

# A Perfect Path to Computational Biology and Quantum Computing

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# A Perfect Path to Computational Biology and Quantum Computing\*

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#### Abstract

I revisit my contributions to the P versus NP millennium problem and the computational complexity of combinatorial problems, especially those arising in Computational Biology and Quantum Computing, through 20 PhD theses, mine and of my students. I explain how the dichotomy NP-complete versus polynomial-time of long-standing problems together with their multivariate analysis is settled. Yet, intriguing questions remain.

Keywords: analysis of algorithms and problem complexity; graph algorithms; structural characterization of types of graphs

## 1 A perfect table

What does it mean today to study a problem from a computational complexity point of view? Together with two former PhD students and an expert on parameterized complexity, I proposed an answer by revising David S. Johnson's "Graph Restrictions and Their Effect" table according to the granularity provided by the parameterized complexity for NP-complete problems [11]. I give here a more personal answer, based on my contributions to the computational complexity of combinatorial problems through 20 PhD theses, mine and of my students. Please refer to Figure 1.

The 1979 book Computers and Intractability, A Guide to the Theory of NP-completeness by Michael R. Garey and David S. Johnson is considered the

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single most important book by the computational complexity community and it is known as The Guide. The book was followed by The NP-completeness Column: An Ongoing Guide where, from 1981 until 2007, D.S. Johnson continuously updated The Guide in 26 columns published first in the Journal of Algorithms and then in the ACM Transactions on Algorithms. My favorite is Column 16 "Graph Restrictions and Their Effect", where several puzzles were proposed by D.S. Johnson and many remain unsolved after 40 years. In his unusual Column 16, D.S. Johnson emphasis is on the restrictions and how they affect the complexity of 10 famous NP-complete graph problems. He selected graph classes having broad algorithmic significance grouped into 4 types: trees and near-trees, planarity and its relations, a catalog of perfect graphs, and intersection graphs. The presentation consisted of a summary table with 30 rows containing the selected classes of graphs, and 11 columns the first devoted to the complexity of determining whether a given graph is in the specified class, followed by 10 of the more famous NP-complete graph problems. The entry for a class and a problem was the complexity of the problem restricted to that class of graphs — polynomial-time solvable or NP-complete, if known. The goal was to identify interesting problems and interesting graph classes establishing the concept of "separation in complexity".

The table revealed among its 330 entries the existence of a substantial collection of 71 open problems classified from entertaining puzzles as P? or O? to may well be hard or are famous as O or O! problems. It is remarkable that only one entry in the entire table deserved a famous open problem O! entry, the recognition for perfect graphs, and just two entries deserved a may well be hard problem O entry, edge-colouring of planar graphs and hamiltonian circuit of permutation graphs. In 1985, the two problems with most open entries were edge-colouring and maximum cut. At that time, maximum cut had 18 proposed entertaining puzzles, and after the recent entry [12], the only NP-complete entry for permutation graphs so far, just 2 entries remain open for maximum cut and just one entry remains open for permutation graphs. At that time, edge-colouring had 19 of its 30 entries classified O?, which meant apparently open but possibly easy to resolve, and 14 of those O? puzzles remain open after 40 years, including the edge-colouring of permutation graphs. It is remarkable that today only two problems still have open entries that resist classification: edge-colouring and maximum cut<sup>1</sup>.

David S. Johnson's choices of NP-complete graph problems and of graph classes were motivated by the famous open problem at the time: the recog-

<sup>1</sup>see the current table at https://www.cos.ufrj.br/~celina/ftp/j/RJ-current.pdf

nition of perfect graphs. A graph G is perfect if for each induced subgraph H of G, the clique number of H equals the chromatic number of H. In the first column of his Ongoing Guide, D.S. Johnson proposed as open problem the recognition of imperfect graphs, since it had recently been established by the ellipsoid method to be a problem in NP. Nowadays, it is known that the recognition of perfect graphs is polynomial, and the famous open problem is to find practically good algorithms for vertex-colouring and clique when restricted to perfect graph inputs. At the time of my thesis, the approach for resolving the complexity of the recognition problem for perfect graphs, as well as the search for algorithms for vertex-colouring and clique, was to consider forbidden induced subgraphs, and Bruce Reed proposed to me the study of bull-free perfect graphs, a task that I finally was able to achieve thanks to Frédéric Maffray [2]. This introductory Section 1 is followed by Section 2 describing a path of twenty theses, grouped into four topics: colouring problems, sandwich problems, genome rearrangements, and graph tessellations; Section 3 giving an account of a selection of 10 significant publications; and Section 4 concluding with four intriguing questions.

## 2 A path of twenty theses

David S. Johnson in his "Graph Restrictions and Their Effect" column proposed the concept of "separation in complexity": Is there a problem that remains NP-hard when restricted to graph class A but is polynomial-time solvable when restricted to graph class B? Starting from the study of bull-free perfect graphs, and through the theses of my students, I pursued, extended and twisted the "separation in complexity" concept. Given a class  $\mathcal{G}$  of graphs and a graph problem  $\pi$  belonging to NP, we say that a full complexity dichotomy of  $\mathcal{G}$  was obtained if one describes a partition of  $\mathcal{G}$  into subclasses such that  $\pi$  is classified as polynomial or NP-complete when restricted to each subclass [23, 24]. The concept of full complexity dichotomy is particularly interesting for the investigation of NP-complete problems: as we partition a class  $\mathcal{G}$  into NP-complete subclasses and polynomial subclasses, it becomes clearer why the problem is NP-complete in  $\mathcal{G}$ . A class  $\mathcal{G}$  of graphs is a separating class for problems  $\pi_1$  and  $\pi_2$  if  $\pi_1$  is NP-complete when restricted to  $\mathcal{G}$  and  $\pi_2$  is polynomial when restricted to  $\mathcal{G}$  — or vice versa. The nice idea about a separating class is that it shows how the same structure may define a polynomial problem and an NP-complete problem. We remark that the "dual" idea of separating problem — a problem that has distinct complexities when restricted to distinct graph classes — was proposed by D.S. Johnson.

Jayme L. Szwarcfiter as my thesis advisor introduced me to Bruce Reed and perfect graphs, and later also at UFRJ as my colleague, Jayme introduced me to most of my co-authors — my students, starting from Luerbio Faria, and my fruitful collaborators Célia Mello and Marisa Gutierrez. Célia Mello was supervised by Jayme at the same time, and so my first papers are all with her. Célia introduced me to João Meidanis and interval graphs, and together we began the study of edge and total colourings [21]. João opened me the world of computational biology, through the doors of genome rearrangements and of sandwich problems, which gave thesis themes for several of my students.

In 2014, Dániel Marx gave a plenary talk at the 9th International Colloquium on Graph Theory and Combinatorics, entitled Every Graph is Easy or Hard: Dichotomy Theorems for Graph Problems<sup>2</sup>. He highlighted three features of dichotomy theorems that have guided the path of twenty theses: dichotomy theorems give good research programmes, easy to formulate, but can be hard to complete; the search for dichotomy theorems may uncover algorithmic results that no one has thought of; proving dichotomy theorems may require good command of both algorithmic and hardness proof techniques.

The theses of Claudia Villela (2005), Raphael Machado (2010), Diana Sasaki (2013), Helio Macêdo (2014), and Caroline Patrão (2021) considered the colouring problem. Claudia considered a generalization of bull-free perfect graphs, supervised by Frédéric Maffray. Raphael studied unichordfree graphs, graphs that do not contain a cycle with a unique chord, a graph class defined by Kristina Vušković and Nicolas Trotignon, and found a surprising complexity dichotomy unmatched in the literature for edge and total colourings [22, 25]. Diana further studied total colourings considering snarks and cubic graphs with Simone, and graph products with Caroline [27]. Taking advantage that unichord-free graphs are diamond-free and so have a polynomial time number of maximal cliques, Helio with Raphael further studied the hierarchical complexity including the third level of the polynomialtime hierarchy and the problems of clique, biclique and star colourings [26]. Recently, I was fortunate to write an invited survey about total colouring, where we assign a colour to each vertex and edge of a graph, so that there are no incidence conflicts. Since, by definition, a total colouring is also a vertex-colouring and an edge-colouring, it is natural to consider successful strategies, both theoretical and algorithmic, towards the solution of these two more studied coloring problems. I was able to summarize the theses on colourings, with recent advances towards a better understanding of the

<sup>&</sup>lt;sup>2</sup>see the slides at https://www.cs.bme.hu/~dmarx/talk.php

challenging total colouring problem, with respect to Hilton's condition, cubic graphs, equitable colourings, vertex-elimination orders, decomposition, and complexity dichotomies [14].

The theses of Simone Dantas (2002), Vinícius Sá (2006), and Rafael Teixeira (2008) considered the sandwich problem, a generalization of the recognition problem arising from applications in computational biology. Let  $G_1 = (V_1, E_1), G_2 = (V_2, E_2), \text{ then } G_2 \text{ is a supergraph of } G_1 \text{ if } V_1 = V_2 = V$ and  $E_1 \subseteq E_2$ . A pair  $(G_1, G_2)$  of graphs so that  $G_2$  is a supergraph of  $G_1$  is called a sandwich instance. The edges in  $E_1$  are called forced, while the edges in  $E_2 \setminus E_1$  are optional. We let  $E_3$  be the set of all edges in the complete graph with vertex set V which are not in  $E_2$ , and call them forbidden edges. A graph G is called a sandwich graph for the sandwich instance  $(G_1, G_2)$  if  $G_2$  is a supergraph of G and G is a supergraph of  $G_1$ . The  $\mathcal{P}$  recognition problem is the problem of deciding whether a given graph G satisfies a graph property  $\mathcal{P}$ . The  $\mathcal{P}$  sandwich problem is the following: For a given sandwich instance  $(G_1, G_2)$ , does there exist a sandwich graph G for  $(G_1, G_2)$  so that G satisfies  $\mathcal{P}$ ? This generalization of the recognition problem was introduced by Golumbic and Shamir [37] in the context of computational biology, when the adjacency relationship between the vertices is only partially specified, and they established that the interval graph sandwich problem is NP-complete<sup>3</sup>. The sandwich problem becomes the recognition problem when  $G_1 = G_2$ , and thus, if the  $\mathcal{P}$  recognition problem is NP-hard, so is the  $\mathcal{P}$  sandwich problem. Vinícius focused on the homogeneous set property, a key property in the study of perfect graphs, celebrated by László Lovász's weak perfect graph theorem — a graph is perfect if and only if its complement is perfect. Vinícius described 10 faster deterministic and randomized algorithms on the homogeneous set sandwich problem [15]. Simone and Luerbio gave me the first full complexity dichotomy, the target family was the generalized split (k,l) -graph sandwich problems [18]. Rafael and Simone achieved the full complexity dichotomy for all three nonempty part sandwich problems, a task of classifying 61 problems into polynomial or NP-complete [28].

Computational biology and genome rearrangements The theses of Rodrigo Hausen (2007) and Luís Felipe Cunha (2015) considered the sorting by transpositions problem. By comparing the orders of common genes between two organisms, one may estimate the series of mutations that occurred

<sup>&</sup>lt;sup>3</sup>see a recent celebration of the 30th anniversary of the landmark paper at http://www.antenabrasil.uff.br/index.php/pt-br/acoes/seminario-combinatoria/seminario-de-combinatoria-visao-unica/815-golumbic-shamir

in the underlying evolutionary process. In a simplified genome rearrangement model, each mutation is a transposition, and the sole chromosome of each organism is modeled by a permutation. A transposition is a rearrangement of the gene order within a chromosome, in which two contiguous blocks are swapped. A classic problem in genome rearrangement is the transposition distance, which consists of the length of a minimum sequence of block moves that transforms one genome into another. Genomes are represented as sequences of segments called syntenic blocks, such sequences are viewed as permutations, elements of the symmetric group  $S_n$ , where one of the genomes can be viewed as the *identity permutation*, the permutation where all elements are in ascending order. The transposition distance of a permutation  $\pi$  is defined by the minimum number of transpositions needed to sort  $\pi$ . Sorting by transpositions is therefore, the problem to determine the transposition distance for any permutation  $\pi$ , and it is of interest for biologists, computer scientists, and mathematicians. Sorting by transpositions was settled as NP-hard, after more than one decade of extensive studies such as: approximation algorithms, with the best known ratio of 1.375-approximation, and tight upper bounds on families of permutations.

Historically, the approach considered regarding sorting by transpositions has been the transposition diameter, i.e., to determine the maximum transposition distance among all possible permutations for a given length n. To this date, the transposition diameter is known only for  $n \leq 15$ . For every  $n \leq 12$ , the reverse permutation, the permutation where all elements are in descending order, is a diametral permutation, i.e., its distance  $\lfloor \frac{n}{2} \rfloor + 1$  equals the diameter, but for odd  $n \geq 13$  the reverse is not diametral and for even n it is not known if there exist permutations whose transposition distance is greater than the reverse permutation. The lower bound of  $\lfloor \frac{n+1}{2} \rfloor + 1$  for the diameter for odd  $n \geq 13$  has been obtained through the union operation, and we were able to construct families that meet the current lower bound  $\lfloor 17 \rfloor$ .

Several approaches to handle sorting by transpositions have been considered exploring approximation algorithms for estimating the transposition distance between permutations, providing better practical results or lowering time complexities. Bafna and Pevzner designed a 1.5-approximation  $O(n^2)$  algorithm, based on the cycle structure of the breakpoint graph. Hartman and Shamir, by considering simple permutations, proposed an easier 1.5-approximation algorithm and, by exploiting a balanced tree data structure, decreased the running time to  $O(n^{\frac{3}{2}}\sqrt{\log n})$ . Feng and Zhu developed the balanced permutation tree data structure, further decreasing the complexity of Hartman and Shamir's 1.5-approximation algorithm to  $O(n \log n)$ . Elias

and Hartman obtained, by a thorough computational case analysis of cycles of the breakpoint graph, a 1.375-approximation  $O(n^2)$  algorithm. We have managed to describe an algorithm that uses the strategy of Elias and Hartman towards bad full configurations, implemented using Feng and Zhu permutation trees, achieving both a 1.375 approximation ratio and  $O(n \log n)$  time complexity, achieving the current best time-approximation trade-off [6].

Quantum computing and tessellations The theses of Luis Antonio Kowada (2006), André Ribeiro (2013), Alexandre Abreu (2020), and Edinelço Dalcumune (2021) considered algorithms for reversible and quantum computing. Random walks play an important role in computer science mainly in the area of algorithms and it is expected that quantum walks, which is the quantum counterpart of random walks, will play at least a similar role in Quantum Computation. In fact, the interest in quantum walks has grown considerably in the last decades, especially because they can be used to build quantum algorithms that outperform their classical counterparts. Recently, the staggered quantum walk model was proposed. This model is defined by an evolution operator, which is described by a product of local unitary matrices obtained from a graph tessellation cover. A tessellation is a partition of the vertices of a graph into vertex disjoint cliques, and a tessellation cover is a set of tessellations so that the union covers the edge set of the graph. To cover the entire edge set is important because a missing edge in the tessellation cover would play no role in the quantum walk dynamics. In order to fully understand the possibilities of the staggered model, it is fundamental to introduce the t-TESSELLABILITY problem. This problem aims to decide whether a given graph can be covered by t tessellations. The simplest evolution operators are the product of few local unitary matrices and, to obtain a non-trivial quantum walk, at least two matrices (corresponding to 2-tessellable graphs) are required. There is a recipe to build a local unitary matrix based on a tessellation. Each clique in a tessellation is associated with a unit vector, and the set of those unit vectors spans a subspace of the model's Hilbert space. A subspace has an associated orthogonal projection  $\Pi$ , which is used to define the local unitary operator  $(2\Pi - I)$  associated with the tessellation. Each clique of the partition establishes a neighbourhood around which the walker can move under the action of the local unitary matrix. The evolution operator of the quantum walk is the product of the unitary operators associated with the tessellations of a tessellation cover.

The study of tessellations in the context of Quantum Computing was proposed by Portugal et al. [38] with the goal of obtaining the dynamics of

quantum walks. Portugal analyzed the 2-tessellable case, showing that a graph is 2-tessellable if and only if its clique graph is bipartite, and examples for the t-tessellable case are also available. The thesis of Alexandre Abreu (2020) supervised with Luis Kowada and Franklin Marquezino is the first systematic study of the graph tessellation cover as a branch of Graph Theory, by establishing graph classes whose tessellation cover number is close or equal to chromatic upper bounds, efficient algorithms, and hardness.

The edge-coloring of a graph G induces a tessellation cover of G: each color class induces a partition of the vertex set into disjoint cliques of size two (vertices incident to edges of that color) and cliques of size one (vertices not incident to edges of that color), which forms a tessellation. The clique graph K(G) is the intersection graph of the maximal cliques of G [39]. Clique graphs play a central role in tessellation covers since a coloring of K(G)induces a tessellation cover of G: two vertices of the same color in K(G)correspond to disjoint maximal cliques of G and every edge of G is in at least one maximal clique, so each color in K(G) defines a tessellation in G by possibly adding cliques of size one (vertices that do not belong to the maximal cliques of G related to vertices of K(G) with that color), such that the union of these tessellations is the edge set of G. Hence, we have the *chromatic upper* bound as the minimum between  $\chi'(G)$  and  $\chi(K(G))$ . We determine graph classes which reach these upper bounds, and provide tools to distinguish several classes for which the t-TESSELLABILITY problem is efficiently tractable (for instance bipartite, triangle-free, diamond-free K-perfect, and threshold graphs) from others where the problem is NP-complete for  $t \geq 3$  (for instance planar, triangle-free, chordal (2, 1)-graphs, (1, 2)-graphs, and diamond-free graphs with diameter at most five) [16].

# 3 Most significant publications

Among my 125 publications in international refereed journals, I have selected the 10 below covering a number of different topics from graph theory and theoretical computer science, 6 of them exhibit long standing central problems that I solved, 5 of them are product of PhD theses that I supervised, and 1 is a survey of a plenary talk. While several research topics like perfect graphs and the computational complexity hierarchy are visible throughout my entire scientific career, I regularly work on new problems and applications such as bioinformatics and quantum computing. I chose the chronological order that emphasizes the regularity of my production, spread along 30 years after my doctoral degree. Among the 28 co-authors below, 8 PhD students and 8

different nationalities are represented, and 8 leading journals in the area of Theoretical Computer Science and Discrete Applied Mathematics.

The paper [1] gave international visibility to my research work and it is my most cited paper. The Skew Partition defined by Chvátal in 1985 is a key decomposition for the Strong Perfect Graph Theorem proved by Chudnovsky et al. in 2002. This paper gives a polynomial-time algorithm for testing whether a graph admits a skew partition. I presented that algorithm at the Latin American Symposium on Theoretical Informatics in 2000, and published the full paper in the very prestigious Journal of Algorithms, at the time edited by Knuth, Johnson, and Galil. In 2001, I was invited to speak about it at closed workshops in Dagstuhl and Princeton, and in 2004 at a conference in honor of Claude Berge, who defined the area of Perfect Graphs. This paper proves that I have Erdös number 2, since Yoshiharu Kohayakawa is the only Brazilian co-author of Paul Erdös.

The paper [2] on polynomial-time combinatorial algorithms for the optimal weighted coloring and clique problems in bull-free perfect graphs solved the problem Bruce Reed gave me when I was a visiting student at the University of Waterloo in 1989. I met Frédéric Maffray in 1989 at a workshop on perfect graphs and we continuously worked together until his premature death in 2018. We co-authored several papers, coordinated joint Brazil-France projects, and co-supervised four female PhD students. We celebrated our close partnership in a Centenary conference in Grenoble in 2010. Optimizing bull-free perfect graphs was a problem proposed by Chvátal in 1987 as a key step towards a combinatorial algorithm to compute the chromatic number of a perfect graph, a central and still open problem in Graph Theory. Frédéric and I were twice guest speakers, consecutive and complementary, about our journey to color these graphs: at the Fields Institute in 2000 and at Dagstuhl in 2007.

In paper [3], my first PhD student Luerbio Faria and I solved the conjecture posed by Erdös in 1973 on the crossing number of the hypercube. Our co-authors are experts in the problem. I met them at WG 1998, the Workshop on Graph-Theoretic Concepts in Computer Science, an important Graph Theory conference. Since then I have been able to continuously participate at WG presenting papers and serving five times as the only Latin American member of its Program Committee. It took us ten years to turn the extended abstract of the WG proceedings into the full paper with Erdös drawings published in the Journal of Graph Theory. In 2014, I gave an invited talk at the Foundations of Computational Mathematics conference about further planarity parameters, which was later also published as a paper in the Journal of Graph Theory.

The time complexity of recognizing clique graphs was a long-standing question open since 1971. I learned about this problem in a survey on clique graphs by my PhD supervisor Jayme Szwarcfiter. In paper [4] we proved that the clique graph recognition problem is NP-complete. The extended abstract was published in the Graph-Theoretic Concepts in Computer Science proceedings in 2006, which we dedicated to Alberto Santos Dumont, aviation pioneer, on the 100th anniversary of the flight of his 14 Bis in Paris in October 1906. My co-authors in this paper are my first PhD student and second most frequent co-author Luerbio Faria, and Marisa Gutierrez and Liliana Alcón from Argentina. Marisa and Liliana are two key long-term collaborators in the context of two series of Latin American conferences where I belong to the steering committee: the Latin and American Algorithms, Graphs and Optimization Symposium, and the Latin American Workshop on Cliques in Graphs.

The survey paper [5] contains my personal approach to the P versus NP problem. I discuss classes of problems for which dichotomy results do exist: every problem in the class is classified into polynomial or NP-complete, and my contribution through the classification of some long-standing open problems in important areas of graph theory: perfect graphs, intersection graphs, and structural characterization of graph classes. The paper is the journal version of my plenary talk given at LAGOS 2009, the Latin-American Algorithms, Graphs and Optimization Symposium. The P versus NP problem is one of the seven Millennium Problems selected by the Clay Mathematics Institute to motivate research on important classic mathematical questions that have resisted solution over the years. The P versus NP problem is the central problem in theoretical computer science: it aims to classify the possible existence of efficient solutions to combinatorial and optimization problems.

In the study of genome rearrangements, Sorting by Transpositions is an NP-hard problem for which several polynomial-time approximation algorithms have been developed. For developing approximation algorithms, one searches for the optimal trade-off between the quality of the approximation and the running time. The algorithm proposed in paper [6] achieves the best trade-off by combining all tools published in leading journals by leading researchers, and by correcting a previous publication in the same prestigious Journal of Computational Biology. My co-authors are three former PhD students: two of them did their theses on genome rearrangements in 2007 and 2017; the third one did his thesis on quantum computing in 2006 and was key with his expertise regarding data structures to handle permutation trees. The research projects that I coordinate benefit from the fact that most

of my former 19 PhD students are research professors at universities in Rio de Janeiro; after finishing their degrees, the young researchers pursue their thesis topics as post-docs, and co-supervising theses with me.

In paper [7], we solve an open problem posed by Kratochvíl and Tuza to determine the complexity of 2-clique-colouring of perfect graphs with all cliques having size at least 3, proving that is complete with respect to the third level of the polynomial-time hierarchy. We also determine a hierarchy of nested subclasses of perfect graphs with all cliques having size at least 3 whereby each graph class is in a distinct complexity class with respect to the polynomial-time hierarchy. Both clique-colouring and perfect graphs have attracted much attention due to a conjecture, posed by Duffus et al. in 1991, that perfect graphs are k-clique-colourable for some constant k, answered negatively by Charbit et al. in 2016. My co-authors are two former PhD students: one did his thesis on the complexity of edge and total coloring problems in 2010, and then co-supervised the thesis of the other one on the complexity of clique and biclique coloring problems in 2013.

The paper [8] solves a problem left open in the PhD thesis of Maria Chudnovsky from Princeton University in 2003: the computational complexity of the Berge trigraph recognition. Maria kindly received me as visiting professor at Princeton in 2016 and generously introduced me to Sophie Spirkl, at the time a PhD student co-supervised by Paul Seymour and herself. I proposed to them a research problem that lies in the intersection of our research interests: the imperfect graph sandwich problem, which is equivalent to Berge trigraph recognition. To prove that the target problem can be solved in polynomial time, we introduce almost monotone properties, for which the sandwich problem can be reduced to the recognition problem. We study the complexity of several graph decompositions related to perfect graphs, with respect to the graph sandwich problem, and the related partitioned and unpartitioned probe problems, resulting in polynomial-time algorithms or NP-hardness results.

Parameterized complexity is a recent branch of computational complexity that provides a framework for refined analysis of hard algorithmic problems. The strict terminal connection is a network design problem whose goal is to decide whether, given a graph and a set of vertices, there exits a tree subgragh having the set as its leaves. Network design problems are combinatorial questions of great practical and theoretical interest. Such problems are challenging tasks closely related to real-world applications. In paper [9], we investigate the parameterized complexity of the strict terminal connection problem with respect to multiple parameters of the input. We establish a Polynomial versus NP-complete dichotomy with respect to the number of

linkers in the tree and the maximum degree of the graph. We prove that the problem parameterized by the number of routers is hard and provide a kernelization when parameterized by the number of linkers. My co-authors are a PhD student and an expert on this new area who co-supervised the thesis, chosen by the Brazilian Computer Society as the best thesis of 2022.

The graph tessellation cover is motivated by its application to quantum walk models, where the evolution operator of the staggered model is obtained from a graph tessellation cover. We investigate the tessellation cover number for extremal graph classes, which are fundamental for the development of quantum walks in the staggered model. These results help to understand the complexity of the unitary operators necessary to express the evolution of staggered quantum walks. We establish tight upper bounds for the tessellation cover number related to chromatic parameters, which gives a complexity dichotomy between edge colorability and tessellability. The paper [10] was published by Theoretical Computer Science Section C, Natural Computing, created in 2004 for research that explores the relationship between nature and computation. Among the co-authors there are three former PhD students: two of them did their theses on quantum computing in 2006 and 2020; the third one did his thesis on genome rearrangements in 2017 and contributed his expertise on computational complexity.

## 4 Intriguing questions remain

I have pursued for many years stubborn questions addressing the structural characterization of types of graphs that would possibly lead to full complexity dichotomies. I highlight four intriguing questions, all address David S. Johnson's puzzles proposed in 1985. The announcement at the International Symposium on Computational Geometry 2021 that the maximum cut problem is NP-complete for the class of interval graphs has been received as an indication that possibly several of the remaining puzzles will be resolved as NP-complete. From my thesis on vertex-colouring bull-free perfect graphs, and through several theses I advised, I have been considering edge and total colourings, trying to explain why edge-colouring provides the stubborn column of D. S. Johnson's table, in particular considering subclasses of chordal graphs such as interval graphs and unit interval graphs. The recognition for perfect graphs provided the famous open problem of D. S. Johnson's table, and the generalization of the recognition problem introduced by Golumbic and Shamir provides a question that since 1995 has received much attention and related research.

Question 1. Is maximum cut polynomial for interval permutation graphs?

In [12], we have proved that the maximum cut problem is NP-complete on permutation graphs. This settles a long-standing open problem that appeared in the 1985 column of the Ongoing Guide to NP-completeness by David S. Johnson, and is the first NP-hardness entry for permutation graphs in such column. Many important graph classes are defined or can be characterized by a geometric intersection model. Two particularly well-studied examples are subclasses of perfect graphs and were among the 30 graph classes selected by D. S. Johnson: the classes of interval graphs and of permutation graphs. In their respective models, the intersecting objects are line segments in the plane, with different restrictions imposed on their positions. In interval graphs, each line segment must have its endpoints on a single line, while in permutation graphs, their endpoints must lie on two distinct parallel lines.

A cut is a partition of the vertex set of a graph into two disjoint parts. The maximum cut problem aims to determine a cut with the maximum number of edges for which each endpoint is in a distinct part. The maximum cut decision problem is known to be NP-complete since the seventies, and only recently its restriction to interval graphs has been announced to be hard by Adhikary, Bose, Mukherjee and Roy, settling one of the puzzles proposed by D. S. Johnson. The NP-completeness proof for permutation graphs presented in [12] is based on Adhikary et al.'s construction used to prove the NP-completeness on interval graphs. Among the problems selected by D. S. Johnson, maximum cut is the only one proven NP-complete for both interval graphs and permutation graphs. Despite that, the interval graph constructed by Adhikary et al. is not a permutation graph, and the constructed permutation graph in [12] is not an interval graph. Thus, a natural open question is the complexity of maximum cut on interval permutation graphs.

The class of  $C_4$ -free co-comparability graphs is precisely the class of interval graphs, and so interval permutation graphs are exactly the class of  $C_4$ -free permutation graphs. Hence a natural question is whether there is a construction that produces a permutation graph that is also  $C_4$ -free (and hence interval). The largest class in the intersection of permutation and interval graphs for which the complexity is known is the class of  $\{C_4, P_4\}$ -free graphs, known as trivially perfect graphs, a class of graphs properly containing the threshold graphs. Maximum cut is polynomial-time solvable on trivially perfect graphs thanks to the algorithm given for  $P_4$ -free graphs, known as cographs, a subclass of permutation graphs that is a superclass

of trivially perfect graphs graphs. Many flawed proofs of polynomiality for maximum cut on the restrictive class of unit interval graphs (or graphs with interval count 1) have been presented along the years, and the classification of the problem is still unknown [13].

#### Question 2. Is chromatic index polynomial for unit interval graphs?

The edge-colouring of a graph G assigns colours to its edges such that no two adjacent edges receive the same colour. The smallest integer k for which an edge-colouring with k colours exists is the chromatic index of G, denoted by  $\chi'(G)$ . Clearly,  $\chi'(G) \geq \Delta(G)$ , where  $\Delta(G)$  is the maximum degree of a vertex in G. Vizing's theorem asserts that every simple graph G has an edge-colouring with  $\Delta(G) + 1$  colours, so  $\chi'(G) = \Delta(G)$  or  $\Delta(G) + 1$ . If  $\chi'(G) = \Delta(G)$ , then G is said to be class 1; otherwise, G is class 2.

The total colouring of a graph G assigns colours to all its elements, vertices and edges, such that no two adjacent or incident elements receive the same colour. The smallest integer k for which a total colouring with k colours exists is the total chromatic number of G, denoted by  $\chi''(G)$ . Clearly,  $\chi''(G) \geq \Delta(G) + 1$ . The total colouring conjecture, posed sixty years ago independently by Behzad and Vizing, states that every simple graph G has a total colouring with  $\Delta(G) + 2$  colours. By the total colouring conjecture,  $\chi'(G) = \Delta(G) + 1$  or  $\Delta(G) + 2$ . If  $\chi''(G) = \Delta(G) + 1$ , then G is said to be type 1; otherwise, G is type 2. The total colouring conjecture has been verified in restricted cases, such as cubic graphs and graphs with maximum degree  $\Delta \leq 5$ , but the general problem has remained challengingly open. The total colouring conjecture has not been settled for regular graphs, for planar graphs, nor for chordal graphs.

Indifference graphs are graphs whose vertices can be linearly ordered so that the vertices contained in the same maximal clique are consecutive in this order. We call such an order an indifference order. Indifference graphs form an important subclass of interval graphs, since they correspond to unit interval graphs — interval graphs that can be represented by intervals of the same size, or equivalently to proper interval graphs — interval graphs that can be represented by intervals not contained in one another.

Despite the powerful restriction imposed by Vizing's theorem, it is very hard to compute the chromatic index in general. The set of graphs in class 1 is NP-complete, whereas class 2 is co-NP-complete. This holds for graph classes, such as comparability and so perfect graphs, and cubic graphs, but besides that very little is known about the complexity of computing the chromatic index. D. S. Johnson's table column for edge-colouring has 14 unresolved entries. Among them edge-colouring planar graphs was highlighted as a

may well be hard open problem. The other 13 unresolved entries, in 1985 classified as entertaining puzzles, consider edge-colouring for well studied classes of graphs such as chordal, split, cographs, interval and permutation. For permutation graphs, edge-colouring gives the only unresolved entry, after hamilton circuit for permutation graphs was classified as polynomial and maximum cut for permutation graphs as NP-complete.

A graph G on n vertices and m edges is said to be overfull if it satisfies  $\Delta(G) \lfloor n/2 \rfloor < m \leq \Delta(G)n/2$ . The more general condition to be subgraph-overfull requires G to have an overfull subgraph with the same maximum degree, can be tested in polynomial time, and ensures that G is class 2. Classes of graphs for which being class 2 is equivalent to being subgraph-overfull are: graphs with a universal vertex and so complete graphs, and split-indifference graphs. Split graphs and indifference graphs with  $\Delta(G)$  odd have  $\chi'(G) = \Delta(G)$ . Moreover, split graphs and indifference graphs are two classes of graphs for which the total colouring conjecture has been proved, and split graphs and indifference graphs with  $\Delta(G)$  even have  $\chi''(G) = \Delta(G) + 1$ . However, the edge-colouring problem and the total colouring problem for these two graph classes are still open. A general question, which we leave open, is to determine the largest graph class for which all of its graphs with odd maximum degree are class 1 and all of its graphs with even maximum degree are type 1.

**Question 3.** What are the complexities of Steiner tree and dominating set on directed path graphs?

Chordal graphs are defined as graphs having no chordless cycle of size bigger than three, and are also known as the intersection graphs admitting a tree model, that is, they are the vertex intersection graphs of subtrees of a characteristic tree. Interval graphs define a subclass of chordal graphs, being the intersection graphs of subpaths of a path. Undirected path graphs, directed path graphs and rooted directed path graphs are intermediate graph classes, defined, respectively, as the intersection graphs of paths of a tree, of directed paths of an oriented tree, and of directed paths of an out branching.

A set  $D \subseteq V(G)$  is dominating if, for every vertex  $v \in V(G), v \in D$  or v has a neighbor that belongs to D. Given a graph G and a positive integer k, the dominating set problem consists of deciding whether G has a dominating set of size at most k. Given a graph G, a subset  $X \subseteq V(G)$ , called terminal set, and a positive integer t, the Steiner tree problem consists of deciding whether there exists a subset  $S \subseteq V(G) \setminus X$  such that  $|S \cup X| \le t$  and  $G[S \cup X]$  is connected — and hence  $G[S \cup X]$  contains a tree subgraph T with  $X \subseteq V(T)$ , called a Steiner tree of G for X. In [11], we proved that

Steiner tree is NP-complete for undirected path graphs, which provides a full dichotomy Polynomial versus NP-complete for the Steiner tree column of D. S. Johnson's table. The proof is a non-trivial adaptation of the NPcompleteness proof for the dominating set restricted to undirected path graphs, presented 40 years before [34]. Recently, we have investigated Steiner tree and dominating set for path graphs [33], proposing to include a missing line in D. S. Johnson's table. According to Johnson's table, undirected path graphs can be modeled by a set of paths in a tree, and directed path graphs are undirected path graphs whose representation is such that for some root vertex in the tree, all paths are subpaths of paths from the root to a leaf. We refer to [35] for the variations called UV, DV and RDV of intersection graphs of a family of undirected or directed vertex paths in an undirected or in a directed tree. According to Johnson's table, the only separating problem for undirected path graphs and rooted directed path graphs was dominating set. The revised version of the table [11] for the 21st century adds two separating problems for these classes: Steiner tree and graph isomorphism. As for problems separating rooted directed path graphs from directed paths graphs, only graph isomorphism is known, which motivates the question.

#### **Question 4.** Is the perfect graph sandwich problem NP-complete?

An induced cycle  $C_k$  with  $k \geq 4$  vertices is called a *hole*; it is called an *odd hole* if k is odd, and an *even hole* if k is even. An *antihole* is the complement of a hole. It is an *odd antihole* if its complement is an odd hole, and an *even antihole* otherwise. Let  $\mathcal{C}$  be a set of graphs. We say that G is  $\mathcal{C}$ -free if no induced subgraph of G is isomorphic to a graph in  $\mathcal{C}$ .

A graph is *Berge* if it contains no odd hole and no odd antihole as an induced subgraph. The strong perfect graph theorem, first conjectured by Claude Berge in 1961, states that a graph is perfect if and only if it is Berge. It is known that Berge graphs can be recognized in polynomial time, resolving the famous open problem O! entry of D. S. Johnson's table. Research has focused on the sandwich problem for subclasses of perfect graphs, and for decompositions related to perfect graphs. The complexity of the perfect graph sandwich problem remains one of the most prominent open questions in this area since 1995.

In the not C-free sandwich problem, we are asking if there exists a sandwich graph in which there exists an induced subgraph isomorphic to a graph in C, whereas in the C-free sandwich problem, we are testing if there exists a sandwich graph G such that for every induced subgraph H of G, H is not in C. The latter problem has an additional alternation, which is an indication that the not C-free sandwich problem might always be easier than

the C-free sandwich problem. For instance, the imperfect graph sandwich problem is polynomial, whereas the complexity of the perfect graph sandwich problem has not been settled. This leads to the question: Is there a set C such that the C-free sandwich problem is P, but the not C-free sandwich problem is P-hard?

Clearly, if the recognition problem for C-free graphs is NP-hard, then the not C-free sandwich problem is NP-hard. This leads to the question: Is there a set C such that recognition of C-free graphs is in P, but the not C-free sandwich problem is NP-hard?

Recently [29], we have shown that the hardness reduction that proves that the  $C_5$ -free sandwich problem is NP-hard [20] actually proves that the odd-hole-free sandwich problem is NP-hard, and thus NP-complete. We were able to modify the hardness reduction that proves that the chordal sandwich problem is NP-hard [19] to prove that the even-hole-free sandwich problem is NP-hard, and thus NP-complete.

Almost monotone properties were introduced in [8], where the sandwich problem was proved to be in P in case the recognition problem was known to be in P. The properties of containing an odd hole and of containing an even hole were proved to be almost monotone. At that time, Berge graphs and even-hole-free graphs were known to be recognizable in polynomial time [30, 31], and the polynomial-time recognition of odd-hole-free graphs was established much later [32]. Together with [29], this implies that the two properties, being odd-hole-free and being even-hole-free, are not almost monotone.

Three path configurations, also known as Truemper configurations, have been studied in relation to perfect graphs, because the existence of these configurations ensures the existence of holes of a certain parity. A 3PC is a graph induced by three internally disjoint chordless paths  $P_1 = x_1, \dots, y_1$ ,  $P_2 = x_2, \ldots, y_2$  and  $P_3 = x_3, \ldots, y_3$  such that any two of them induce a hole. If  $x_1 = x_2 = x_3$  and  $y_1 = y_2 = y_3$ , we say that  $P_1 \cup P_2 \cup P_3$  induces a  $3PC(x_1,y_1)$ . If  $\{x_1,x_2,x_3\}$  and  $\{y_1,y_2,y_3\}$  induce triangles, then we say that  $P_1 \cup P_2 \cup P_3$  induces a  $3PC(x_1x_2x_3, y_1y_2y_3)$ . If  $\{x_1, x_2, x_3\}$  induces a triangle and  $y_1 = y_2 = y_3$ , we say that  $P_1 \cup P_2 \cup P_3$  induces a  $3PC(x_1x_2x_3, y_1)$ . We say that a graph G contains a  $3PC(\cdot,\cdot)$  if it contains a 3PC(x,y) for some  $x, y \in V(G)$ . Similarly we say that a graph G contains a  $3PC(\Delta, \Delta)$  (resp.  $3PC(\Delta, \cdot)$  if it contains a  $3PC(x_1x_2x_3, y_1y_2y_3)$  (resp.  $3PC(x_1x_2x_3, y_1)$ ) for some  $x_1, x_2, x_3, y_1, y_2, y_3 \in V(G)$  (resp.  $x_1, x_2, x_3, y \in V(G)$ ). Graphs  $3PC(\cdot,\cdot)$ ,  $3PC(\Delta,\Delta)$  and  $3PC(\Delta,\cdot)$  are also known as thetas, prisms and pyramids, respectively. If a graph contains a pyramid, then it contains an odd hole, whereas if a graph contains a prism or a theta, then it contains an

even hole.

Truemper configurations, such as prisms, thetas, and pyramids, were considered for the  $\mathcal{C}$ -free sandwich problem [20] and for the not  $\mathcal{C}$ -free sandwich problem [8]. The prism-free and not prism-free sandwich problems are NP-hard, because the recognition problem is NP-hard. However, the theta-free sandwich problem is NP-hard [20], but the not theta-free sandwich problem is in P [8]. The polynomial time algorithm to test if a graph is Berge presented in 2005 tests as first step for pyramids. The not pyramid-free sandwich problem is in P [8], but the complexity of the pyramid-free sandwich problem remains open.

Concluding remarks My students are my most frequent co-authors and they brought me subjects that I have explored with them through research that is registered in papers and books. When I wrote the preface for Jayme's book on the Computational Theory of Graphs [40], I acknowledged his courses, books and papers that have shaped the area of graph algorithms in Latin America. Jayme's course on Algorithms and Complexity has three parts: efficiency, inefficiency, and dealing with inefficiency. When I wrote with Manoel, Guilherme and Vinícius a book on Randomized Algorithms [36], we dedicated the book to Jayme, acknowledging the importance of having always teaching and research together.

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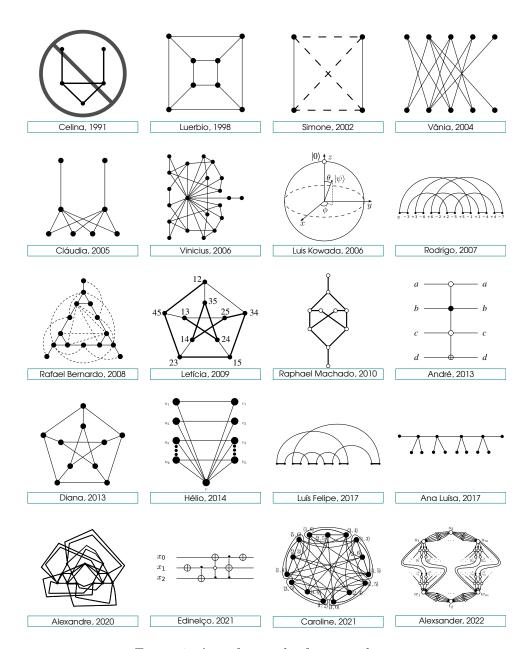


Figure 1: A perfect path of twenty theses