Limits and Potential Solutions to Represent and Analyze Multidimensional and Heterogeneous Situations

Yolène Berrou, Maxime Guery, Eddie Soulier

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Yolène Berrou*
Informatic and digital society laboratory (LIST3N), team Tech-CICO, University of Technology of Troyes
Computer Science and Artificial Intelligence Laboratory (CSAI), ENGIE Lab CRIGEN
France
yolene.berrou@utt.fr

Maxime Guery*
Data Nostra, R&D lab
Université de Reims Champagne Ardenne (URCA), CReSTIC EA 3804, Equipe MODECO
France
mguery@datanostra.ai

Eddie Soulier
Informatic and digital society laboratory (LIST3N), team Tech-CICO, University of Technology of Troyes
France
eddie.soulier@utt.fr

ABSTRACT
The universe is made of multidimensional and heterogenous interactions which can be represented by a graph. These interactions and the terms they connect are heterogeneous and multidimensional, and therefore current graph representations and analytics techniques are insufficient. Our article aims to show two issues: firstly, how these representations and analytics methods are limited and secondly, the possible solutions to overcome the multidimensionality and the heterogeneity of situations at the same time.

CCS Concepts
Graph theory – Entity relationship models – Modeling methodologies

Keywords
Graph – Multidimensionality – Heterogeneity – Complex system – Hypernetwork

1. INTRODUCTION
It is easy to find examples of real situations composed of relations between things, the assumption being that the universe is lurking in interactions. For example, in a network of citations, authors *come* from laboratories, researchers *write* articles to *present* them during conferences; in a communication system, there are means of communication (cellphones, tablets, computers, servers, etc.) *interacting* with each other in networks in different ways; finally, in social networks, persons *write* posts, *share* pictures and *like* contents, etc. [41].

More recently, Shackel came up with the metaphysical idea that the universe could be seen as an infinite graph made up of nodes and relationships [45], as graphs are supposed to represent interactions. A graph is, in its simplest form, a set of vertices and a set of edges which connect two vertices. While this graph representation is used in many cases, reality is often more complex: a relation between two things can be unidirectional (for example, a graph representing the water flow of a water supply system), there can be multiple types of vertices or relations between two things (for example, a social network consists in many different objects such as people, photos, comments, etc., with multiple kinds of relations between them: friendship between two people, people-comment relationship, etc.) [48], etc. Thus, this kind of graphs can hardly represent some phenomena if they are composed of heterogeneous relations or entities, and if they are multidimensional.

The analytical techniques which can be associated with the characterization of relationships between things can be of interest to better characterize them. Analytical techniques allow to obtain information from graphs. However, current methods do not succeed to fully handle the characteristics of the more complex kinds of graphs, such as the multidimensionality of edges or the heterogeneity of nodes and edges – for example, community detection. Current solutions tinker with the graph to make it compatible with classical analytics methods.

Therefore, the aim of this article is to present an overview of the representation and analytics techniques of graphs. Starting from this overview, the idea is to highlight what is not currently considered and has to be developed, especially regarding heterogeneity and multidimensionality in order to work on phenomena whose components are in interaction and are heterogeneous and multidimensional.

This paper is organized as follow: first, the mathematical definition of a simple graph is given in Section 2. Then, Section 3 presents two paradigms to tackle graphs, as well as more complex techniques developed to represent and analyze them. In Section 4, some limits of the existing approaches are highlighted, before potential solutions presented to overcome them in Section 5. Finally, a summary of this work and research paths are exposed in Section 6.

2. Background
The origins of graphs date back the eighteenth century. The mathematician Euler described a new method to solve problems such as the Königsberg bridges and answer to the question: is it possible to find a path that would cross only one time each of the seven bridges of the city? [16] This new method consisted in representing the bridges by edges and the lands connected by the bridges by vertices. In this section we start by giving the mathematical definition of a graph, while section 3.2 presents more elaborated graphs.

A finite graph is represented by a finite set of vertices (V) as well as a finite set of edges (E) with each edge connecting two different vertices [12]. Formally, the graph G is defined as a

*These authors contributed equally.

couple such that G = (V; E). Unlike a finite graph, an infinite graph has an uncountable number of vertices and edges. In this paper, we will use the terms vertices and nodes interchangeably, as well as for edges and relation.

Moreover, graphs are exploited in four different ways, to:

- model or represent a situation (e.g., ontologies, knowledge graphs)
- store data (e.g., graph-oriented database)
- visualize data (e.g., Human Machine Interface)
- exchange data (e.g., GEXF or GDF)

The research in this paper is based on the first category of use: the representation of phenomena as a graph, that is that the phenomenon consists in "some things" connected together. However, it can be more complex than just pairs of things that are connected: these phenomena can hold multidimensionality and heterogeneity. In this paper, the multidimensionality of relations means that a relation can connect from one to an infinity of nodes and not only two as in simple graphs. The heterogeneity allows a graph to have multiple node labels and multiple relationship types. Therefore, simple graphs are too weak to represent complex systems, thus several classes of graph generalization have been developed in the literature.

3. Graphs: an overview

This part intends to give an overview of graphs and is split in three parts. First, two paradigms are presented. Then, we present some classes of graphs as well as methods to analyze them. This state of the art is not intended to be exhaustive but representative in order to have an overview of how graphs can be addressed, what it is possible to represent and how to analyze them.

3.1 Paradigms

Most of the time graphs concentrate on the nodes, which are the starting point of the analysis. However, there is another paradigm to tackle graphs. This section briefly presents those two paradigms, which are deeply rooted in specific philosophical trends. They both use the term "entity" which designates "something that exists".

3.1.1 Entity's point of view

The most common paradigm focuses on the entities. This means entities have their own characteristics like a substance and we start by detecting entities before relations. Entities always exist whether they are connected or not. For example, when we analyze a text with an NLP (Natural Language Processing) program, you first extract the entities then the relations between them.

3.1.2 Relation's point of view

Another approach considers the relation first: for Abbott, it is the relations (which he calls "boundaries") that pre-exist before the entities [1]. With this paradigm, the entities are "empty", we do not presuppose them. They only exist when they are connected. The relations will give entities and modify them. This paradigm is dynamic in a way because relations make entities evolve. In the case of an NLP program, the idea would be to first extract relations that will give you entities and how they evolve. This paradigm is more pragmatic: it follows what is happening, what are the relations, and then, what are the entities.

3.2 Graph classes

The representation of multidimensionality and heterogeneity in a graph is not placed at the same level. Indeed, multidimensionality is a question of structure of the graph while heterogeneity is given by its characteristics, and can refer to nodes or relations types.

3.2.1 Structures

As an analogy to object-oriented programming, there is an inheritance between the simple graph and the other graphs. The simple graph is the parent of the whole classes of graphs. The definition of a simple graph is given in Section 2.

In 1973, then 1984, through his books [12], [13], Claude Berge developed the notion of hypergraph. Formally, a hypergraph H is defined as a couple such that H = (V; E). A hypergraph H is a set of vertices (V) and a set of subsets of V (E) called hyperedges (as represented in Figure 1.B). Unlike the edges of ordinary graphs, a hyperedge can be related to k nodes such that: $k \in [1, n]$ where $n = |V|$, number of vertices of the set V, whereas a relation of a simple graph can only be linked to two nodes maximum. A hypergraph is a good way to represent sets like members of an organization [2]. Each hypergraph has a double (or conjugate) hypergraph [12], [13]. That is, from two sets and a relation between these two sets, it is possible to construct two hypergraphs. The hypergraph can be seen as a bipartite graph [12], [13].

The notion of hypergraph can lead to that of simplicial complex, a concept having its source in the field of algebraic topology. As it is composed of two sets (a set V of vertices and a subset S of V called simplices), it can be approached as a bipartite graph (as represented in Figure 1.C). In this regard, this makes it possible to represent a hypergraph in a geometrical way. Atkin worked on simplicial complexes and developed methods to apply them to various application domains such as social systems [3], [5], [6], [8]. In his conception, a simplex have a meaning as a whole [7].

A multilayer network with N levels is formally defined as a couple such that M = (G, C) where (G) is a set of simple graphs and (C) is a set of edges between graphs of (G) [15] (see Figure 1.D). Multilayer networks have been used in a wide variety of fields such as social networks, communication, economy, computer science, etc.

Hypergraphs are the generalization of graphs in a sense they allow edges to connect more than two nodes. It is the same for multilayer hypergraphs which are the generalization of multilayer networks. In a multilayer hypergraph, (G) is a set of hypergraphs [10].

In 2013, Johnson used the term hypernetwork to unify several structures cohesively including hypergraphs, simplicial complexes and networks [29]. The definition of this term should not be confused with the different definitions given in other fields. Readers should refer to [26] for more details. A hypernetwork is a set of hypersimplexes. A hypersimplex is a simplex with an explicit *n-ary* relation. Formally, a hypersimplex is noted $\sigma = \langle v_1, v_2, v_3; R\rangle$ where v_1, v_2, v_3 are vertices and R the named relation. This notation allows two hypersimplexes to be discriminated while two simplexes cannot. Johnson idea is to be able to represent complex hierarchical systems as well as to obtain a global structure facilitating the relational analysis and the different dynamics of the systems. Nevertheless, it should be noted that the unification of all these structures remains a theory, and that some bricks remain to be developed. He illustrated how works a hypernetwork with the robot football (not the American one) [30], [31], [36]–[38], [43] which is the most popular example in hypernetworks.

3.2.2 *Characteristics*

The graph structures previously presented can be augmented by some characteristics. Structures will be said *directed*, *weighed*, *attributed*, or *labeled*.

A directed graph (also called digraph) is a graph where its edges can carry an orientation [12]. A digraph can represent a road network: a one-way road between two neighborhoods will be represented by a single directed relation while a two-way road will be materialized by two opposite directed relations. Extending this concept to hypergraphs, a directed hypergraph makes it possible to connect k nodes by directed relations [9]. Directed hypergraphs have been used to represent implication systems [24].

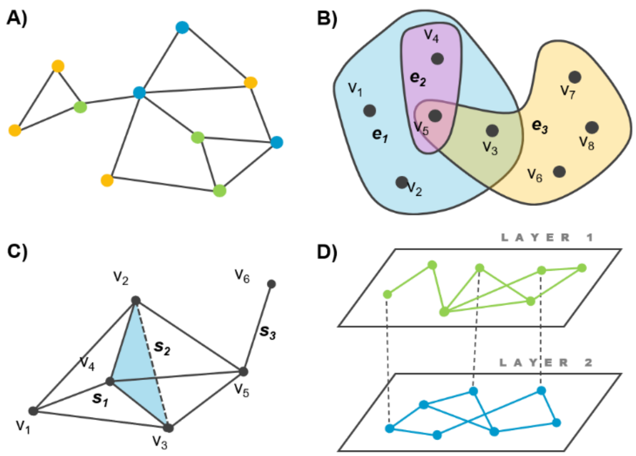

Figure 1. Representation of A) a graph with heterogeneous nodes, B) a hypergraph with eight vertices and three hyperedges, C) a simplicial complex with three simplices and six vertices, and D) a multilayer network composed of two layers.

When weights are added on nodes and/or relations, it is called a weighted graph [12] or a weighted hypergraph [47]. Still taking the example of a road network, the weights of the relationships can represent the distance between the two neighborhoods. The weights of the nodes can represent the number of inhabitants of the districts. In the case of hypernetworks and simplicial complexes, the notion of weights is called the traffic [11], [32].

Graph structures can also carry properties which are represented as key/value pairs on nodes and relations. It is called an attributed graph or a property graph [44].

A labeled graph is a structure which have labels on nodes and type on relations. Labels and types can come from data or functions associated to set of vertices (vertex labelling) and set of edges (edge labelling). Figure 1.A presents graph with three types of nodes.

Some readers might point out that we are not talking about dynamic graphs. Indeed, we consider these graphs as evolutions of the different classes that we have presented, and not as a class. For example, a property graph can support a temporal graph with temporal property at different clock time, but at the end it remains a property graph.

3.3 Graph analytics

In the same way as the graph classes, there are multiple techniques to get a deeper understanding on the graph and the phenomena it tries to represent. Here, we present a non-exhaustive list of metrics, functions and methods to give an overview of existing techniques.

3.3.1 *Metrics*

Many metrics allow to analyze the structural properties of graphs. For example we can measure its length, that is its number of nodes or links; its density, that is the ratio between nodes and relations; the similarity between vertices; or the degree of the nodes, that is the number of relations that are connected to it [41]. This last metric leads to the concept of centrality, which aims to determine the importance of central nodes in a graph. It can be seen as the simplest centrality measure and is sometimes called "degree centrality". However, many other centrality measures exist, such as the eigenvector centrality (which takes into account the importance of the nodes that are connected to the node); betweenness centrality, that indicates if a vertex belongs to many or few paths between other vertices; or the PageRank, which is a centrality measure of a node that takes into account the importance of the nodes connected to it, counterbalanced by the number of connections of the important nodes [41]. Specific centrality measures can be computed for directed graphs: the authority centrality (centrality of nodes that contain useful information on a topic) and the hub centrality (ability of a node to "know" where to find information on a topic of interest) [41].

Other techniques consider the graph topology and how groups or communities can be detected. The identification of cliques in undirected graphs, which are maximal subsets of vertices where each two vertices are adjacent, gives insights on the existence of a cohesive subgroup and is widely used to analyze social networks and how people form groups [41]. The level of transitivity (implying that if vertex v_1 is connected to vertex v_2, and v_2 is connected to v_3, then v_1 is connected to v_3) leads to the clustering coefficient, that measures the probability that two nodes are connected if they have a node in common [41]. The modularity is a measure to quantify the quality of a clustering for a given node [41].

These measures give information about the graph and its structure. For a more extensive review on topology metrics in graphs, please refer to [19].

With the increasingly growing size of graphs—such as online social networks, which can have billion nodes—applying algorithms becomes challenging in terms of computational memory. Graph embedding techniques allow to overcome this problem by converting a large graph into a lower dimensional space, where graph information such as structural properties or attributes are preserved [20], [25], [39].

3.3.2 *Functions*

To go deeper in graph analytics, multiple functions have been developed. While there exists metrics to give insights on how nodes can group together, there is also much deeper methods.

The clustering consists in finding how nodes are grouping together in the graph – or forming communities [41]. A group is characterized by a set of nodes tightly connected, with fewer edges connecting nodes outside the group. Generally, one distinguishes between graph partitioning and community detections. In the first case the number and size of the groups are specified whereas, in the second case, the groups are detected in the network itself. Examples of heuristic methods for graph partitioning are the Kernighan-Lin algorithm and the spectral partitioning. Regarding community detection, some algorithms are based on the modularity metric [18], [41], [42] or in finding cliques [18]. Other method consists in using the Louvain method [17] or in finding the strongly connected components (see for example the Tarjan's algorithm [49]).

Other functions consist in finding the shortest path between two nodes [41]. It can consider some constraints or condition, such as the weights of links; one famous algorithm for this task is the Dijkstra's algorithm [23].

Tasks such as prediction can also be performed. At the graph structure's level, links prediction consists in predicting if a link exists between two nodes in a graph [40]. Regarding nodes, they can be classified (that is, a given label can be allocated to a node) according to the graph topology and the information contained in the nodes (labels or attributes) [14].

3.3.3 *Methodologies*

Other methods or frameworks can be used to analyze graphs. Carley [21] developed DyNet, a tool to study inter-linked and dynamic networks to represent cellular organizations. The inter-link aspect is studied with a meta-matrix made up of the networks considered in the problem.

Algebraic topology can be used to study graphs, as a graph can be viewed as a 1-dimensional simplicial complex [27] (see Section 3.2.1). Thus, some metrics or methods of algebraic topology can be applied to graphs such as the computation of the Betti numbers, which gives an insight on the number of topological holes in a graph [27], [28]. Following this, the Q-analysis [2], [4] is a method developed by Atkin to analyze the connectivity structure of simplicial complexes. The author applied this method to many application domains, such as social systems [4], chess [2] or road traffic systems [33].

4. Limits of existing approaches

While much work has been conducted to enhance the representation of graphs and to analyze them, there is still some limits to existing approaches.

4.1 Representation

There are several solutions to represent multidimensionality and heterogeneity in graphs. As mentioned in Section 2 and in Section 3.2.1, some graph classes can handle and represent multidimensional relations (or n-ary relations) as opposed to binary relations. Table 1 shows what each class of graph can represent in terms of multidimensionality. The crosses indicate that the graph class supports a characteristic.

Moreover, all graphs can support the heterogeneity of nodes and relations since it is a characteristic given to the graph structure (possibility to add labels). The heterogeneity can be given by the data, or by a function associated to the set of nodes and the set of relations.

Table 1. Which graph structures can represent multidimensionality or n-ary relation?

Representation	Multidimensionality
Simple graph	
Hypergraph	×
Simplicial complex	×
Multilayer network	
Multilayer hypergraph	×
Hypernetwork	×

However, some structures have limits which could encroach on the correct representation of multidimensionality and heterogeneity.

Simplicial complexes have an orientation which can be positive or negative while it is possible to make more than two different combinations with the vertices as well as different topological representations. Looking at the aforementioned problems, simplicial complexes allow the issue of multidimensionality to be completely addressed but present a limitation regarding the heterogeneity of nodes and relations. Indeed, a simplicial complex makes it possible to represent two sets of distinct nodes. There is therefore a certain consideration of heterogeneity. Likewise for relations: two types of relations can be considered in a simplicial complex: the relation between the two defined sets, as well as the relation of connectivity between simplices. But the complexes do not allow to represent several different relations at the same time between more than two types of sets of nodes. In other words, it is possible to represent several relations simultaneously between two sets of nodes: the complex will represent the intersection of these relations; but it cannot represent several relations between more than two sets of nodes.

Hypergraphs are a basic structure in a way that multilayer hypergraphs have a better power of representation since they have several layers. Multilayer hypergraphs can express a hierarchy whereas hypergraphs cannot.

The main limitation of the graph representation is the visualization, especially when the size of the graph becomes larger, but this should be developed in another article.

Finally, the existing representations allow to address the two paradigms presented in Section 3.1 (that either gives more importance to nodes or relations). However, much work has to be produced to build the graphs with the second paradigms. In particular, identify the relations before entities, and do not consider what are the characteristics of the entities beforehand.

4.2 Analytics

Regarding the graphs analytics, most of them consider homogeneous graphs [46] even though recent work have been conducted to address heterogeneous graphs [22], [46]. For example, multiple clustering methods have been developed for attributed graphs [18]. They are based on grouping nodes according to the similarity of their attributes and their position in the graph. Most of the time, these clusters do not overlap (one node belongs to only one cluster), which can be limiting according to the use case. Whereas nodes are taken into account in the analysis, there are few methods considering heterogeneous edges for clustering. One method presented by Bothorel to cluster edge-attributed graphs, which is the most common one, consists in reducing the heterogeneous types into single weighted edges [18]. This approach is also used for multilayer network, where the edges of the layers are flattened to build a single weighted graph, and where classical clustering algorithm can then be applied [18]. However, this method may cause a loss of information, such as the fact that some attributes (or edges types) may be more important than others for the cluster definition [18].

Considering Carley's DyNet tool and, more specifically, the meta-matrices, their aim is to analyze inter-linked network, represented in the same meta-matrix [21]. Heterogeneous nodes and edges can be represented in it, but they cannot be analyzed at the same time: the analysis can be conducted only by edge type, for two sets of nodes.

Q-analysis and Atkin's way to approach simplicial complexes [4] allow to represent a given type of relation (explicitly named) as well as an underlying relation, which is the connectivity relation between simplices. This representation also allows to represent two sets of distinct nodes and their multidimensional relations. Those sets are built according to the considered relation. Atkin's theory can also take into account the notion of hierarchy [2]. Thus, this approach allows to analyze several relations between two sets at the same time, if the study of these relations (or the intersection of these relations) make sense. However, it does not allow to study multiple types of relations between multiple nodes sets at the same time.

To conclude, there are many studies to enrich graph's representation and analytics techniques in order to study more complex problems. But it still seems difficult to take into account all the aspects (specially, the multidimensionality and the heterogeneity) in one single approach. It seems to be even more difficult to address the heterogeneity of relations in the analysis, and thus to address the second paradigm mentioned in Section 3.1.

5. Potential solutions

Based on previously discussed limits, some structures and analytics methods seem to be suitable to answer the problems of multidimensionality and heterogeneity. In term of structures, multilayer hypergraphs and hypernetworks are the candidates.

Nevertheless, hypernetworks are above multilayer hypergraphs because Johnson developed hypernetworks to unify all the structures presented in Section 3.2.1 [32]. A multilayer hypergraph is only a set of hypergraphs with edges between them whereas a hypernetwork has a lot more to offer.

Theoretically, hypernetworks make it possible to improve simplices by adding an explicit relation to the simplex in order to obtain a relational simplex (hypersimplex). This notation makes it possible to describe two simplexes having the same orientation but a different representation according to the relations considered. In addition, Q-analysis can be used on a hypernetwork and allows to compute information on a heterogeneous dataset in terms of nodes or relationships. Indeed, the vertices of a simplex can be heterogeneous regarding their substance (i.e., what the things actually are): heterogeneous entities could compose a simplex according to the relation. For example, "flowers", "smell of freshly baked bread" and "board games" can be associated together in the same simplex called "Annie" if the relation considered is "—likes—".

Hypernetworks can model dynamic phenomena thanks to traffic. The negative point that remains to be resolved is the representation of a hypernetwork when the dataset is large. The other negative point is to find the dataset which can fully use the Q-analysis methodology, especially in term of traffic.

So, hypernetwork theory seems to be the best solution as far as we know but there are several gray areas to fill in the theory. For example, can a level N support heterogenous relations? Moreover, Atkin and Johnson focused their work on small examples: defining two sets and a known relation. However, in everyday life, it is never the case. Communication use cases based on a directed graph could highlight the hypernetwork theory while avoiding people to define sets and relations like Atkin and Johnson did. Johnson explained a procedure to obtain a hypernetwork from a network, but there is still the need to find the right example and try its procedure [35].

6. Conclusion

To conclude, this paper expose limitations and solutions to represent and analyze multidimensional and heterogenous data through a graph. From social graphs to biological networks, there are multiple examples of the wide use of graphs these lasts decades, and of proposed solution to enrich the simple graphs. Section 3 presents two philosophical paradigms to tackle graphs, an overview of different kinds of graph classes, from simple ones (simple graphs) to more sophisticated ones (for example, hypernetworks); and some metrics and analytics developed to be able to address more complex problems. From our research and as far as we know, currently there is no working solutions that could address multidimensionality and nodes and edges heterogeneity at the same time (see Section 4 and 5). While hypergraphs can represent those three characteristics, the available analytics methods have difficulties to take into account these three aspects all at once.

The hypernetwork seems to be a step in the right direction for the representation as a graph and the Q-analysis is a relevant methodology for the analysis of complex systems. Hypernetworks could, in theory [34], address the aforesaid issues.

However, there are still a lot of shadows to clear up:

- Find a multidimensional, heterogenous and hierarchical dataset to highlight the representational power of the hypernetwork and analysis quality of Q-analysis methodology.
- Can a simplicial complex support heterogeneous relation? Mathematically, there is restrictions but is there a meaning?

Further work will consist in working on hypernetworks, such as developing an application to manage hypernetworks, find the right visualization for larger hyper networks and consider heterogenous relations in a simplicial complex. On the other side, some research work must be done to build graphs with the second paradigms. This means identifying relations before entities.

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