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Quantitative Graph Theory: A new branch of graph theory and network science

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ABSTRACT

In this paper, we describe some highlights of the new branch QUANTITATIVE GRAPH THEORY and explain its significant different features compared to classical graph theory. The main goal of quantitative graph theory is the structural quantification of information contained in complex networks by employing a *measurement approach* based on numerical invariants and comparisons. Furthermore, the methods as well as the networks do not need to be deterministic but can be statistic. As such this complements the field of classical graph theory, which is descriptive and deterministic in nature. We provide examples of how quantitative graph theory can be used for novel applications in the context of the overarching concept network science.

1. Introduction

The research in graph theory has started in the thirties by König [46]. Afterwards many deep research problems like planarity [47], graph minors [66] and other fundamental problems [39] have been explored. Seminal work was done by Harary [38,39] who investigated numerous problems in graph theory. For example, Harary [38] defined graph measures for analyzing social networks as one of the first. In the nineteens, many other emerging areas in graph theory such as Extremal Graph Theory [9], Random Graph Theory [10] and Algebraic Graph Theory [36] have been established. There is no doubt that graph-theoretical approaches and methods have been applied extensively in many areas. A small subset thereof is pattern recognition [19], computational biology [31,44], chemoinformatics [63,64,78], cognitive modeling [72], computational linguistics [55] and web mining [25]. Other problems in network analysis can be found in [32].

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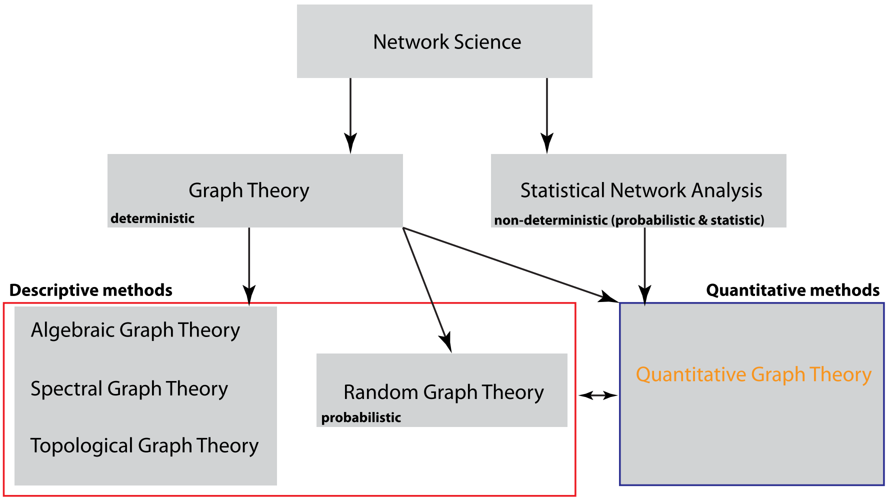

Fig. 1. Quantitative graph theory as a branch of graph theory and network science.

In [21,24], we explained that most of the results which have been achieved in Graph Theory so far are *descriptive* approaches for describing graphs structurally. In contrast, Dehmer and Emmert-Streib [21,24] defined *Quantitative Graph Theory* as the quantification of structural information of graphs instead of characterizing graphs only descriptively. As pointed out in [21,24], the aspect of *measurement* is crucial for this theory. The quantification of structural information has been mainly performed by using graph-theoretical measures (local and global).

In this paper, we highlight important issues of Quantitative Graph Theory and classify this graph-theoretical branch. Quite generally speaking, it could be understood as a subarea of *Data Science* as seen in Fig. 1. In particular, we demonstrate why it is useful to distinguish between classical Graph Theory and *Statistical Network Analysis*. Understanding these differences is crucial for an efficient analysis of the underlying mathematical apparatus [21,24] as well as novel applications. As in Network Science one starts thinking from data, it is important to know and understand what kind of methods are available to analyze a particular data set. Hence, we believe that this contribution can be valuable to perform and classify Quantitative Graph Theory in the context of Data Science efficiently.

2. Quantitative graph theory

In [24], Quantitative Graph Theory has been defined as a measurement approach to quantify structural information of networks. In general, local, global or comparative graph measures can be employed for measuring structural information. See also Section 3. We emphasize that this definition complements (classical) graph theory which mainly deals with the description of structural properties of graphs, see [39]. Examples for pure descriptive graph theory methods are graph colorings, graph embeddings and decompositions, and characterizations of graphs like the Theorem of Kuratowski [47]. In contrast, pure quantitative methods are quantitative graph measures that are based on estimating structural features of networks [20]. The latter class of methods can be interpreted as graph complexity measures. Seminal work in this area was done by Mowshowitz [56] and Bonchev [11]. Note that the ambiguity of some methods belonging to both Descriptive and Quantitative Graph Theory has been explained in [24].

In Fig. 1, we present a conceptual overview that shows the connection of Quantitative Graph Theory within some other related fields. First, we note that Network Science comprises both, Graph Theory and Statistical Network Analysis because it is the most generic field. The major difference between Graph Theory and Statistical Network Analysis is that the graphs as well as the methods of Graph Theory are purely deterministic, whereas in statistical network analysis the networks and the methods may be non-deterministic. A cause for the structural non-deterministicness may be given by, e.g., measurement errors or signal variability used to infer such networks [31]. Hence, the methods applied are based on probabilistic and statistical principles. Furthermore, Quantitative Graph Theory is also a branch of Graph Theory which relates to quantify structural information of networks. This is in contrast to classical Graph Theory which mainly deals with descriptive graph analysis, as discussed above. Interestingly, one can see that random graph theory is on one hand deterministic, when describing properties of random graphs. On the other hand, the methods and the random graphs themselves are often probabilistic and, hence, this subfield is also non-deterministic in nature.

As known, quantitative graph theory has many important applications in various scientific areas. Using web algorithms like PageRank and analyzing properties of social network analysis are two well-known examples, see [16,60,79]. For instance, the famous PageRank algorithm [60] operates on web graphs and it's based on employing quantitative techniques and graph invariants such as eigenvalues. Social network analysis already emerged in the forties and fifties. Classical contributions thereof deal with developing graph-theoretical measures based on shortest paths and vertex degrees. Those were firstly