ProteinKG65: A Knowledge Graph for Protein Science

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Abstract. Existing data-centric methods for protein science generally cannot sufficiently capture and leverage biology knowledge, which may be crucial for many protein tasks. To facilitate research in this field, we create ProteinKG65, a knowledge graph for protein science. Using gene ontology and Uniprot knowledge base as a basis, we transform and integrate various kinds of knowledge with aligned descriptions and protein sequences respectively to GO terms and protein entities. ProteinKG65 is mainly dedicated to providing a specialized protein knowledge graph, bringing the knowledge of Gene Ontology to protein function and structure prediction. The current version contains about 614,099 entities, 5,620,437 triples (including 5,510,437 protein-go triplets and 110,000 GO-GO triplets). We also illustrate the potential applications of ProteinKG65 with a prototype. We hope our released knowledge graph can help promote studies in AI for science.

Keywords: Knowledge Graph · Protein Science · Gene Ontology

1 Introduction

Recent decays have witnessed the success of protein science with neural networks \cite{1–3}, achieving remarkable performance in understanding the structure and functionality of the protein. However, existing approaches cannot sufficiently capture biological knowledge, which may be crucial for many protein tasks. Note that biologists have contributed lots of domain knowledge in knowledge bases like Gene Ontology\textsuperscript{4} (GO), which are summaries of expert experience. Thus, it is intuitive to leverage knowledge graphs (KGs) as vital support for protein understanding. For example, it is advantageous to identify protein’s functions with the knowledge of functionally similar proteins having similar shapes since protein’s shape determines its function \cite{4}. Yet one major stumbling block is the limitation of high-quality knowledge graphs that can cover the biology knowledge and protein sequences.

\textsuperscript{4} http://geneontology.org/
Research Challenge. Various biological knowledge bases and protein data are publicly available in different formats on the Web; however, it is a non-trivial task to integrate those heterogeneous sources of data. For example, Gene Ontology contains extensive biological functional knowledge but is not directly associated with protein sequences. Conversely, the UniProt Knowledge base (UniProtKB\textsuperscript{5}) consists of the functional information on proteins reviewed by experts without biological facts. Another major challenge is the extremely unbalanced distribution. Statistically, we observe that 97.9\% of relational triples evolve in relations of is_a, part_of and enables, which makes it challenging to leverage long-tailed semantic knowledge for protein understanding.

Contributed Resource. To address the challenges mentioned above and facilitate research in this area, we construct a knowledge graph, ProteinKG65, as shown in Fig. 1. We collect experimentally verified high-quality data from Gene

\textsuperscript{5} https://www.uniprot.org/
Table 1. According to the GO term classification in Gene Ontology (GO), there are three types of ontology: Cellular Component (CC), Biological Process (BP), and Molecular Function (MF).

| Aspects            | Description                                                                 |
|--------------------|-----------------------------------------------------------------------------|
| Molecular Function | Molecular-level activities performed by gene products.                      |
| Cellular Component | The locations relative to cellular structures in which a gene product performs a function. |
| Biological Process | The larger processes, or biological programs accomplished by multiple molecular activities. |

Ontology and UniProtKB as a basis and utilize gene ontology and protein alignment to construct the KG. We further propose relation refinement to address the unbalanced distribution issue. All relational triples in ProteinKG65 are identified by permanent dereferenceable URIs in w3id and are also available on Zenodo. We release the resources under CC BY-SA 4.0 and will continue to maintain the ProteinKG65. We also provide a prototype of the potential applications with ProteinKG65. The contributions of this study can be summarized as follows:

- We contribute a protein knowledge graph containing all the experimentally verified high-quality proteins with biological knowledge.
- We provide a prototype with an online demo to predict the secondary structure and function based on ProteinKG65. For details, please refer to the demo website: https://proteinkg.zjukg.cn.

2 Overview of ProteinKG65

This section describes the schema and data sources of ProteinKG65.

2.1 Schema

We build ProteinKG65 based on Gene Ontology [5] and UniprotKB [6]. Thus, there are two primary types of nodes in ProteinKG65, one is the Protein type, and the other is the GO type.

As shown in Fig. 1, there are two kinds of relational triples in ProteinKG65: GO-GO triplet (e.g., (GO:0007601, is_a, GO:0050953)) and Protein-GO triplet (e.g., (Q14028, involved_in, GO:0007601)).

For the GO nodes, they can be divided into three categories, namely MF (Molecular Function), CC (Cellular Component), and BP (Biological Process), as shown in Table 1. The specific relations between GO terms are listed in Table 2.

6 https://w3id.org/proteinkg65
Table 2. The main relations between GO terms.

| Abbreviation | Relation   | Symbol          | Example                                                                 |
|--------------|------------|-----------------|-------------------------------------------------------------------------|
| i            | is a       | $A - i \rightarrow B$ | maltose metabolic process is a disaccharide metabolic process          |
| P            | part of    | $A - P \rightarrow B$ | meiotic strand invasion part of meiotic cell cycle                      |
| R            | regulates  | $A - R \rightarrow B$ | regulation of arginine metabolic process regulates arginine metabolic process |
| hP           | has part   | $A - hP \rightarrow B$ | cytokinesis has part membrane fission                                  |
| R+           | positively regulates | $A - R^+ \rightarrow B$ | positive regulation of metabolic process positively regulates metabolic process |
| R-           | negatively regulates | $A - R^- \rightarrow B$ | photoinhibition negatively regulates photosynthetic electron transport chain |

2.2 Gene Ontology

Gene Ontology describes the knowledge of the biological domain concerning molecular function, cellular component, and biological process. Gene Ontology resources provide structured, computable knowledge about the function of genes and gene products in many different organisms, from humans to bacteria. The structure of Gene Ontology can be described in terms of a graph, where each GO term is a node, and the relations between the terms are edges between the nodes.

Gene Ontology has been expanding since its establishment in 1998, and the IDs of some previous GO terms are no longer applicable. We filter those invalid Go term nodes to construct ProteinKG65.

2.3 UniprotKB

The UniProtKB\(^7\) is the central hub for the collection of functional information on proteins with accurate, consistent and rich annotation. The UniProtKB consists of two sections: UniProtKB/TrEMBL and UniProtKB/Swiss-Prot. UniProtKB/TrEMBL (unreviewed) consists of protein sequences associated with computationally generated annotation and large-scale functional characterization.

\(^7\) [https://www.uniprot.org/](https://www.uniprot.org/)
Fig. 2. Construct of ProteinKG65: Step 1 and Step 2: Extract gene annotations and gene ontology information from the gene ontology knowledge base. Step 3: Obtain all the proteins involved in the annotation and retrieve the corresponding protein sequence from the Swiss-Prot database. Step 4: Align and merge three data sources according to ID. Step 5: Refine the relations in ProteinKG25 and obtain fine-grained knowledge.

UniProtKB/Swiss-Prot (reviewed) is a non-redundant and high-quality manually annotated protein sequence database.

UniProtKB data is primarily derived from the translation of protein sequences from coding sequences (CDS), and all of these sequences, along with associated other data, are integrated into UniProtKB/TrEMBL. To reduce redundancy between two databases, once a protein in UniProtKB/TrEMBL was manually annotated, the protein was added to UniProtKB/Swiss-Prot and deleted from UniProtKB/TrEMBL.

3 Construction of ProteinKG65

In this section, we mainly discuss the construction process of ProteinKG65 and how to mitigate the unbalanced distribution. The specific process of the construction is shown in Fig. 2. It should be noted that the total number of relations is 25 after knowledge integration, and after relation refinement, the number of relations is 65.

3.1 Data Acquisition and Integration

We obtain data from the files below and utilize the off-the-shelf toolkit to construct ProteinKG65:

- go.obo: the structure data from Gene Ontology\(^8\). This file contains all GO terms information up to July 2021, including the accession, definition, ontology type, and relationship with other GO terms. Depending on the relations between the terms, we generate GO-GO relational triples.

\(^8\) [http://geneontology.org/docs/download-ontology/](http://geneontology.org/docs/download-ontology/)
uniprot_sprot.dat: UniProtKB/Swiss-Prot protein sequence database\textsuperscript{9}. This file includes the protein set used in ProteinKG65 and the corresponding protein sequences. Since Swiss-Prot is manually reviewed and non-redundant, all proteins in this database are of high quality.

goa_uniprot_all.gpa: GO Annotation data\textsuperscript{10}. A GO annotation in this file represents a single association between a gene product (maybe a protein or RNA, etc.) and a GO term. Each annotation is attached to the GO Evidence Code, which reflects whether the annotation is reviewed by an expert biocurator. In this work, we mainly use the GO annotations for proteins as the relational facts in the ProteinKG65.

GOATOOLS: a Python-based library\textsuperscript{11}, which can process the obo-formatted file from the Gene Ontology. With this toolkit, researchers can conveniently conduct functional analysis, e.g., reporting the level and depth of GO terms or determining the semantic similarities between GO terms.

In terms of the existing abundant functional knowledge of proteins in the Gene Ontology knowledge base, we extract the relational facts between proteins and GO terms (named Protein-GO triplet) from goa_uniprot_all.gpa, and loosely hierarchical relationship between GO terms (named GO-GO triplet) from go.obo. Especially to avoid information redundancy and to ensure the reliability of annotations in the ProteinKG65, we only consider proteins from the Swiss-Prot database so that we can obtain high-quality protein knowledge.

For each protein in ProteinKG65, we retrieve the corresponding sequence in uniprot_sprot.dat from UniProtKB/Swiss-Prot. All data is merged and aligned according to the unique ID. So far, we could obtain the raw protein knowledge graph, and we will introduce the relation refinement procedure in the following section.

3.2 Relation Refinement

We empirically observe that there exists a severe unbalanced distribution problem in the raw protein knowledge graph as shown in Fig 3. Specifically, 97.9% of protein-GO triples data are all gathered in relations of involved_in, located_in and enables, which may cause poor performance for representation learning. Thus, we propose relation refinement to generate fine-grained relational triples, which can better represent the relational knowledge between proteins and GO terms. We take the following steps for relation refinement:

\textit{Step 1: Top-k GO term sampling.} We select the top-k GO terms with the highest occurrences in the Gene Ontology annotations. Specifically, we sample top-10 GO terms from Molecular Function ontology and Cellular Component Ontology and top-20 GO terms from Biological Process Ontology. Due to the higher number of GO terms in the BPO, we sample more GO terms from BPO than the other two ontologies.

\textsuperscript{9} https://www.uniprot.org/downloads
\textsuperscript{10} https://ftp.ebi.ac.uk/pub/databases/GO/goa/old/UNIPROT/
\textsuperscript{11} https://github.com/tanghaibao/goatools
Step 2: Subtree extraction. We use the goatools toolkit to extract corresponding descendant GO term sets (i.e., subtrees) of the previously selected top-k GO terms. There may be overlap between the descendant sets of different top-k GO terms, i.e., one top-k GO term is an ancestor of the other. In this case, we follow the “descendant-prior” principle to remove the overlapped GO terms from the subtree of ancestor top-k GO term.

Step 3: Fine-grained relation extension. We then update the original ProteinGO triplets. For each triple, if GO term or its ancestor is a top-k GO term, we concatenate the top-k GO term name with the current relation using the template [relation name]_[GO term name]. For example, given a triple (A0A023-GS28, enables, oxidoreductase activity (GO:0016491)), in which the ancestor of GO term is catalytic activity (GO:0003824), it will become (A0-
Table 3. Comparison of ProteinKG65 with previous biological knowledge graphs.

| Dataset          | #Type | Protein | GO  | Protein-GO | GO-GO | Protein-Protein | #Triplet |
|------------------|-------|---------|-----|------------|-------|----------------|----------|
| ProteinKG65      | 2(2)  | 566,996 | 47,103 | 5,510,437 | 110,000 | 0              | 5,620,437 |
| HetioNet         | 17(19)| 19.116  | 1,454 | 133,613    | 0      | 97,938         | 1,608,168 |
| InteractomeNet   | 4(6)  | 17,660  | 9,798 | 34,777     | 22,545 | 387,626        | 478,728  |

Fig. 4. (a) GO terms distribution in the three sub-ontologies of Gene Ontology. GO terms belonging to Biological Process Ontology occupy most of the whole GO term set of Gene Ontology. (b) Sequence length distribution of proteins in ProteinKG65. Sequence lengths less than 1024 account for the vast majority.

A023GS28, enables_catalytic_activity(GO:0016491)). After relation refinement, the relational fact can better reflect the function of the protein. Due to the transitivity in the Gene Ontology annotation principles, which annotation to a GO term implies annotation to all its parents, we could extend the number of relations to 65 through the above procedures, and parts of the triples contain informative fine-grained relations.

3.3 Statistics About ProteinKG65

In this section, we compare ProteinKG65 with previous biological knowledge graphs, such as HetioNet [7] and InteractomeNet [8], from two aspects of the number of entity and relation types, and the scale of proteins, GO terms and relational facts. From Table 3, we notice that ProteinKG65 has fewer types of nodes than HetioNet and InteractomeNet, but contains much more proteins that are advantageous for real-world applications. Besides, we analyze the relation distribution before and after relation refinement. From Fig. 3, we notice that after adding more fine-grained relations, the overall relation distribution is relatively flat. Moreover, those fine-grained relations contain more semantic knowledge.

Protein in ProteinKG65 We further analyze some essential characteristics of proteins in ProteinKG65, such as the distribution of protein sequence length.
Table 4. The statistic of Protein-GO triplets in ProteinKG65. We remove all the proteins that appeared in the train dataset, and the remaining data was used as the inductive dataset.

| Setting | Protein Entity | GO Entity | Relation | Triplet |
|---------|----------------|-----------|----------|---------|
| train   | 543,110        | 28,524    | 57       | 4,884,034 |
| Transductive valid | 25,241 | 5,009 | 44 | 51,243 |
| test    | 217,463        | 17,908    | 57       | 575,160  |
| train   | 543,110        | 28,524    | 57       | 4,884,034 |
| Inductive valid | 855   | 270      | 31       | 2,216   |
| test    | 3,085          | 1,062     | 50       | 11,127   |

We count the length of protein sequences ranging from (0, 256] to the interval over 2048.

From Fig. 4, we observe that there exist significant differences in the length distribution for proteins. Some proteins can be as long as 35214, and some are extremely short, which brings out challenges for protein representation learning. We leave this for future work.

3.4 Transductive & Inductive

To make the ProteinKG65 consistent with the real-world application setting, we take two different settings for the Protein-GO triplets dataset: the transductive and the inductive settings. The inductive setting (protein sequence in the test set does not exist in the training set) is more suitable for predicting new proteins without GO annotations when the GO term is relatively fixed. Generally, the inductive setting is more challenging than the transductive setting. We detail the statistics of different settings in Table 4.

3.5 Data Splitting

In the application scenario, the new protein sequences will usually be added to the UniprotKB. To facilitate the usage of ProteinKG65, we divide the dataset following the timeline released by the goa_uniprot_all.gpa. All the protein data released before April 2020 is regarded as the training set, the data from April to August 2020 is used for the validation dataset, and the data from August 2020 to November 2021 is used for the test dataset. Thus, we can guarantee that the test Protein-GO triples are not seen in the train set, which conforms to the real-world prediction of new proteins. We will maintain the ProteinKG65 to add new proteins in the future.
3.6 Quality of ProteinKG65

Since it is non-trivial to thoroughly evaluate the quality of a large-scale KG, thus, we evaluate the quality of the dataset from the data source and construction process. Specifically, we filter and clean the KG twice during the construction procedure. For the first time, only the protein data reviewed by experts are retained, which ensures that the proteins are all artificially verified data and are highly credible. For the second time, after initially generating the ProteinKG65 dataset, we clean all the duplicate data (duplicate protein sequences) evolving in the training, valid and test set.

4 Applications of ProteinKG65

To illustrate the potential applications of ProteinKG65, we develop a prototype protein understanding system with ProteinKG65.

4.1 Prototype: A Protein Understanding System

Recent years have witnessed breakthroughs in predicting protein structure and function using artificial intelligence technologies such as AlphaFold [3], ProteinBERT [9]. With the proposed ProteinKG65, we have implemented a prototype protein understanding system\(^\text{12}\) based on a knowledge-enhanced pre-trained protein language model OntoProtein\(^\text{13}\) [10]. Biologists, computer scientists, and other users can utilize the prototype to analyze proteins for structure and function prediction. We will introduce the potential applications as follows:

\(^\text{12}\) http://proteinkg.zjukg.cn

\(^\text{13}\) https://github.com/zjunlp/OntoProtein
Secondary Structure Prediction Analysis of protein structure can help understand the role of protein, how the protein performs its biological function, and the interaction between protein and protein (or other molecular drugs), which is essential for biology, medicine and pharmacy. The secondary structure of a protein refers to the structure of each amino acid corresponding to the amino acid chain, which is mainly divided into eight categories: H (alpha helix), B (residue in isolated beta-bridge), E (extended strand, participates in beta ladder), G (3-helix), I (pi helix), T (hydrogen-bonded turn), S (bend), Blank (loop or irregular).

We utilize a slightly rough classification setting for structure prediction following [9], and consider three classes: H, E, and C, representing helix, sheet, and coil, respectively. Users can enter their own protein sequences or choose running examples to obtain the corresponding secondary structure sequence. From Fig. 5, we illustrate the results predicted by the model below and use different colors to distinguish different secondary structures.

Protein Function Prediction Protein function prediction is a critical task in biological research. With the development of post-genome, many protein sequences with unknown structures and functions appear in protein databases. The function prediction of protein can understand the specific properties of the protein, including the biological process that the protein can participate in, the location of the protein, and whether it has specific catalytic or other functions.

As shown in Fig. 6, user can enter the sequence or PDB ID [11] (the id of the protein database) to obtain their functions. Specifically, the system will first check the Neo4J graph database to determine whether the protein is already in the database. The system will directly return all GO nodes (functions).
4.2 Other Applications

In addition to predicting protein structure and function, as shown in Fig. 7 there are many other potential applications for ProteinKG65, such as protein-drug molecule binding prediction and biological QA systems. The research on the binding of proteins and drug molecules is mainly in pharmacy, and the study of the interaction between drug molecules and proteins is of great significance for elucidating the transport of drugs in the body and targeted therapy. The proposed ProteinKG65 contains rich sequence–structure–function relationships with biological expert experience. Intuitively, those prior knowledge of the biological process and cellular components of proteins is beneficial for recognizing its interaction with drugs or proteins.

Concretely, data-centric methods for protein representation learning pose challenges for dynamically updating learned knowledge (e.g., correcting biases or enriching knowledge sources), which may not satisfy users’ needs in real-world applications. In other words, one main drawback of existing models is the lack of ability to leverage explicit knowledge, and our proposed ProteinKG65 provides such a scaffold for knowledge-enhanced protein representation learning.

5 Related Work

KG is a structured semantic knowledge base for describing concepts and their interrelationships in the physical world in symbolic form, which can provide back-
end support for a variety of tasks such as recommender systems [12]. In the biological domain, KG has been investigated for a long time [13–15]. CKG [16] collects annotations from 26 biomedical databases using ten ontologies. BioKG [17] proposes a new biological knowledge graph that compiles curated relational data from open biological databases in a unified format with standard, interlinked identifiers.

For protein science, biologists have contributed lots of domain knowledge bases. Hetionet [7] is an integrative network encoding knowledge from millions of biomedical studies. InteractomeNet [8] integrates disease-perturbed proteins, drug targets, and biological functions into a multiscale interactome network. Gene Ontology (GO) [5] is a widely used biomedical ontology that describes protein function. Some researchers have noticed the use of GO for protein prediction tasks, such as GO2Vec [18]. evoKGsim [19] uses a knowledge graph that integrates Gene Ontology and proteins for protein-protein interaction prediction. However, those proteins are tiny, only some human proteins and yeast proteins are used, and relevant annotation text information is not considered.

Inspired by these works, we create ProteinKG65, which integrates protein sequences into the Gene Ontology and provides rich semantic knowledge of proteins from domain experts, benefiting widespread tasks.

6 Conclusion and Future Work

We construct and release a knowledge graph for protein science. We also provide the potential application of ProteinKG65 with a prototype. We hope our released knowledge graph can help to promote studies in AI for science. However, our work still has some limitations, as follows.

**KG Refinement.** Currently, we leverage a relatively crude method to collect proteins (directly putting all the protein sequences into the graph). We believe that detailed discrimination of protein species is helpful. For example, we will try to classify proteins by homology, or classify proteins from the perspective of different species, and distinguish the proteins of humans, mice, bacteria and other species, which can make the KG more informative and be able to make contributions to specific fields of species.

**KG Enhancement.** Since previous studies have shown that protein functions are inseparably related to its structure, we will consider incorporating more helpful knowledge into protein graphs, such as introducing three-dimensional protein structure information into knowledge graphs. In other words, this will also convert the ProteinKG65 to a multimodal KG. Besides, our ProteinKG65 still misses some vital knowledge. For example, we do not consider the relations between protein pairs, which is very helpful for understanding protein-protein interactions. We also leave this for future work.

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