Arc-pancyclicity in multipartite tournaments
&
GTECS – An application in crystallography

Von der Fakultät für Mathematik, Informatik und Naturwissenschaften der RWTH Aachen University zur Erlangung des akademischen Grades eines Doktors der Naturwissenschaften genehmigte Dissertation

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Preface

In graph theory as a part of discrete mathematics, there has always been a close connection between theoretical results and their applications. Many problems arising in the everyday life concerning topics like logistics, scheduling, routing, (social) networks etc. can be solved by algorithms based on the solutions of corresponding theoretical problems. Therefore, the aim of this thesis is to deal with questions from both areas of graph theory: theory and application.

Well-studied classes of directed graphs are tournaments which are orientations of the complete graph, and multipartite tournaments as one kind of generalisation of tournaments. One property of these digraphs is of special interest right from the beginning of the research in this area: the existence of cycles. Thus, the main focus in the first part of this thesis is on answering questions concerning this topic.

Very much attention has been given to one of the first results published by Moon [47] in 1966, who presented his well-known theorem about cycles in tournaments which says that every vertex in a strong tournament on n vertices is pancyclic, i.e. it is contained in cycles of length $3, 4, \ldots, n$. This theorem can be seen as a starting point for investigations on the cycle structure of tournaments. One year later Alspach [1] considered pancyclic arcs instead of vertices and he proved that every arc in a regular tournament is pancyclic. A question which naturally arises in this context, is the question of the number of pancyclic arcs in a tournament in general. Moon [48] showed that $h(T)$, the maximum number of pancyclic arcs belonging to the same Hamiltonian cycle of a strong tournament T, is at least three which is also a lower bound for $p(T)$, the number of all pancyclic arcs in T. Additionally, he presented all tournaments with $h(T) = 3$ and $p(T) = 3$. In Chapter 2, we will generalise this result of Moon by showing that $h^t(T)$, the maximum number of t-pancyclic arcs, i.e. arcs which are contained in cycles of length $t, t+1, \ldots, n$, belonging to the same Hamiltonian cycle, is at least t. With $p^t(T)$ the number of all t-pancyclic arcs in T, we also get $p^t(T) \geq t$. Moreover, we will characterise all tournaments with $h^t(T) = t$ or $h^t(T) = t + 1$ and $p^t(T) = t$ or $p^t(T) = t + 1$.

Instead of asking for the number of pancyclic arcs in the whole tournament, Yao, Guo and Zhang [63] considered vertices whose all out-arcs are pancyclic. After Thomassen [56] showed the existence of a vertex whose all out-arcs are contained in Hamiltonian cycles, they improved his result by characterising a vertex whose all out-arcs are pancyclic. Chapter 3 discusses the problem whether this result can be generalised for multipartite tournaments which contain tournaments as a subclass. A well-known theorem by Bondy [9] shows, that each strong c-partite tournament contains an m-cycle for each $m \in \{3, 4, \ldots, c\}$. Furthermore, he presented a c-partite tournament which does not contain cycles of lengths exceeding c. Thus, instead of the length of a cycle, we consider the number of partite sets which have at least one vertex in common with the cycle. Additionally, we use the concept of outpaths introduced by Guo [27] as a generalisation of cycles and show that every 2-strong c-partite tournament has a vertex whose all out-arcs are contained in an outpath containing vertices from exactly k partite sets for all $k \in \{4, \ldots, c\}$. Moreover, we present a counterexample showing that $k = 3$ is generally not possible.

In Chapter 4, we consider digraphs D in general and look for approximating spanning subdigraphs H such that the distance between every pair of vertices in H is bounded by the original distance plus a constant t. Dragan et al. [17] introduced the class of (α, r)-decomposable graphs and proved that every such graph has a so called additive $2r$-spanner with at most $(n-1)\log_{\frac{1}{\alpha}}(n)$ edges as well as a system of at most $\log_{\frac{1}{\alpha}}(n)$ additive tree $2r$-spanners. As Cai and Corneil [11] showed that only acyclic digraphs may have a tree spanner, we first introduce the concept of pairs of tree spanners to have a tool for general digraphs and adapt the results of Dragan et al. to the class of (α, r)-decomposable digraphs.

The second part of this thesis considers an application in the field of crystallography. Since every molecule and, in a more complex way, every crystal structure can be represented by a graph, the visualisation and analysis of particularly large structures are in the focus of nowadays' research. A few software tools to support the user already exist, but most of them either have an old visualisation technique or important features for the user to interact with the represented structure are missing. Therefore, the three-dimensional visualisation- and analysis-tool GTECS, as a result of an interdisciplinary project of chemists, computer scientists and mathematicians, has been developed.

Chapter 5 introduces the main idea of GTECS. Since the software tool should be able to handle large structures consisting of a repetition of a so-called unit cell in all dimensions, we additionally introduce the concept of (infinite) periodic graphs. Furthermore, we focus on molecular topology, since the aim of GTECS is to simplify the given structure in a way that its topology does not change.

For such a simplification, algorithms to contract paths and to detect cycles of a given length in periodic graphs are represented in Chapter 6. Additionally, we discuss problems which arise in the context of cycle contraction and show an algorithm for those cases in which a unique contraction is possible.

Chapter 7 contains the main algorithm of GTECS which determines the components of a periodic graph, their dimensionality as well as the right size of the visualised part of the structure containing all important information for the user.

Various possibilities of characterising a crystal structure are presented in Chapter 8. As in the most cases it is impossible to have one parameter to describe the whole topology, we will introduce different topological symbols by regarding the local topology around a single atom. Algorithms to calculate these symbols will be provided.

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