CS520

Knowledge Graphs

What should AI Know ?

What is a Knowledge Graph?

1. Introduction

Knowledge graphs have emerged as a compelling abstraction for organizing world's structured knowledge over the internet, and a way to integrate information extracted from multiple data sources. Knowledge graphs have also started to play a central role in machine learning as a method to incorporate world knowledge, as a target knowledge representation for extracted knowledge, and for explaining what is learned.

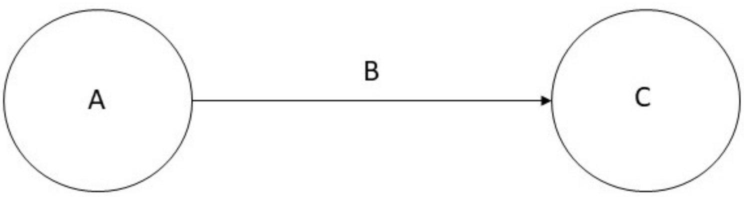
Our goal here is to explain the basic terminology, concepts and usage of knowledge graphs in a simple to understand manner. We do not intend to give here an exhaustive survey of the past and current work on the topic of knowledge graphs.

We will begin by defining knowledge graphs, some applications that have contributed to the recent surge in the popularity of knowledge graphs, and then use of knowledge graphs in machine learning. We will conclude this chapter by summarizing what is new and different about the recent use of knowledge graphs.

2. Knowledge Graph Definition

A knowledge graph is a directed labeled graph in which the labels have well-defined meanings. A directed labeled graph consists of nodes, edges, and labels. Anything can act as a node, for example, people, company, computer, etc. An edge connects a pair of nodes and captures the relationship of interest between them, for example, friendship relationship between two people, customer relationship between a company and person, or a network connection between two computers. The labels capture the meaning of the relationship, for example, the friendship relationship between two people.

More formally, given a set of nodes N, and a set of labels L, a knowledge graph is a subset of the cross product $N \times L \times N$. Each member of this set is referred to as a triple, and can be visualized as shown below.



The directed graph representation is used in a variety of ways depending on the needs of an application. A directed graphs such as the one in which the nodes are people, and the edges capture friendship relationship is also known as a data graph. A directed graph in which the nodes are classes of objects (e.g., Book, Textbook, etc.), and the edges capture the *subclass* relationship, is also known as a taxonomy. In some data models, *A* is referred to as *subject*, *B* is referred to as *predicate*, and *C* is referred to as object.

Many interesting computations over graphs can be reduced to navigation. For example, in a friendship knowledge graph, to calculate the friends of a friends of a person *A*, we can navigate the knowledge graph from *A* to all nodes *B* connected to it by a relation labeled as friend, and then recursively to all nodes *C* connected by the friend relation to each *B*.

A ***path*** in a graph *G* is a series of nodes (v_1, v_2,..., v_n) where for any $i \in N$ with $1 \leq i < n$, there is an edge from v_i to v_{i+1}. A ***simple path*** is a path with no repeated nodes. A ***cycle*** is a path in which the first and the last nodes are the same. Usually, we are interested in only those paths in which the edge label is the same for every pair of nodes. It is possible to define numerous additional properties over the graphs (e.g., connected components, strongly connected components), and provide different ways to traverse the graphs (e.g., shortest path, Hamiltonian path, etc.).

3. Recent Applications of Knowledge Graphs

There are numerous applications of knowledge graphs both in research and industry. Within computer science, there are many uses of a directed graph representation, for example, data flow graphs, binary decision diagrams, state charts, etc. For our discussion here, we have chosen to focus on two concrete applications that have led to recent surge in popularity of knowledge graphs: organizing information over internet and data integration.

3.1 Knowledge Graphs for organizing Knowledge over the Internet

We will explain the use of a knowledge graph over the web by taking the concrete example of Wikidata. Wikidata acts as the central storage for the structured data for Wikipedia. To show the interplay between the two, and to motivate the use of Wikidata knowledge graph, consider the city of Winterthur in Switzerland which has a page in Wikipedia. The Wikipedia page for Winterthur lists its twin towns: two are in Switerzland, one in Czech Republic, and one in Austria. The city of Ontario in California that has a Wikipedia page titled *Ontario, California*, lists Winterthur as its sister city. The sister city and twin city relationships are identical as well as reciprocal. Thus, if a city A is a sister city of another city B, then B must be a sister city of A. This inference should be automatic, but because this information is stated in English in Wikipedia, it is not easy to detect this discrepancy. In contrast, in the Wikidata representation of Winterthur, there is a relationship called *twinned administrative body* that lists the city of Ontario. As this relationship is symmetric, the Wikidata page for the city of Ontario automatically includes Winterthur. Thus, when Wikidata knowledge graph will be fully integrated into Wikipedia, such discrepancies will naturally disappear.

Wikidata includes data from several independent providers, for example, the Library of Congress that publishes data containing information about Winterthur. By using the Wikidata identifier for Winterthur, the information released by Library of Congress can be easily linked with information available from other sources. Wikidata makes it easy to establish such links by publishing the definitions of relationships used in it in *Schema.Org*.

The vocabulary of relations in *Schema.Org* gives us, at least, three advantages. First, it is possible to write queries that span across multiple datasets that would not have been possible otherwise. One example of such a query is: Display on a map the birth cities of people who died in Winterthour? Second, with such a query capability, it is possible to easily generate structured information boxes within Wikipedia. Third, structured information returned by queries also can appear in the search results which is now a standard feature for the leading search engines.

A recent version of Wikidata had over 80 million objects, with over one billion relationships among those objects. Wikidata makes connections across over 4872 different catalogs in 414 different languages published by independent data providers. As per the recent estimate, 31% of the websites, and over 12 million data providers publish Schema.Org annotations are currently using the vocabulary of *Schema.Org*.

Let us observe several key features of the Wikidata knowledge graph. First, it is a graph of unprecedented scale, and is the largest knowledge graph available today. Second, it is being jointly created by a community of contributors. Third, some of the data in Wikidata may come from automatically extracted information, but it must be easily understood and verified as per the Wikidata editorial policies. Fourth, there is an explicit effort to provide semantic definitions of different relation names through the vocabulary in *Schema.Org*. Finally, the primary driving use case for Wikidata is to improve the web search. Even though Wikidata has several applications using it for analytical and visualization tasks, but its use over the web continues to be the most compelling and easily understood application.

3.2 Knowledge Graphs for Data Integration in Enterprises

Data integration is the process of combining data from different sources, and providing the user with a unified view of data. A large fraction of data in the enterprises resides in the relational databases. One approach to data integration relies on a global schema that captures the interrelationships between the data items represented across these databases. Creating a global schema is an extremely difficult process because there are many tables and attributes; the experts who created these databases are usually not available; and because of lack of documentation, it is difficult to understand the meaning of the data. Because of the challenges in creating a global schema, it is convenient to sidestep this issue, and convert the relational data into a database with the generic schema of triples, ie, a knowledge graph. The mappings between the attributes are created on as needed basis, for example, in response to addressing specific business questions, and can themselves be represented within a knowledge graph. We illustrate this process using a concrete example.

Many financial institutions are interested in creating a company knowledge graph that combines the internal customer data with the data licensed from third parties. Some examples of such third party datasets include Dunn & Bradstreet, S&P 500, etc. An example usage of a company knowledge graph is to assess the risk while making loan decisions. The external data contain information such as the suppliers of a company. If a company is going through financial difficulty, it increases the risk of awarding loan to the suppliers of that company. To combine this external data with the internal data, one has to relate the external schemas with the internal company schema. Furthermore, the company names used in the external sources have to be related to the corresponding customer identifiers used by the financial institutions. While using a knowledge graph approach to data integration, determining such relationships can be delayed until they are actually required.

4. Knowledge Graphs in Artificial Intelligence

Knowledge graphs, known as semantic networks, have been used as a representation for Artificial Intelligence since the early days of the field. Over the years, semantic networks were evolved into different representations such as conceptual graphs, description logics, and rule languages. To capture uncertain knowledge, probabilistic graphical models were invented.

A widely known application of the representation languages that originated from semantic networks is in capturing ontologies. An ontology is formal specification of the conceptualization of a domain. An ontology plays important role in information exchange and in capturing the background knowledge of a domain that could be used for reasoning and answering questions.

World Wide Web Consortium (W3C) standardized a family of knowledge representation languages that are now widely used for capturing knowledge on the internet. We will consider one such language known as the Resource Description Frame (RDF) in the next chapter. This family of languages also includes the Web Ontology Language (OWL), and the Semantic Web Rule

Language (SWRL).

Orthogonal to the representation of knowledge, a central challenge in AI is knowledge acquisition bottleneck, ie, how to capture knowledge into the chosen representation in an economically scalable manner. Early approaches relied on knowledge engineering. Efforts to automate portions of knowledge engineering led to techniques such as inductive learning, and the current generation of machine learning.

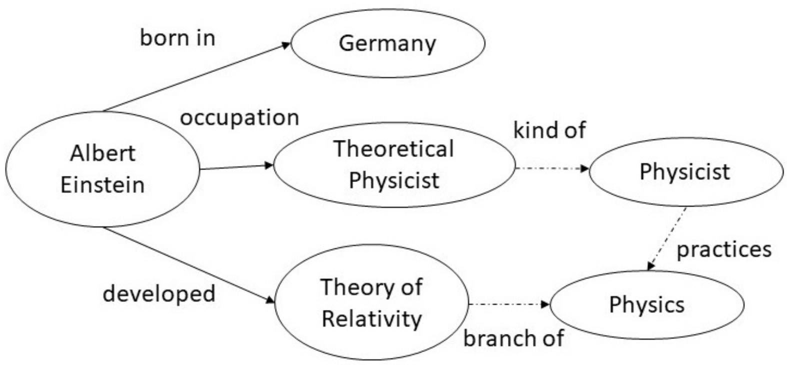
Therefore, it is natural that the knowledge graphs are being used as a representation of choice for storing the knowledge automatically learned. There is also an increasing interest to leverage domain knowledge that is expressed in knowledge graphs to improve machine learning.

4.1 Knowledge Graphs as the output of Machine Learning

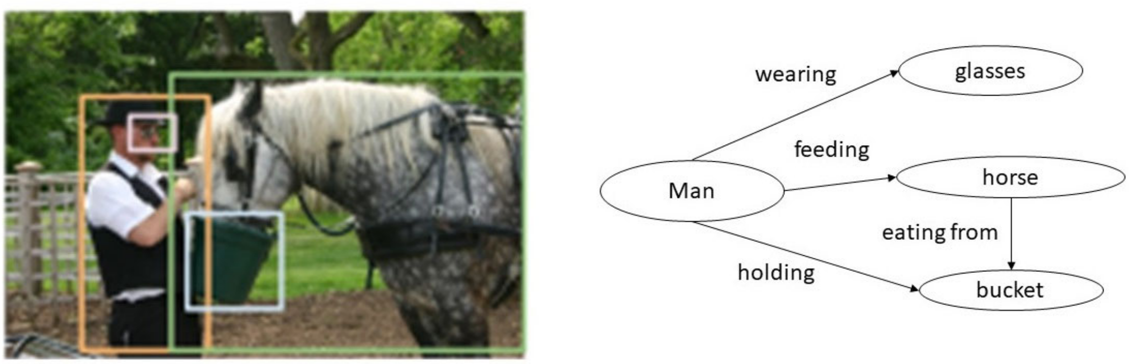
We will consider how graphs are being used as a target output representation for natural language processing and computer vision algorithms.

Entity extraction and relation extraction from text are two fundamental tasks in natural language processing. The extracted information from multiple portions of the text needs be correlated, and knowledge graphs provide a natural medium to accomplish such a goal. For example, from the sentence shown on the left, we can extract the entities *Albert Einstein*, *Germany*, *Theoretical Physicist*, and *Theory of Relativity*; and the relations *born in*, *occupation* and *developed*. Once this snippet of the knowledge graph is incorporated into a larger knowledge graph, we get additional links (shown by dotted edges) such as a Theoretical Physicist is a *kind of* Physicist who *practices* Physics, and that Theory of Relativity is a *branch of* Physics.

Albert Einstein was a **German-born theoretical physicist** who developed the **theory of relativity**.



A holy grail of computer vision is the complete understanding of an image, that is, creating a model that can name and detect objects, describe their attributes, and recognize their relationships. Understanding scenes would enable important applications such as image search, question answering, and robotic interactions. Much progress has been made in recent years towards this goal, including image classification and object detection.



For example, from the image shown above, an image understanding system should produce a knowledge graph shown to the right. The nodes in the knowledge graph are the outputs of an object detector. Current research in computer vision focuses on developing techniques that can correctly infer the relationships between the objects, such as, man *holding* a bucket, and horse *feeding* from the bucket, etc. The knowledge graph shown to the right is an example of a knowledge graph.

4.2 Knowledge Graphs as input to Machine Learning

Popular deep machine learning models rely on a numerical input which requires that any symbolic or discrete structures should first be converted into a numerical representation. *Embeddings* that transform a symbolic input into a vector of numbers have emerged as a representation of choice for input to machine learning models. We will explain this concept and its relationship to knowledge graphs by taking the example of *word embeddings* and *graph embeddings*.

Word embeddings were developed for calculating similarity between words. To understand the word embeddings, we consider the following set of sentences.

I like knowledge graphs.
I like databases.
I enjoy running.

In the above set of sentences, we will count how often a word appears next to another word, and record the counts in a matrix shown below. For example, the word *I* appears next to the word *like* twice, and next to word *enjoy* once, and therefore, its counts for these two words are 2 and 1 respectively, and 0 for every other word. We can calculate the counts for other words in a similar manner to fill out the table.

counts	I	like	enjoy	knowledge	graphs	databases	running	.
I	0	2	1	0	0	0	0	0
like	2	0	0	1	0	1	0	0
enjoy	1	0	0	0	0	0	1	0
knowledge	0	1	0	0	1	0	0	0
graphs	0	0	0	1	0	0	0	1
databases	0	1	0	0	0	0	0	1
running	0	0	1	0	0	0	0	1
.	0	0	0	0	1	1	1	0

Above table constitutes a matrix which is often referred to as *word cooccurrence* counts. We say that the meaning of each word is captured by the vector in the row corresponding to that word. To calculate similarity between words, we can simply calculate the similarity between the vectors corresponding to them. In practice, we are interested in text that may contain millions of words, and a more compact representation is desired. As the above matrix is sparse, we can use techniques from Linear Algebra (e.g., singular value decomposition) to reduce its dimensions. The resulting vector corresponding to a word is known as *word embedding*. Typical word embeddings in use today rely on vectors of length 200. There are numerous variations and extensions of the basic idea presented here. Techniques exist for automatically learning word embeddings for any given text.

Use of word embeddings has been found to improve the performance of many natural language processing tasks including entity extraction, relation extraction, parsing, passage retrieval, etc. One of the most common applications of word embeddings is in auto completion of search queries. Word embeddings give us a straightforward way to predict the words that are likely to follow the partial query that a user has already typed.

As a text is a sequence of words, and word embeddings calculate co-occurrences of words in it, we can view the text as a knowledge graph in which every word is a node, and there is a directed edge between each word and another word that immediately follows it. Graph embeddings generalize this notion for general network structure. The goal and approach, however, remains the same: represent each node in a knowledge graph by a vector, so that the similarity between the nodes can be calculated as a difference between their corresponding vectors. The vectors for each node are also referred to as graph embeddings.

To calculate knowledge graph embeddings, we define a method for encoding each node in the graph into a vector, a function to calculate similarity between the nodes, and then optimize the encoding function. Encoding of a node into a vector is also known as a *node embedding*. One possible encoding function is to use *random walks* of the knowledge graph (typically 32 to 64 such random walks) and calculate co-occurrence counts of nodes on the knowledge graph yielding a matrix similar to co-occurrence counts of words in text. There are numerous variations of this basic method to calculate knowledge graph embeddings. Just like we have encoded a node into a vector, we can also encode the whole graph into a vector which is known as graph embedding. There are many approaches to calcuate graph embeddings, but perhaps, the simplest approach is to add the vectors for each of nodes in the graph and obtain a vector representing the whole graph.

We have chosen to explain graph embeddings by first explaining word embeddings because as it is easy to understand them, and their use is common place. Graph embeddings are a generalization of the word embeddings. They are a way to input domain knowledge expressed in a knowledge graph into a machine learning algorithm. Graph embeddings do not induce a knowledge representation, but are a way to turn symbolic representation into a numeric representation for consumption by a machine learning algorithm.

Once we have calculated knowledge graph embeddings, they can be used for a variety of applications. One obvious use for the knowledge graph embeddings calculated from a friendship graph is to recommend new friends. A more advanced task involves link prediction (ie, the likelihood of a link between two nodes). Link prediction in a company graph could be used to identify potential new customers.

5. Summary

Graphs are a fundamental construct in discrete mathematics, and have applications in all areas of computer science. Most notable uses of graphs in knowledge representation and databases have taken the form of data graphs, taxonomies and ontologies. Traditionally, such applications have been driven by a top down design. As a knowledge graph is a directed labeled graphs, we are able to leverage theory, algorithms and implementations from more general graph-based systems in computer science.

Recent surge in the use of knowledge graphs is driven because of the confluence of three different advances: data linking and sharing over the web graph computations over data, and progress in in NLP and vision to extract relations from texts and images. A common thread across all three of these advances is scale. The knowledge graphs that are available today are of unprecedented scale. We have already noted that a recent version of Wikidata had over 80 million objects, and over 1 Billion relationships. Several industry knowledge graphs are even bigger, for example, a recent version of the Google knowledge graph had over 570 million entities, and over 18 Billion relationships. This large scale of knowledge graphs makes the efficiency and scalability of the graph algorithms paramount.

For organizing information on the web, and in many data integration applications, it is extremely difficult to come up with a top down design of a schema. The machine learning applications are driven by the availability of the data, and what can be usefully inferred from it. Bottom up uses of knowledge graphs do not diminish the value of a top down design of the schema or an ontology.

Indeed, the Wikidata project leverages ontologies for ensuring data quality, and most enterprise data integration projects advocate defining the schema on as needed basis. Machine learning applications also benefit significantly with the use of rich ontology for making inferences from the information that is learned even though a global ontology or a schema is not required at the outset.

Word-embeddings and graph-embeddings both leverage a graph structure in the input data, but they are necessarily more general than *knowledge graphs* in that there is no implicit or explicit need for a schema or an ontology. For example, graph embeddings can be used over the network defined by exchange of messages between nodes on the internet, and then used in machine learning algorithms to predict rogue nodes. In contrast, for the Wikidata knowledge graph, knowledge graphs in the enterprises, and in the output representation of machine learning algorithms, a schema or ontology can play a central role.

We conclude by observing that the recent surge in interest in knowledge graphs is primarily driven by the bottom up requirements of several compelling business applications. Knowledge graphs in these applications can certainly benefit from the classical work on the top down representation design techniques, and in fact, we envision that eventually the two will converge.

Exercises

Exercise 1.1. Identify which of the following satisfies the definition of a knowledge graph introduced in this chapter.

(*a*) A *data graph* defined among data items representing real-world entities.
(*b*) A *schema graph* defined among classes in a schema.
(*c*) A *process graph* representing the steps of a process, their order, and branching conditions.
(*d*) A *parse tree* is an ordered, rooted tree that represents the syntactic structure of a string according to some context-free grammar.
(*e*) An *entity relationship diagram* shows the relationships of entity sets stored in a database.

Exercise 1.2. Which of the following counts as a well-defined meaning of the labels in a knowledge graph?

(*a*) Names of the labels in a human understandable language.
(*b*) Everything in (a) plus a documentation string that explains the label in sufficient detail.
(*c*) Embeddings calculated for the relation names over a large corpus of text.
(*d*) Everything in (a) plus a specification in a formal language.
(*e*) Everything in (b) plus a specification in a formal language.

Exercise 1.3. Identify which of the following statements about knowledge graphs are true.

(*a*) Knowledge graphs are the only way to achieve data integration in enterprises.
(*b*) Edges in a knowledge graph are like the links between web documents except that the edges have semantically defined labels.
(*c*) A knowledge graph is the best representation for recording the output of NLP and vision algorithms.
(*d*) Semantic networks were the earliest knowledge graphs in AI.
(*e*) Understanding is to brain as a knowledge graph is to AI.

Exercise 1.4. Identify if the following statements are true or true or false.

(*a*) If word embeddings of two words show high similarity, they are likely to be synonyms.
(*b*) A word embedding calculation views the text as a knowledge graph.
(*c*) A sentence is to a word embedding as a path is to a graph embedding.
(*d*) Edge detection is to computer vision as relation extraction is to NLP.

(*e*) Calculating similarity using word embeddings is always better than using hand curated sources.

Exercise 1.5. What is not new about the knowledge graphs in their recent usage?

(*a*) Directed labeled graph representation

(*b*) The large sizes of the knowledge graphs

(*c*) Creating a knowledge graph using automated methods

(*d*) Publicly available curated graph data sets

(*e*) Ability to make high value predictions using graph data