardinality:** Relation cardinality describes the numerical relationship between the possible
 188 head and tail entities of the relation (i.e., how many entities a relation can have as a tail or head).
 189 The possible types are: (i) one-to-one (1-1), (ii) one-to-many (1-M), (iii) many-to-many (M-M), (iv)
 190 many-to-one (M-1) (Widjaja et al., 2022). For illustration, the relation GeneActivationGene (from
 191 the OpenBioLink dataset) is M-M because various genes can activate multiple other genes. Fig. 2
 192 plots the relation cardinality distribution for each dataset considered. We observe several different
 193 dataset profiles: **(i) 1-1 dominance:** In 15 of the 28 datasets in Fig. 2 the leading relation type is 1-1
 194 including many semantic datasets. Overall, the number of 1-1 relations is more pronounced in the
 195 semantic datasets than in the biomedical datasets. **(ii) M-M dominance:** In 11 of the 28 datasets, the
 196 leading relation type is M-M. Biological datasets (e.g. BioKG, Hetionet, OpenBioLink, PharmKG8k)
 197 are dominated by M-M relations with the exception of PharmKG and Globi which exhibit a distinct
 198 profile. All societal datasets also fall in this category. **(iii) mixed cardinalities:** We observe that
 199 some of the most frequently used semantic datasets (FB15k, FB15k-237, Yago310) have a significant
 200 number of all 4 cardinalities unlike the rest of the analyzed datasets. **(iv) mixed profile with a 1-1 or**
 201 **M-M skew:** All biomedical datasets tend to be skewed towards M-M relations, except PharmKG and
 202 Globi. All semantic datasets tend to be skewed towards 1-1 relations, with the notable exception of
 203 Yago310.

204 **Relational patterns.** We considered four relation types described in the literature (Ali et al., 2021a;
 205 Toutanova and Chen, 2015). A relation $r \in R$ is: (i) **asymmetric** if $(h, r, t) \in T \implies (t, r, h) \notin T$. (ii)
 206 **symmetric** if $(h, r, t) \in T \implies (t, r, h) \in T$. (iii) **inverse** to $r_{inv} \in R$ if $(h, r, t) \in T \implies (t, r_{inv}, h) \in T$
 207 If there exists a $r' \in R$, s.t. $r' \neq r$ and r' is inverse of r then r is an inverse relation. (iv) **composite**
 208 of two relations $r_1, r_2 \in R$ if $(x, r_1, y) \in T \wedge (y, r_2, z) \in T \implies (z, r, z) \in T$. Fig. 3 plots the relation
 209 pattern distribution for each dataset considered. Notably, some semantic datasets such as DB100K,
 210 OpenEA and DBpedia50 have a small amount of inverse relations which may affect benchmarking
 211 on these datasets in light of the ‘inverse relation problem’ discussed above. Across all datasets we
 212 observe dominance of anti-symmetric relations, with the exception of the societal datasets and some
 213 of the most frequently used benchmarking datasets in NLP, such as FB15 and WN18RR, which show
 214 presence of all 4 relation types. Some semantic and societal datasets have composite relations, while
 215 none of the biomedical do.

216 **Metapaths:** KG metapaths are widely used in the biomedical literature for assessing the connectivity
 217 of KGs and deriving insights about the clinical or biological relevance of interactions such as gene-
 218 gene or drug effects (Su et al., 2020; Fu et al., 2016; Himmelstein et al., 2017; Zhang et al., 2020). A
 219 metapath is defined as a sequence of relations separated by edge types (metanodes). For example, a
 220 metapath of length ℓ is of the form $e_1 \xrightarrow{r_1} e_2 \xrightarrow{r_2} \dots \xrightarrow{r_{\ell-1}} e_\ell$ where each of $e_1, e_2,$ and e_ℓ belongs to
 221 a specific metanode. For example, in the Hetionet dataset (Himmelstein et al., 2017) the metanodes
 222 Compound, Gene and Disease form the metapath Compound $\xrightarrow{\text{binds}}$ Gene $\xrightarrow{\text{associates}}$ Disease of
 223 length 2. The number of metapaths of a given length provides a way for quantifying the level of
 224 relational composition without having explicit composite relations encoded in the KG. Interestingly,
 225 Cohen et al. (2023) test the reasoning abilities of PLMs by a prompting strategy that forces them
 226 to survey entity neighborhoods; although the authors do not put their work in the context of KG
 227 metapaths.

228 In practice, metapaths of length of greater than 4 are considered too long to make a significant
 229 contribution in link prediction task (Himmelstein et al., 2017; Fu et al., 2016). Fig. 1 (btm., right)
 230 compares the metapath length distribution over paths of length 2, 3 and 4 for all KGs (see Appx for
 231 additional details). From the figure we see that the biomedical datasets contain a significantly higher

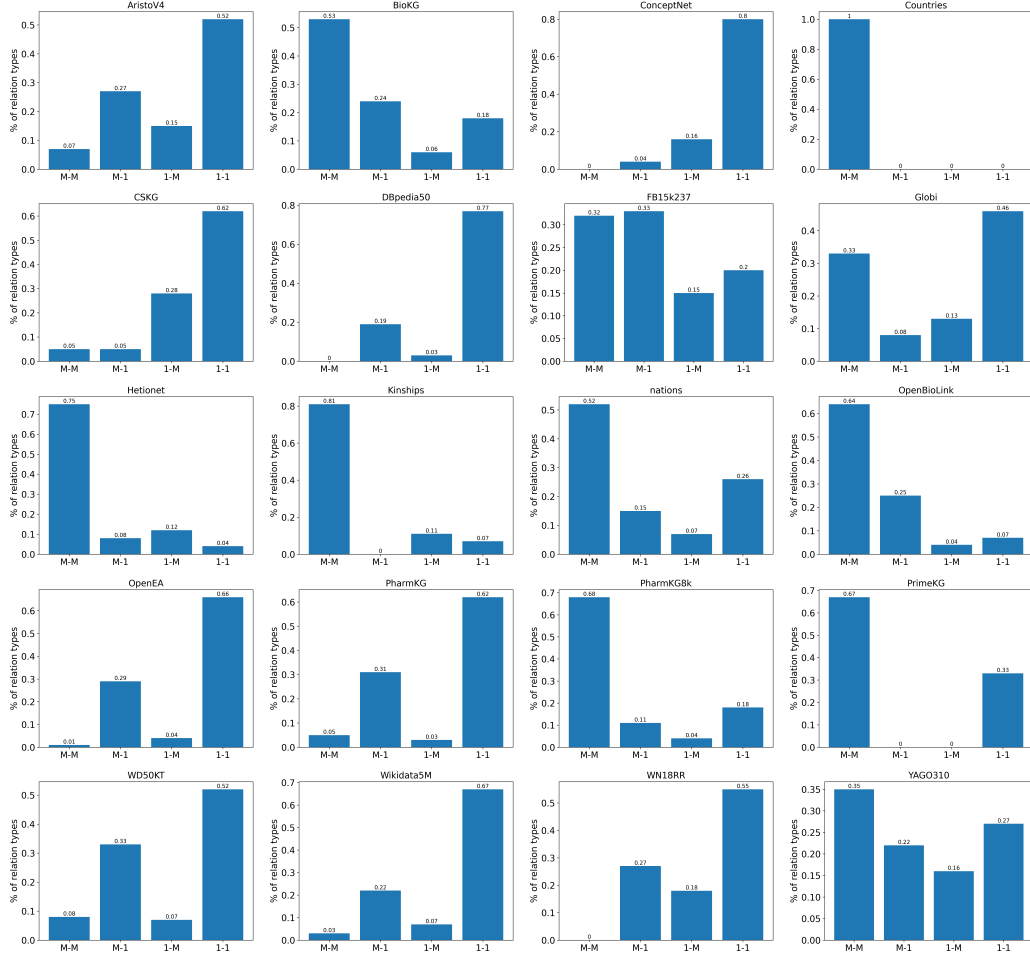


Figure 2: Distribution of relation cardinalities in different KGs. Each bar is marked with the # number of relations of the specified type. Due to space limits, the remaining datasets are shown in the Appx.

232 number of metapaths than the other types of datasets with the exception of Globi. However, among
 233 the semantic dataset FB15k and the societal datasets Kinship and Nations datasets exhibit a profile
 234 which is similar to the biomedical datasets.

235 5 Findings and Future Work

236 Below we highlight the key takeaways from our analysis and make several recommendations:

- 237 • Given the KG diversity observed in this study, we conclude that not all KGs are created equal. This
 238 has implications for model evaluation in all scientific domains KGs are used. Thus, we recommend
 239 that researchers consider a broader set of datasets beyond their target domain (biomedical, NLP,
 240 etc.) for their KG model development and evaluation. Fine-grained model evaluation – for example,
 241 as function of relation type, cardinality, KG density or degree distribution – has the potential to
 242 further drive the development of new KG-based models or inform model selection given the specific
 243 KG properties.
- 244 • Inverse relations are present in some datasets, including some released after the ‘inverse relation’
 245 leakage problem was reported by Toutanova and Chen (2015). Given the implications of this
 246 problem in downstream applications, we recommend KG libraries and benchmarks consider adding
 247 tools for handling/removing inverse relations in order to bring visibility to the leakage problems.
- 248 • The overall negligible amount of composite relations in many datasets (including biological,
 249 semantic, and societal) is one interesting observation that merits further analysis. Composite

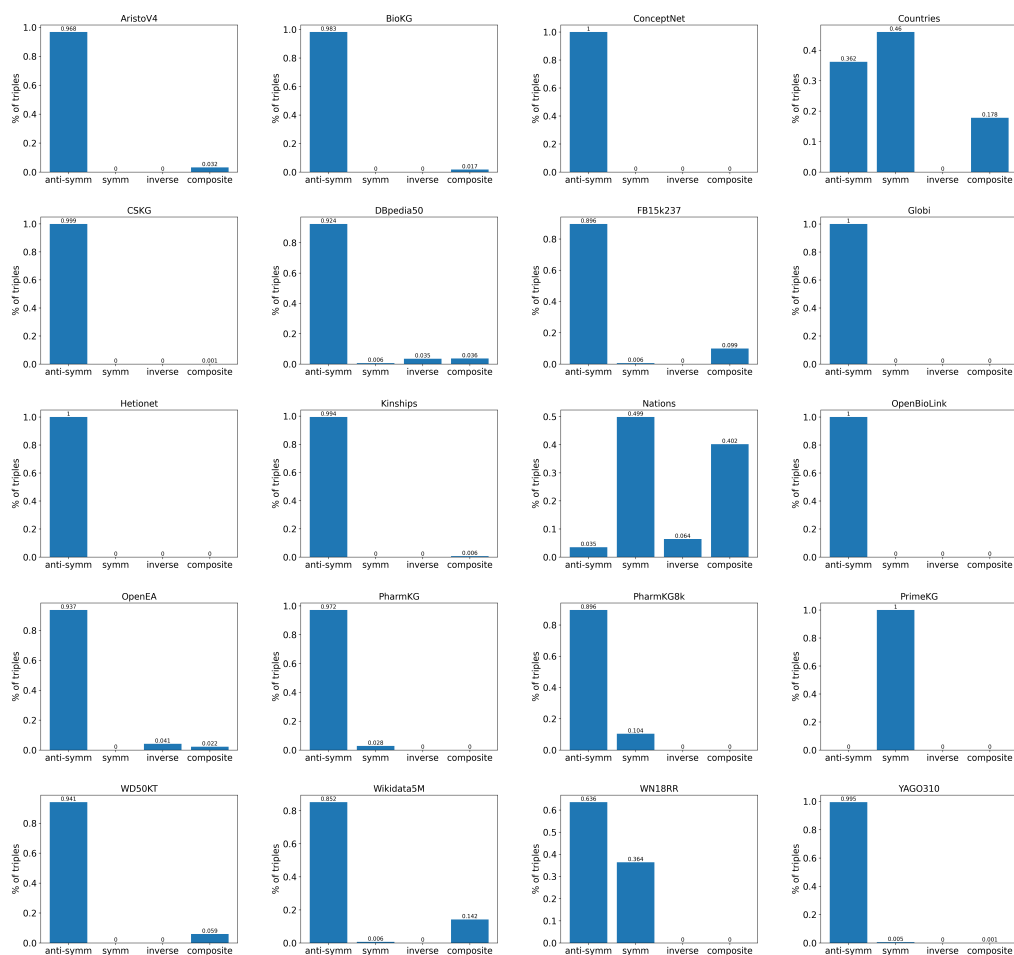


Figure 3: Proportion of (anti-)symmetric, inverse and composite relations in different KGs. Each bar is marked with the # of relations of the specified type with the y -axis showing the corresponding triples (as a % of all triples). Due to space limits, the CoDEXMedium dataset is shown in the Appx.

250 relations lead to triangles in KGs and intuitively imply diminished reasoning pathways in KGs
 251 which may have an effect on downstream model performance. Additionally, the distinct presence
 252 of composite relations in FB15k237 (one of the most frequently used datasets in NLP research)
 253 may lead to flaws in KG-based NLP model evaluation, unless performance on a variety of other
 254 datasets is also considered.

- 255 • Breit et al. (2020) hypothesize that the size of biomedical KGs tends to be large, which calls into
 256 double whether model results from smaller datasets are informative. We argue that beyond size,
 257 practitioners should consider the role KG properties and structural patterns during the design and
 258 testing of hypotheses and model development.
- 259 • We believe that analyzing the properties and structure of existing KGs can also benefit the future
 260 design of more robust KG datasets which incorporate diversity along different dimensions, such as
 261 the ones explored in this paper.

262 In conclusion, our study has implications for the broader KGs use in research: given the proliferation
 263 of models (KG link prediction, EA, LM-as-KG evaluation) across domains (natural sciences, medicine,
 264 ML and other disciplines), it is worth investigating whether (and how) structural patterns, as well as
 265 their inter-domain variability across KGs, may correlate or influence KG model performance. Given
 266 the scope and scale of such an investigation, we leave it for a follow up study and encourage others –
 267 within the ML, NLP and the ‘ML for sciences’ communities – to further explore this topic.

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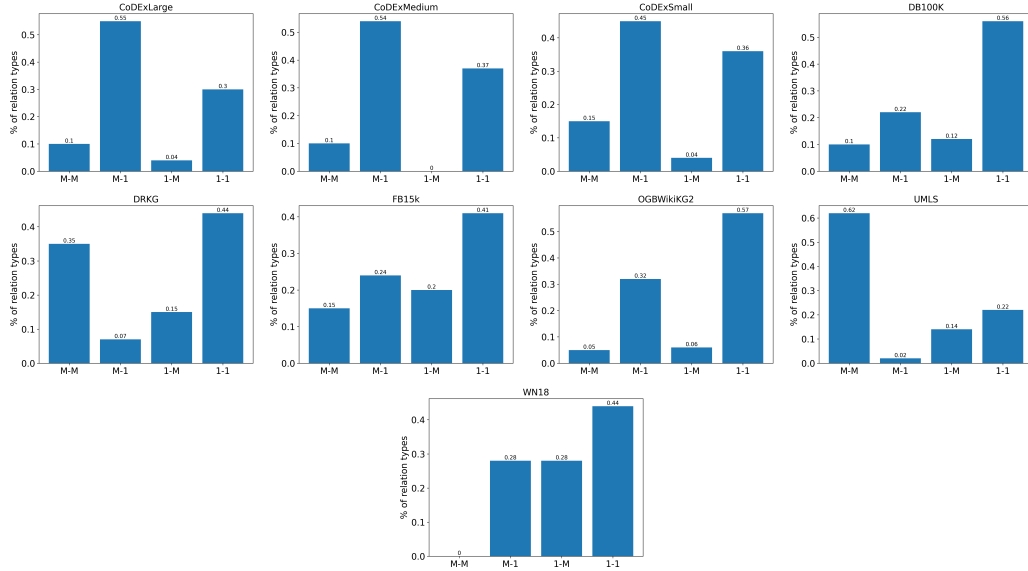


Figure 4: Supplemental panels for Fig. 2.

392 A Appendix

393 A.1 Datasets used

394 We used all the datasets in the PyKEEN library as described in the paper with the exception of several
 395 datasets (e.g., WK3115k, WK31120k, CN3l, and CKG) whose underlying files are no longer available
 396 for download on the URLs the library points to.

397 A.2 Degree plots

398 The Nations and Kinship datasets were not included in Fig. 1 due to the high number of high degree
 399 nodes in them which leads to plot scaling issues of the remaining 26 datasets. The Nation’s 14 entities
 400 have degrees in the range 146 – 514; the Kinship’s entities have degrees in the 192 – 206 range. For
 401 similar reasons we exclude the highest-degree entity (men) of the ConceptNet dataset in the plot in
 402 Fig. 1.

403 A.3 Relation types, cardinalities, and metapaths

404 Relationship type determination, i.e. whether a relation is (anti)-symmetric, inverse, composite, is
 405 based on association rule mining. The relation classifications are based on checking whether the
 406 corresponding rules hold with sufficient support and confidence – we calculated the support using a
 407 confidence of 95%. We used the reference implementation in available in PyKEEN Ali et al. (2021b).
 408 Note that a relation can be of several different types.

409 Relation cardinality is computed similarly to the relation type.

410 Metapath lengths are approximated by sampling (uniformly at random) an entity e from each KG and
 411 counting all the paths of length 2, 3 and 4 originating from e . Each KG was sampled 3 times, so the
 412 metapath numbers reported in Fig. 1 (right) are averaged over 3 independent entity samples, for each
 413 KG.

414 A.4 Additional plots for Fig. 2 and Fig. 3

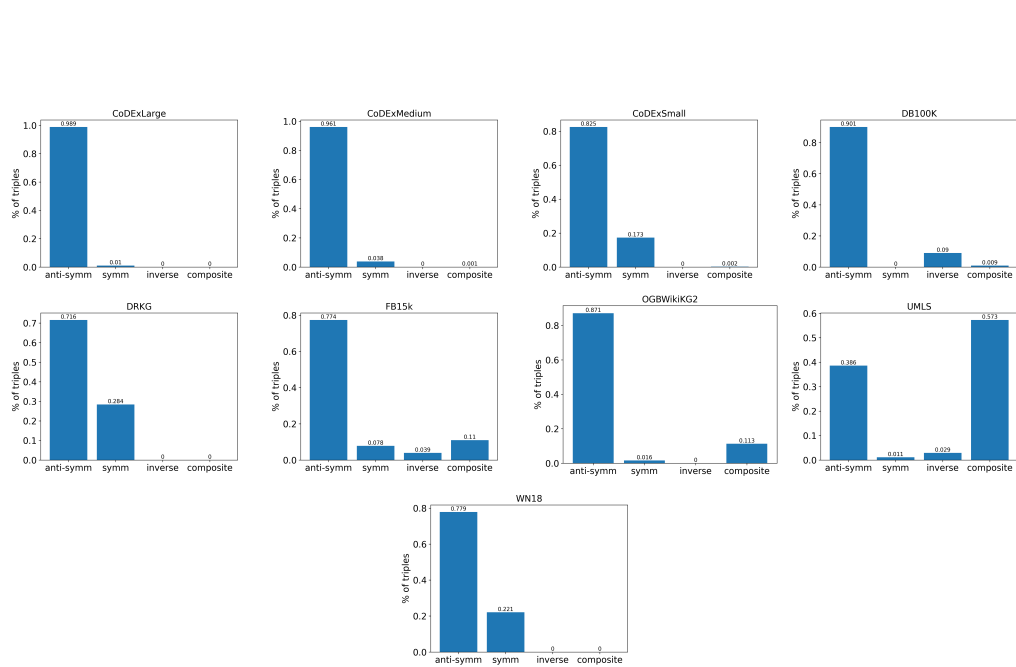


Figure 5: Supplemental panels for Fig. 3