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Advanced Graph Theory and Combinatorics

Michel Rigo



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Foreword

The book content reflects the (good) taste of the author for solid mathematical concepts and results that have exciting practical applications. It is an excellent textbook that should appeal to students and instructors for its very clear presentation of both classical and more recent concepts in graph theory.

Vincent BLONDEL Professor of Applied Mathematics, University of Louvain September 2016

Introduction

This book is a result of lecture notes from a graph theory course taught at the University of Liège since 2005. Through the years, this course evolved and lectures were given at different levels ranging from second-year undergraduates in mathematics to students in computer science entering master's studies. It was therefore quite challenging to find a suitable title for this book.

Advanced or not so advanced material?

I hope that the reader will not feel cheated by the title (which is always tricky to choose). In some aspects, the material is rather elementary: we will start from scratch and present basic results on graphs such as connectedness or Eulerian graphs. In the second part of the book, we will analyze in great detail the strongly connected components of a digraph and make use of Perron–Frobenius theory and formal power series to estimate asymptotics on the number of walks of a given length between two vertices. Topics with an algebraic or a combinatorial flavor such as Ramsey numbers, introduction to Robertson–Seymour theorem or PageRank can be considered as more advanced.

In the history of mathematics, we often mention the *seven bridges of Königsberg problem* as the very first problem in graph theory. It was studied by the famous mathematician L. Euler in 1736. It took two centuries to develop and build a complete theory from a few scattered results. Probably the first book on graphs is *Theorie der endlichen und unendlichen Graphen* [KÖN 90] written by the Hungarian mathematician D. König in 1936, a student of J. Kürschák and H. Minkowski. In the middle of the 20th Century, graph theory matured into a well-defined branch of discrete mathematics and

combinatorics. We observe many mathematicians turning their attention to graph theory with books by C. Berge, N. Biggs, P. Erdős, C. Kuratowski, W. T. Tutte, K. Wagner, etc. We have seen an important growth during the past decades in combinatorics because of the particular interactions existing with optimization, randomized algorithms, dynamical programming, ergodic or number theory, theoretical computer science, computational geometry, molecular biology, etc. On MathSciNet, if you look for research papers with a Primary Mathematics Subject Classification equal to 05C (which stands for graph theory and is divided into 38 subfields ranging from planar graphs to connectivity, random walks or hypergraphs), then we find for the period 2011–2015 between 3, 300 and 3, 700 papers published every single year.

In less than a century, many scientists and entrepreneurs have seen the importance of graph theory in real-life applications. In a recent issue of Wired magazine (March 2014), we can read an article entitled *Is graph theory a key* to understanding big data? by R. Marsten. Let us quote his conclusion: "The data that we have today, and often the ways we look at data, are already steeped in the theory of graphs. In the future, our ability to understand data with graphs will take us beyond searching for an answer. Creating and analyzing graphs will bring us to answers automatically". Later, in the same magazine (May 2014), E. Eifrem wrote: "We're all well aware of how Facebook and Twitter have used the social graph to dominate their markets, and how Facebook and Google are now using their Graph Search and respectively, to gear up for the next wave of Knowledge Graph, hyper-accurate and hyper-personal recommendations, but graphs are becoming very widely deployed in a host of other industries".

This book reflects the tastes of the author but also includes some important applications such as Google's PageRank. It is only assumed that the reader has a working knowledge of linear algebra. Nevertheless, all the definitions and important results are given for the sake of completeness. The aim of the book is to provide the reader with the necessary theoretical background to tackle new problems or to easily understand new concepts in graph theory. Algorithms and complexity theory occupy a very small portion of the book (mostly in the first chapters).

This book, others and inspiration

Many other books on graphs do exist and the reader should not limit himself or herself to a single source. The Internet is also a formidable resource. Even if we have to be cautious when looking for information on the Web, Wikipedia contains a wealth of relevant information (but keep a critical eye). The present book starts with some unavoidable general material, then moves on to some particular topics with a combinatorial flavor. Powers of the adjacency matrix and Perron theory have a predominant role. The reader could probably start with this book and then move to [BRU 11] as a good companion to get a deeper knowledge of the links between linear algebra and graphs. See also [BAP 14] or the classical [GOD 01] in algebraic graph theory. Similarly, a comprehensive presentation of PageRank techniques can be found in [LAN 06]. The authors of that book, A. Langville and C. D. Meyer, also specialized in ranking techniques (see [LAN 12]). Another general reference discussing partially the same topics as here – and I do hope, with the same philosophy – is by R. Diestel where much more material and a particular emphasis on infinite graphs may be found. The present book is smaller and is thus well suited for readers who do not want to spend too much time on a specialized topic.

Having given a graph theory course for more than 10 years, I'm probably unconsciously tempted to take ownership of the proofs that I found somewhere else. It is no easy task to cite and give credits to all the sources that inspired me in this process. Let me mention [BIG 93] for algebraic aspects and chromatic polynomial, [TUT 01] for its first chapters and [ORE 90] for planar graphs and his proof of the 5-color theorem. I should also mention [BOL 98] (with an impressive collection of exercises) and [BER 89]. Finally, I remember that projects available on the Web and run by D. Arnold (College of Redwoods) were inspiring.

Practical organization

For a one-semester course, here is the time I usually devote to selected topics with 15 lectures of 90 min. Moreover, sessions for exercises take the same amount of time. The book contains extra material and more than 115 exercises:

- digraphs, paths, connected components (sections 1.1 and 1.2);
- Eulerian graphs, distance and shortest path (sections 1.3 and 1.5);
- introduction to Hamiltonicity, applications (sections 1.4 and 1.6);
- trees (section 4.1);
- homomorphisms, group of automorphisms (sections 7.1 and 7.2);
- Hamiltonian graphs (sections 3.1–3.4);
- topological sort (Chapter 4);

- adjacency matrix, counting walks (sections 8.2 and 8.3);
- primitivity, Perron's theorem and asymptotics (sections 9.1 and 9.4);
- irreducibility and asymptotics (sections 9.2 and 9.4);
- applications of Perron-Frobenius theory (section 9.3);
- Google's PageRank (Chapter 10);
- planar graphs and Euler's formula (sections 6.1–6.3);
- colorings, the five-color theorem (section 6.5);
- Ramsey numbers (section 7.4).

Definitions are emphasized and the most important ones are written in bold face, so that definitions of recurrent notions can be found more easily. Labels of bibliographic entries are based on the first three letters of the last name of the first author and then the year of publication. In the bibliography, entries are sorted in alphabetical order using these labels.

I address special thanks to Émilie Charlier, Aline Parreau and Manon Stipulanti for their great feedback leading to some major improvements in this book. Of course, Valérie Berthé always plays a special role. I am very pleased to blame her (indeed, this adventure produced some pressure from time to time) for what this project finally looks like. She is always supportive and enthusiastic. I also thanks several colleagues: Benoît Donnet, Eric Duchêne, Fabien Durand, Narad Rampersad, Eric Rowland and Élise Vandomme for the valuable time they spent reading drafts of parts of this book. I will not forget Laurent Waxweiler who gave and prepared the very first exercise classes for my course. I also thank my many students along the years. Their questions, queries and enthusiasm allowed me to improve, over the time, the overall presentation and sequencing of this book.

Michel RIGO September, 2016

A First Encounter with Graphs

1.1. A few definitions

There is not much fun in listing basic definitions about graphs (this is quite a bad introduction to start with!) but if we seek a rigorous presentation of results and proofs, then we cannot avoid giving accurate definitions of the objects that we will manipulate, but hopefully nice examples will also come quickly. In this book, we assume that the reader has a basic (or, at least a naive) knowledge of sets and operations on them.

As usual in mathematics, a pair (u,v) made up of two elements is implicitly assumed to be ordered: it has a first component u and a second component v. It has to be compared with a set with two elements u and v denoted by $\{u,v\}$. A set does not carry any ordering information about its elements. In particular, if $u \neq v$, then we can build two pairs but a single set: $(u,v) \neq (v,u)$ and $\{u,v\} = \{v,u\}$. If S is a finite set, we will write #S to denote the number of elements in S, i.e. the cardinality of S. We can also find the notation |S| but we will use it to denote lengths of paths.

1.1.1. Directed graphs

DEFINITION 1.1.— Let V be an arbitrary set. A directed graph, or **digraph**, is a pair G = (V, E) where E is a subset of the Cartesian product $V \times V$, i.e. E is a set of pairs of elements in V. The elements of V are the vertices of G—some authors also use the term nodes—and the elements of E are the edges,

also called oriented edges or arcs^1 , of G. An edge of the form (v,v) is a **loop** on v. Another way to express that E is a subset of $V \times V$ is to say that E is a binary relation over V. If either (u,v) or (v,u) belongs to E, the vertices u and v are adjacent. If neither (u,v) nor (v,u) belong to E, then u and v are independent. Given a digraph G, the set of vertices (respectively of edges) of G is denoted by V(G) (respectively E(G)).

The vast majority of the graphs that we will encounter are *finite* meaning that the set V of vertices is finite, and thus E contains at most $(\#V)^2$ edges.

REMARK 1.2.— It is common to speak of the order of G for #(V(G)) and the size of G for #(E(G)).

There are a few examples of infinite graphs in this book; see examples 1.47 and 4.11 (in formal language theory) and section 7.2 about colorings. Infinite graphs usually require more sophisticated arguments such as the axiom of choice. Implementation of infinite graphs in a computer could be tricky or impossible. From a practical point of view, particular instances of infinite graphs with a countable number of vertices and edges can be implemented. Think about a periodic graph that permits one to store only a finite amount of information to be repeated or a relation among vertices that can be computed and implemented as a function (see exercise 6 and example 1.5).

A digraph G=(V,E) is said to be **simple** if E is a subset of $(V\times V)\setminus\{(v,v)\mid v\in V\}$. In that case, the relation E is *irreflexive*. Otherwise stated, loops are not allowed.

The elements belonging to a set are pairwise distinct: there is no repeated element. What we need to define a directed multigraph, i.e. a digraph where multiple edges between two vertices are allowed, is to permit repetitions of an element belonging to a set. In set theory, we can introduce the notion of a *multiset*. First, we restrict ourselves to multisets with finite integer multiplicities. A **multiset** M is a pair (S,m) where S is a set, in the "classical" sense, and $m:S\to\mathbb{N}_{\geq 1}$ is a *multiplicity function* that specifies the number m(s) of occurrences of $s\in S$ in the multiset. As an example, the multiset denoted by $\{u,u,v,v,v,w\}$ is built from $S=\{u,v,w\}$ and

¹ If we really have to distinguish the directed graphs from the undirected graphs that we will soon introduce, then we could restrict the use of the word "edge" to the undirected case and use the word "arc" solely in the directed case. But usually the context permits one to avoid any misunderstanding.

m(u)=2, m(v)=3, m(w)=1. If the occurrences of an element have to be distinguished², we can index elements $s\in S$ by $s_1,\ldots,s_{m(s)}$. To continue the example, $\{u_1,u_2,v_1,v_2,v_3,w_1\}$ denotes the same multiset as above. If S is a finite set, then the cardinality of the multiset M=(S,m) with finite multiplicities is

$$\#M:=\sum_{s\in S}m(s).$$

Observe that a multiset (S, m) where m(s) = 1, for all $s \in S$, is simply a set. Equivalently, we could have defined the multiplicity function to map every element s of S to a finite subset of \mathbb{N} : the set of indices used for s.

Second, we could consider countable multiplicities³. In that case, an element of a multiset can be repeated infinitely many times and the multiplicity function maps every element to a subset of \mathbb{N} (which is the set of indices used for that element). As an example, a vertex u could be repeated infinitely many times with prime indices: $\{u_2, u_3, u_5, u_7, u_{11}, \ldots\}$. Thus, the multiplicity function maps u to the set of prime numbers.

We now introduce a **directed multigraph** as a pair G=(V,E) where V is a set of vertices and E is a multiset of edges built from a subset of $V\times V$. For a directed multigraph G=(V,E), the fact that V is finite does not imply that E is also finite. Indeed, we could have infinitely many edges between two vertices. Thus, a directed multigraph is *finite* if both the set V and the multiset E are finite.

REMARK 1.3.— It is common (and quite visual) to represent the vertices of a digraph by points in the plane (but we can also draw graphs on other surfaces like on a torus). Edges of the form (u, v) are represented by arrows going from u to v. We say that u (resp. v) is the **origin** (respectively, **destination**) of the edge. Actually any oriented arc of a curve can be used to join two vertices, not only straight vectors. Since positions of the vertices and arcs of curves joining the vertices can be freely chosen, there are usually infinitely many ways to represent a given graph. There is no reason that two edges that are intersecting in one representation are also intersecting in another representation of the same graph. We will rediscuss these notions with great care in section 6.1.

² For instance, to define a walk using different edges between two vertices.

³ Recall that a set is *countable* if it is in one-to-one correspondence with a subset of \mathbb{N} . Of course, from a mathematical point of view, further generalizations of multiplicity function and multisets can be considered; see section 1.7 for comments and pointers.

In Figure 1.1, we have depicted representations of a simple digraph, digraph and directed multigraph.

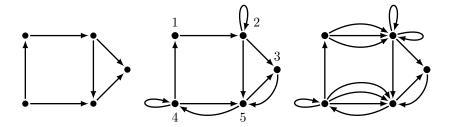


Figure 1.1. From left to right: a simple digraph, a digraph and a directed multigraph

A digraph G can be stored as an *adjacency list*: with each vertex u is associated the list of vertices v such that $(u,v) \in E(G)$. For the central digraph in Figure 1.1, the corresponding adjacency list is given in Table 1.1. A similar data structure can be used for directed multigraphs.

1	2		
2	2	3	5
3	5		
4	1	4	5
5	3	4	

Table 1.1. An adjacency list

EXAMPLE 1.4 (Tournament).— A simple digraph G = (V, E) where, for all pairs of distinct vertices u and v, either (u, v) or (v, u) belongs to E (but exactly one of these two edges belongs to E) is said to be a tournament. Indeed, it corresponds to an all-play-all tournament: each player plays against every other player and there are no ties. If u wins the confrontation against v, then we take the edge (v, u). See Figure 1.2.

EXAMPLE 1.5.— For an example of infinite simple digraph, take $\mathbb{N}_{>1}$ as set of vertices and a pair (m,n) of integers greater than 1 is an edge if and only if m divides n. The first few vertices and some edges of this digraph are depicted in Figure 1.3. Note that the relation E is transitive. If (m,n) and (n,p) belong to E, then (m,p) belongs to E.



Figure 1.2. A tournament among four players or teams

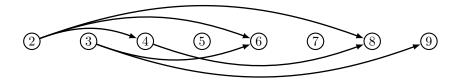


Figure 1.3. A divisibility relation (first few vertices only)

EXAMPLE 1.6.— We consider the digraph made up of Webpages and there is an edge from a page p to a page q if there is a link on p referencing q. This digraph is finite but contains several billions of vertices. Independently of the content of the pages, here we are interested in the links that one user can follow by browsing through pages. Based on Perron's theorem (theorem 9.2), we will discuss the basis of the Google's PageRank algorithm in Chapter 10.

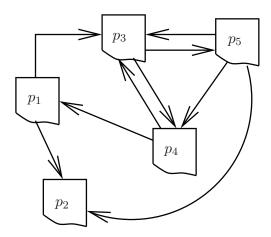


Figure 1.4. Some links and Webpages

Similarly to pages referencing other pages, we can also think about scientific papers that are citing other papers. In that case, we get a digraph where it is meaningful to try to identify relevant or influential papers. Which are the papers that are cited by many other papers, which are the "best" journals? The website http://www.eigenfactor.org/ uses a similar strategy to rank journals instead of Webpages [BER 07, WES 10].

EXAMPLE 1.7.— The digraph that we may associate with Twitter is another example about social networks. There is an edge from a user account u to a user account v, if u is following the tweets of v. Therefore, all the tweets posted by v are displayed in the follower's timeline. Such a digraph captures who is following who. For instance, see [YAM 10] for an example of a User–Tweet digraph.

REMARK 1.8.— The reader may wonder about this triple definition of digraphs: simple digraphs, digraphs and directed multigraphs. Why should we take into account the case of simple or multiple digraphs? The answer is a pragmatic one. We choose the model that best fits the situation that we are considering. If we are interested in finding a shortest path between two vertices, it is meaningless to consider loops or multiple edges; going through a loop just makes the path longer. We just want to know if the two vertices are connected or not. In such a case, we will deal with simple digraphs. On the other hand, assume that we have to model the fact that between two cities, there is a road, a river but also a railway. Here multigraphs are useful to take this fact into account. Note that simple digraphs are special cases of digraphs that are themselves special cases of directed multigraphs. We reach same conclusions when we have to choose between digraphs and the unoriented graphs that we will soon introduce to model a particular situation.

DEFINITION 1.9.— In a directed graph G = (V, E), we may associate two sets with every vertex v, respectively, the sets of outgoing edges and incoming edges:

$$\omega^+(v) := \{(v,w) \in E \mid w \in V\}, \quad \omega^-(v) := \{(u,v) \in E \mid u \in V\}.$$

These definitions are extended to directed multigraphs and in that case, the corresponding sets are multisets. If, for all vertices v, the multisets $\omega^+(v)$ and $\omega^-(v)$ are finite, then we say that G is of *finite degree*. The **successors** (respectively, **predecessors**) of a vertex v are the vertices w (respectively, w) such that v, w (respectively, v) belongs to v0 (respectively, v0). The set of successors (respectively, predecessors) of v1 is denoted by v1 (respectively, v2). Note that there is a loop on v3 if and only if

 $v \in \operatorname{succ}(v) \cap \operatorname{pred}(v)$. The **neighbors** of v are the vertices in $\operatorname{succ}(v) \cup \operatorname{pred}(v)$, they are the vertices adjacent to v. If there is no loop on v, then v is not a neighbor of itself. The set of neighbors of v, $\operatorname{N}(v) := \operatorname{succ}(v) \cup \operatorname{pred}(v)$, is sometimes called the *(open) neighborhood* of v. If v has to be included in the neighborhood, we speak of the *closed neighborhood* of v and is denoted by $\operatorname{N}[v]$.

In a directed multigraph of finite degree, the **indegree** of the vertex v is the number of incoming edges of v. It is denoted by $\deg^-(v) := \#\omega^-(v)$. The **outdegree** of the vertex v, denoted by $\deg^+(v) := \#\omega^+(v)$, is the number of outgoing edges of v. If $\deg^-(v) = 0$, v is a *source*. If $\deg^+(v) = 0$, v is a *sink*. If there exists k such that $\deg^+(v) = k$ for all vertices v, then the directed multigraph is said to be k-regular.

EXAMPLE 1.10.— In theoretical computer science, a (complete) deterministic finite automaton is a k-regular directed multigraph where k is the size of the alphabet. Automata are, for instance, useful when working with regular expression and searching a word in a text. An example is given in Figure 1.5 where the alphabet is $\{R, B\}$ and the directed multigraph is 2-regular. See, for instance, $[SUD\ 06]$ for a general reference.

With infinite digraphs having infinitely many edges, indegrees or outdegrees may be infinite. For instance, the outdegree (respectively, indegree) of every vertex in the digraph of example 1.5 is infinite (respectively, finite). Indeed, every positive integer n is a divisor of all numbers of the form kn but every integer m has a finite number of divisors. Sources in this simple digraph are exactly the prime numbers.

The following observation is a direct consequence of the fact that every edge (in particular, loop) has exactly one origin and one destination.

LEMMA 1.11 (Handshaking Formula).— Let G = (V, E) be a finite directed multigraph. We have

$$\sum_{v\in V} \operatorname{deg}^+(v) = \sum_{v\in V} \operatorname{deg}^-(v) = \#E.$$

DEFINITION 1.12 (Labeled Graphs).— We can add some relevant information on the edges or vertices of a digraph. Formally, edges can receive a label or a weight (the latter term usually refers to numerical assignments). If G=(V,E) is a directed multigraph, then we consider a map $\ell:E\to S$ where S is a set. For instance, S can be a finite set if we need to distinguish several types of edges (e.g. colors) or S could be equal to $\mathbb N$ or $\mathbb R$ if we need to add numerical

information (e.g. cost, capacity and distance). Similarly, we can define a map of domain V to add information about the vertices.

EXAMPLE 1.13.— Consider the 197 countries in the world and the flow of migrants moving from one country to another. So an edge from a country c to a country d will receive extra information to count the number of migrants from c to d during a given period. For instance, between 2005 and 2010, 1.8 million migrants moved from Mexico to the United States. Summing up the weights of the edges in-going to the United States give the total number of migrants entering the United States [ABE 14].

EXAMPLE 1.14.— On the Internet, Internet service providers represent their local network by a digraph where each edge is weighted by the capacity of the link.

EXAMPLE 1.15.— Consider the digraph depicted in Figure 1.5. Here, we have added labels B or R to edges corresponding to the two colors "Blue" or "Red". This is an example of a synchronized digraph: starting from any vertex, following a sequence of three consecutive edges of color blue, red and blue leads to vertex 1. This is a solution to the road coloring problem (See section 1.7).

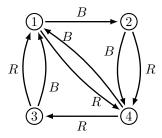


Figure 1.5. Adding labels to edges

DEFINITION 1.16.— Let G = (V, E) be a directed multigraph. Let W be a subset of V and F be a subset of $^4E \cap (W \times W)$. The directed multigraph

⁴ Here, the intersection of a multiset E and a set $W \times W$ has to be understood as follows: we keep the multiplicities carried by E but we restrict ourselves to edges with both endpoints in W. Now if we take a *subset* of $E \cap (W \times W)$, the multiplicity of an edge in this multiset is less than or equal to the corresponding multiplicity in E.

G'=(W,F) is a **subgraph** of G. We can also say that G is a supergraph of G'. A proper subgraph of G is a subgraph G' of G such that $G'\neq G$. The directed multigraph

$$(W, E \cap (W \times W))$$

is the subgraph of G induced by W. If e is an edge, G-e denotes the subgraph where e has been deleted. If v is a vertex, G-v denotes the subgraph of G induced by $V\setminus \{v\}$. These two operations can be extended to G-F and G-W where F is a multiset of edges and W is a set of vertices.

Now, we keep all the vertices of the original directed multigraph. A directed multigraph H = (W, F) is a **spanning subgraph** of G = (V, E) if W = V and $F \subseteq E$. We also say that H is a factor of G. Otherwise stated, we only remove some of the edges of G. We will reconsider this notion in definition 4.5 with spanning subtrees. If a directed multigraph has m edges, then it has 2^m spanning subgraphs.

1.1.2. Unoriented graphs

We now consider particular digraphs: the unoriented graphs.

DEFINITION 1.17.— A multigraph G=(V,E) is unoriented if, for every edge (u,v) belonging to E, the edge (v,u) belongs to E. Moreover, the edges (u,v) and (v,u) have the same multiplicities. Otherwise, stated E is symmetric. In that case, we allow ourselves to denote an edge between two distinct vertices by a set $\{u,v\}$, instead of taking the two pairs (u,v) and (v,u) into account. So the two oriented edges are identified⁵ with a single (unoriented) edge $\{u,v\}$. This is just an abuse of notation. We say that u and v are adjacent. Similarly a loop on u can be designated by the multiset $\{u,u\}$. By abuse of notation, we may write $\{u,v\} \in E$ or $\{u,u\} \in E$. In a representation of an unoriented graph, we use segments or arcs of curves without any orientation. We can define accordingly unoriented graphs where multiple edges are not allowed and simple unoriented graphs where also loops are not allowed.

REMARK 1.18.– Even though it may sound awkward, note that an unoriented multigraph is a special case of a directed multigraph where

⁵ When discussing walks it is important to note when there is an edge $\{u, v\}$, an agent can move from u to v and also from v to u. Thus in the unoriented case, we will not distinguish any orientation from u to v or from v to u.

orientation is neglected. Thus, definitions given for digraphs usually hold for unoriented graphs.

If not specified, the term *graph* (respectively, *multigraph*) is used only for unoriented graphs (respectively, multigraphs). From now on, we will use, respectively, the words graph and digraph to distinguish between the unoriented case and the general case.

EXAMPLE 1.19.— Again from the world of social networks, we can view Facebook as a graph where the vertices are the Facebook users and there is an edge between two users whenever they are friends. "Being friends" is a symmetric relation, so there is no need to consider an orientation.

EXAMPLE 1.20.— A map of Belgium with the main cities connected by highways is an example of a simple graph where the edges have weights (distances in kilometers). If there is a highway from a to b, there is always a highway from b to a. One representation of the graph is depicted in Figure 1.6.

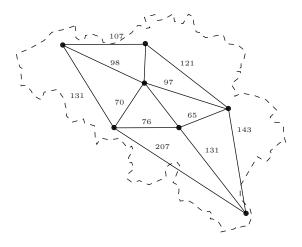


Figure 1.6. Brugge, Antwerp, Brussels, Mons, Namur, Liège, Arlon (from north to south and from west to east)

As a result of remark 1.18, the notions of degree, neighborhood or subgraph can be adapted to unoriented graphs. Let v be a vertex. We let

 $\omega(v):=\{\{v,w\}\in E\mid w\in V\}$ be the set of edges adjacent to v. For a multigraph, $\omega(v)$ is usually a multiset. If $\omega(v)$ is finite, the **degree** of v, denoted by $\deg(v)$, is equal to the number of edges of the form $\{v,w\}\in E$ with $v\neq w$ plus twice the number of loops on v. Therefore, for a finite multigraph the handshaking formula becomes

$$\sum_{v \in V} \deg(v) = 2 \# E. \tag{1.1}$$

We transpose the notion of k-regularity to undirected graphs. Let k be an integer. The multigraph G is k-regular, if every vertex has degree k. As an example, the complete graph K_n introduced below is an (n-1)-regular graph. Regularity provides structural information about the graph.

The notion of k-regular graphs will be encountered several times in this book: about their spectrum with Hoffman theorem and algebra of matrices in section 8.5 and proposition 9.8, with PageRank in section 10.2. Similarly, complete graphs will be encountered in section 6.5, about coloring of planar graphs and Kuratowski's theorem (see proposition 6.13) or about Ramsey numbers in section 7.5.

EXAMPLE 1.21.— The **complete graph** with n vertices is a simple graph where every edge between any two distinct vertices is present, i.e. every vertex is adjacent to all the other vertices. It is denoted by K_n . A clique in a graph G is a complete subgraph of G. The knowledge of the maximal cliques occurring in G provides structural information (for instance, think about a subgroup of people where everyone knows everyone else or a network where a region is densely connected) about G. Two examples are depicted in Figure 1.7.

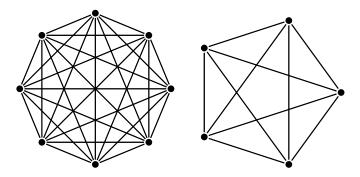


Figure 1.7. The complete graphs K_8 and K_5

REMARK 1.22.— Every simple graph with n vertices is a (spanning) subgraph of K_n .

There are several extra notions that we usually encounter in an unoriented context (of course, it would not be hard to adapt them in the general case of digraphs). Roughly speaking, a vertex cover is about a subset of vertices that meets every edge of the graph and a dominating set is a subset of vertices "close" to every vertex.

DEFINITION 1.23 (Covering and domination).— Let G be a graph. Let W be a subset of V(G). If, for every edge $e \in E(G)$, there exists a vertex $v \in W$ such that v is an endpoint of e, then W is a vertex cover of G. A minimum vertex cover is a vertex cover of G of minimal size. A vertex cover of the Petersen graph G is represented in Figure 1.8 (left). It is a minimum vertex cover (see section 1.8).

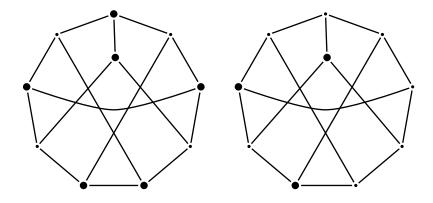


Figure 1.8. A vertex cover (left) and dominating set (right) of the Petersen graph represented by large vertices

With the same philosophy, a subset W of V(G) is a dominating set of G, if every vertex of V(G) is either in W or adjacent to a vertex in W, i.e. V(G) =

⁶ In a second reading, make also the connection with lemma 7.29.

⁷ The *Petersen graph* is recurrent in graph theory. It is common to find it as example or counterexample for many problems. Petersen built this graph as the smallest bridgeless 3-regular graph with no 3-edge-coloring [PET 98]. (These notions will be defined later on in this book).

 $(\bigcup_{w \in W} \mathsf{N}(w)) \cup W = \bigcup_{w \in W} \mathsf{N}[w]$ where we recall that $\mathsf{N}(w)$ (respectively, $\mathsf{N}[w]$) is the neighborhood of w (respectively, closed neighborhood of w). A dominating set of the Petersen graph is represented in Figure 1.8 (right). Note that this set of three vertices is not a vertex cover: at least five edges have no endpoints in this set.

DEFINITION 1.24.— A simple graph G=(V,E) is bipartite if there exists a partition of V into two subsets V_1 and V_2 in such a way that every edge in E is of the form $\{v_1,v_2\}$ with $v_1 \in V_1$ and $v_2 \in V_2$. The pair (V_1,V_2) is said to be a **bipartition** of G. The complete bipartite graph $K_{\ell,m}$ is a bipartite graph with $\ell+m$ vertices such that there is a bipartition (V_1,V_2) with $\#V_1=\ell$ and $\#V_2=m$ and for every $u\in V_1$ and every $v\in V_2$, the edge $\{u,v\}$ is present. A complete bipartite graph of the form $K_{1,m}$ is said to be a star.

This notion of partition can easily be generalized. Let $n \geq 2$. A simple graph G = (V, E) is n-partite if there exists a partition of V into n subsets V_1, \ldots, V_n in such a way that every edge in E is of the form $\{u, v\}$ with $u \in V_i$ and $v \in V_j$ for some i, j such that $i \neq j$. The complete n-partite graph K_{m_1, \ldots, m_n} has a set of vertices partitioned into n subsets V_1, \ldots, V_n in such a way that $\#V_i = m_i$; for all i, there is no edge between two vertices of the same subset V_i and for all vertices u in V_i and v in V_j , $i \neq j$, the edge $\{u, v\}$ is present.

Compared with Figure 1.9, the complete tripartite graph $K_{3,3,2}$ has 21 edges.

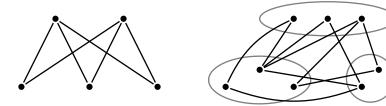


Figure 1.9. The complete bipartite graph $K_{2,3}$ and a 3-partite graph

Example 1.25.— Consider a graph where the vertices represent either workers, or tasks to be completed. So there is a natural partition of this set. There is an edge between a worker W_i and a task T_j if W_i has the skills to perform T_j . Usually the question is to assign tasks to workers in such a way that every task will be realized. In Figure 1.10, a spanning subgraph of the bipartite graph is represented with black edges.

For a modeling of the Internet topology by bipartite graphs, see [TAR 13].

EXAMPLE 1.26.— Another example of modeling is to consider patients needing kidney transplants and donors. With blood or tissue incompatibility, some matchings are impossible. A bipartite graph can model the possible compatible patient—donor pairs. We can consider a two-way kidney exchange that involves two patients, each of whom is incompatible with his/her own donor but compatible with the other donor (see, for instance⁸, [ROT 07]).

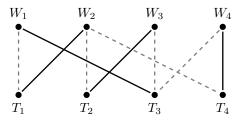


Figure 1.10. Workers and tasks, in black a spanning subgraph

1.2. Paths and connected components

Let us place an agent on a vertex of a graph. This agent is allowed to move from vertex to vertex along the edges of the graph. This leads to the notion of a walk. If the agent moves forever, even though the graph is finite, this will gives infinite paths (the same vertex can be visited several times). For a general presentation, we consider the directed case. We refer again to remark 1.18.

DEFINITION 1.27.— Let G=(V,E) be a directed multigraph. A walk in G is a finite or infinite sequence of edges $((v_{i,1},v_{i,2}))_i$ such that $v_{i,2}=v_{i+1,1}$ for all i. The length of a finite walk is the number of edges in the sequence. To a walk $((v_{i,1},v_{i,2}))_{i=1,\dots,n}$ of length n corresponds the sequence of the n+1 visited vertices $(v_{1,1},v_{2,1},\dots,v_{n,1},v_{n,2})=(v_{1,1},v_{1,2},v_{2,2},\dots,v_{n,2})$. This is a walk from (or joining) $v_{1,1}$ to $v_{n,2}$.

The walk is **closed** if $v_{1,1} = v_{n,2}$. A closed walk is defined up to a cyclic permutation of the edges in the sequence. In a digraph (where there are no multiple edges), a walk is completely determined by the sequence of visited vertices.

⁸ Alvin Elliot Roth won the Nobel prize in economic sciences in 2012.

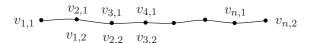


Figure 1.11. A walk

A trail is a walk where all the edges occurring in the sequence are pairwise distinct. Finally, a path (some authors use the term simple path to emphasize the special case) is a walk where all the visited vertices (except maybe the first one and the last one when defining a closed path) are pairwise distinct. This implies that every path is a trail. A closed path is usually called a cycle. A graph without cycle is said to be acyclic.

For the digraph in Figure 1.12, (e_1,e_4,e_5,e_4,e_6) is a walk joining 1 to 5; (e_1,e_4,e_5,e_2,e_3) is a closed trail (no repeated edges but the vertex 2 is visited twice); (e_1,e_4,e_6,e_7) is a path joining 1 to 6. There are exactly three cycles: (e_1,e_2,e_3) , (e_4,e_5) and (e_6,e_7,e_8) and three closed trails which are not cycles: (e_1,e_4,e_5,e_2,e_3) , (e_4,e_6,e_7,e_8,e_5) and $(e_1,e_4,e_6,e_7,e_8,e_5,e_2,e_3)$. For the simple graph on the right, $(f_1,f_4,f_5,f_6,f_7,f_4,f_2)$ is a walk joining a and c.

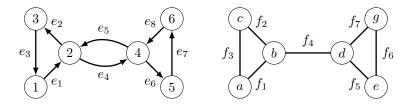


Figure 1.12. A simple digraph and a simple graph

Here is a major difference with the oriented case: There is no trail joining a to c and passing through d because, for any such walk, the (unoriented) edge f_4 must be repeated. In particular, in an unoriented graph, there is no cycle of length exactly 2. To have a such a cycle, we need two edges between two given vertices, i.e. a multigraph. Thus, there are exactly two cycles: (f_1, f_2, f_3) and (f_5, f_6, f_7) .

EXAMPLE 1.28 (Collaboration Graphs).— In science, a majority of published research papers are coauthored by several researchers. We may build a graph where the vertices are the scientists and two scientists are connected if they share a publication. For instance, the so-called Erdős number of a mathematician M is the distance in this graph, i.e. the length of the shortest path (assuming that it exists), between M and the famous Hungarian mathematician Paul Erdős⁹. See the paper [ODD 79] written by R. Graham (using a pseudonym) or [EAS 10, p. 34]. It seems that every living mathematician has a quite small Erdős number (less than seven). This is not a theorem, it just reflects the fact that the community of researchers is quite dense. This "fact" is known as the small world phenomenon. See the comments in section 1.7.

If you are a tennis player, you can try to compute your own Federer number: players who played once (winning or losing) an official game against Roger Federer have a Federer number equal to 1, players who played against a player with a Federer number 1 but who never played against Federer himself, have a number equal to 2 and so on.

EXAMPLE 1.29.— On various operating systems, you can find the tool traceroute that reveals the presence of intermediate-level equipment (routers) on the route (or path) of packets of data taken from an IP network on their way to a given host on the Internet.

1.2.1. Connected components

Let G=(V,E) be a directed multigraph. Let u,v be two vertices. We say that u is connected to v and we write $u \to v$, if there exists a walk from u to v. In particular, we assume that every vertex u is connected to itself (with a length-0 walk). If u is connected to v, we let d(u,v) denote the minimal length of a walk from u to v. Note that there is always a path achieving d(u,v). A strongly connected component (SCC) is a maximal subset C of V such that for all $u,v\in C$, $u\to v$ (in particular, we also have $v\to u$). The term "strongly" reflects the fact that orientation is taken into account. If V(G) is an SCC, then G is said to be (strongly) connected.

⁹ Paul Erdős (1913–1996) has had more than 500 collaborators, he worked in several fields ranging from combinatorics and graph theory to number theory, analysis and probability. For instance, see [HOF 99] for an account about this colorful mathematician.

An SCC is *trivial* if it is restricted to a single vertex with no loop. In every non-trivial SCC, there exists a closed walk visiting all the vertices of the component. We write $u \leftrightarrow v$ if and only if $u \to v$ and $v \to u$. Since every vertex is connected to itself, we have $u \leftrightarrow u$ for all vertices u. Note that \leftrightarrow defines an equivalence relation over V(G) and the corresponding equivalence classes are exactly the SCCs of G.

Since (unoriented) multigraphs are special cases of directed multigraphs (see remark 1.18), we have thus defined connected vertices and connected components in a multigraph.

A directed multigraph G=(V,E) is *weakly connected* if the unoriented graph obtained by taking the symmetric closure of E is connected. That is to say, if one disregards the orientation of the oriented edges, then the graph is connected.

EXAMPLE 1.30.— The digraph depicted in Figure 1.13 is not strongly connected but weakly connected. We have $1 \rightarrow 9$ but $9 \not\rightarrow 1$ or simply, $2 \rightarrow 5$ but $5 \not\rightarrow 2$. It has four SCCs: $\{1, 2, 3, 4\}, \{5\}, \{6, 7\}$ and $\{8, 9\}$.

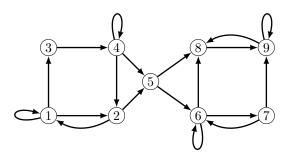


Figure 1.13. A digraph and its four SCCs

REMARK 1.31 (Distance).— The fact that u is connected to v does not imply, in a digraph, that v is also connected to u. The relation "being connected" over V is not necessarily symmetric. But for an unoriented multigraph G, since E(G) is symmetric, so is the relation "being connected". In that case, the relations \rightarrow and \leftrightarrow coincide and the map d restricted to a connected

component is a distance 10 . Note that we usually still refer to the term distance in a strongly connected digraph even if the map d is not symmetric. In Figure 1.13, we have d(1,3) = 1 but d(3,1) = 3.

The procedure given in Table 1.2 allows us to compute the reflexive and transitive closure of $\mathrm{succ}(v)$, i.e. the set $\mathrm{succ}^*(v) := \{u \in V \mid v \to u\}$. Note that since $v \to v$, v belongs to $\mathrm{succ}^*(v)$. In the following algorithm, the data are a finite digraph G = (V, E) and a vertex $v \in V$, the output is the set $\mathrm{succ}^*(v)$. The idea is to let the set Component grow by adding elements in $\mathrm{succ}(u)$ for the vertices u that have been recently added to Component and stored in New. When no new vertices are added, the procedure stops.

```
TRANSITIVECLOSURESUCC(G, v)
    Component \leftarrow \{v\};
2
    New \leftarrow \{v\};
   while New \neq \emptyset,
3
4
         do Neighbors \leftarrow \emptyset;
5
             for all u \in New,
                  do Neighbors \leftarrow Neighbors \cup succ(u);
6
7
             New \leftarrow Neighbors \setminus Component;
8
             Component \leftarrow Component \cup New;
9
   return Component;
```

Table 1.2. Algorithm to compute $succ^*(v)$

Similarly, we compute $\operatorname{pred}^*(v) := \{u \in V \mid u \to v\}$. The SCC¹¹ of u is simply $\operatorname{succ}^*(u) \cap \operatorname{pred}^*(u)$. The procedure can be adapted to detect connected components of an unoriented graph. In particular, a graph is connected if and only if V = Component. Also see the Roy–Warshall algorithm in section 1.8.

1.2.2. Stronger notions of connectivity

To conclude this section, we mention stronger notions related to connectedness. All notions and results are stated in an unoriented setting.

¹⁰ In the mathematical sense, $\forall u, v, \, \mathsf{d}(u, v) \geq 0$ and $\mathsf{d}(u, v) = 0$ if and only if $u = v, \, \mathsf{d}(u, v) = \mathsf{d}(v, u)$ and d satisfies the triangular inequality: $\forall u, v, w, \, \mathsf{d}(u, v) \leq \mathsf{d}(u, w) + \mathsf{d}(w, v)$.

¹¹ For more insight, consider Tarjan's SCCs algorithm [TAR 72].

DEFINITION 1.32.— In a multigraph, a **bridge** (also called isthmus or cut-edge) is an edge whose removal increases the number of connected components in the graph. In particular, if G is a connected multigraph, a bridge is an edge e such that G-e is not connected. Observe that in that case, G-e has exactly two connected components. Since E is connected, every vertex in G-e is connected to an endpoint of e.

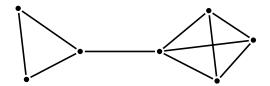


Figure 1.14. A graph with a single bridge

Clearly, an edge is a bridge if and only if it does not belong to any cycle. Equivalently, e is a bridge if and only if there exist two connected vertices u and v such that all paths joining u and v go through e. As an example, the edge f_4 in Figure 1.12 is a bridge. In a directed multigraph, a $strong\ bridge$ is an edge such that removing that edge increases the number of SCC in the digraph.

THEOREM 1.33 (Robbin's theorem — strong orientation).— Let G be a simple graph. There exists an orientation for every edge, turning it into a strongly connected digraph, if and only if G is connected and has no bridge.

The proof is left as an exercise: it is clear that if G has a bridge, then no orientation may exist. Notice that this result is still valid for a multigraph. Indeed, if there are at least two edges between two vertices u and v, locally the task is easy: one simply takes the two orientations (u,v) and (v,u) (see [ROB 39]).

The notion of a bridge extends to a *cut-set*.

DEFINITION 1.34 (Cut-set).— Let G be a multigraph. A subset F of E(G) is a cut-set if G-F has more connected components than G. In particular, when G is a connected multigraph, a set F such that G-F is disconnected is a cut-set.

DEFINITION 1.35.— Let us introduce a quantity $\lambda(G)$ (some authors use $\kappa'(G)$). If G is a disconnected multigraph, we set $\lambda(G)=0$. If G is a

connected multigraph, $\lambda(G)$ is defined as the cardinality of a cut-set of minimal size. Let $k \geq 1$. We say that a multigraph G is k-edge connected when

$$\lambda(G) \geq k$$
.

This means that G is connected and removing any subset of at most k-1 edges leaves the graph connected. Note that if $\lambda(G)=k$, then removing k well-chosen edges leads to a disconnected graph (with exactly two connected components).

For instance, $\lambda(K_n) = n - 1$ and a connected graph with no bridge is 2-edge connected: we have to delete at least two edges to disconnect the graph. See, for instance, the graph depicted in Figure 5.1.

Dual notions (edges versus vertices) can be defined when removing some vertices of the graph (and, of course, the edges adjacent to them).

DEFINITION 1.36.— A cut-vertex is a vertex such that its removal increases the number of connected components in the multigraph. A subset W of V(G) is a separating set if G-W has more connected components than G. In particular, if G is connected, a vertex v (respectively, a set W) such that G-v (respectively, G-W) is disconnected, is a cut-vertex (respectively, a separating set).

REMARK 1.37.— When removing a bridge, the number of connected components increases by 1. The situation is quite different when removing a cut-vertex. Removing the central vertex in Figure 1.15 leads to three connected components.

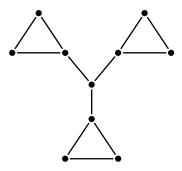


Figure 1.15. A cut-vertex

Every connected non-complete multigraph has a separating set. It is thus legitimate to introduce the next notion.

DEFINITION 1.38 (Vertex Connectivity).— Let G be a multigraph. We define a quantity $\kappa(G)$ as follows. We set $\kappa(G)=0$ whenever G is disconnected. For a complete graph K_n , we set $\kappa(K_n)=n-1$ because it cannot be disconnected when removing vertices. In all other cases, G is a connected and non-complete graph, $\kappa(G)$ is the cardinality of a separating set of minimal size.

Let $k \geq 1$. We say that a multigraph G is k-connected (more precisely, k-vertex connected) if

$$\kappa(G) \geq k$$
.

This means that G is connected and removing any subset of at most k-1 vertices leaves the graph connected C. The least integer k such that G is k-connected is the vertex connectivity of G. If $\kappa(G)=k$, then removing k well-chosen vertices leads to a disconnected graph or to a trivial graph reduced to a single vertex.

For instance, every cycle of length at least 3 is 2-connected. The next result gives an interpretation of the vertex-connectivity.

THEOREM 1.39 (Menger's theorem).— Let G = (V, E) be a finite graph. Let u, v be two non-adjacent vertices. Let $k \geq 0$ be the smallest integer such that there exists $W \subset V$ with #W = k and $u \not\leftrightarrow v$ in the subgraph G - W. The maximal number of vertex-independent paths joining u and v, i.e. any two such paths have no common vertex except for u and v, is equal to k.

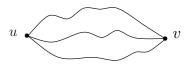


Figure 1.16. Three vertex-independent paths

A proof can be found in [DIR 66]. For extension to infinite graphs, see [HAL 74]. There is also an analogous version of this result in terms of edge connectivity and edge-independent paths.

¹² It could be left with a single vertex but recall that a trivial graph reduced to a vertex is connected.

COROLLARY 1.40.— Let $k \ge 2$. A graph is k-connected if and only if every pair of distinct vertices is connected by at least k vertex-independent paths.

To conclude this section, we mention the following result.

THEOREM 1.41 (Whitney [WHI 32]).— For every graph, we have

$$\kappa(G) \le \lambda(G) \le \min_{v \in V(G)} \deg(v).$$

PROOF.— The right inequality is clear: if we remove all the edges adjacent to a vertex of minimal degree, then this vertex will be disconnected from the other vertices.

If $\lambda(G) \leq 1$, then $\kappa(G) = \lambda(G)$. Now assume that $\lambda(G) = k \geq 2$. There exist k edges $\{u_1, v_1\}, \ldots, \{u_k, v_k\}$ whose removal leads to a disconnect graph with a partition of the vertices into two sets V_1 and V_2 corresponding to the two connected components of the resulting graph I^3 . Note that the u_i 's and v_i 's are not necessarily different. We may assume that the u_i 's belong to V_1 and the v_i 's to V_2 . If there exists $w \in V_1 \setminus \{u_1, \ldots, u_k\}$, then removing u_1, \ldots, u_k will disconnect w from the vertices in V_2 . So we remove at most (some of the u_i 's could be identical) k vertices to disconnect G. The other case is when $V_1 = \{u_1, \ldots, u_k\}$. The argument is that u_1 has at most k neighbors, i.e. $\deg(u_1) \leq k$. Indeed, u_1 has at most $(\#V_1) - 1$ neighbors in V_1 and at most $k - ((\#V_1) - 1)$ in V_2 because we know that there are exactly k edges between V_1 and V_2 and every vertex in V_1 is the endpoint of at least one such edge. Since $\lambda(G) = k$ and from the right inequality of the statement, we deduce that $\deg(u_1) \geq k$. Hence, $\deg(u_1) = k$. Thus, we may remove the k neighbors of u_1 to disconnect the graph, meaning that $\kappa(G) \leq k$.

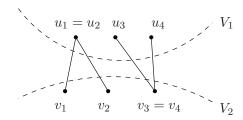


Figure 1.17. Illustration of Whitney's theorem

¹³ Removing $\{u_1, v_1\}, \dots, \{u_{k-1}, v_{k-1}\}$ leaves the graph connected and $\{u_k, v_k\}$ becomes a bridge whose removal gives two connected components.

1.3. Eulerian graphs

In a directed multigraph, an **Eulerian trail** is a trail visiting all the edges, i.e. a walk going exactly once through all edges.

A directed multigraph is **Eulerian** if it has a closed Eulerian trail, i.e. a walk starting and ending in the same vertex and going exactly once through all edges. Such a closed Eulerian trail is usually said to be an *Eulerian circuit*. The fact that a digraph is or is not Eulerian is easy to check and the constructive proof below gives an algorithm for finding an Eulerian circuit.

LEMMA 1.42.— A weakly connected (finite) directed multigraph G = (V, E) is Eulerian if and only if, for all vertices $v \in V$, $\deg^-(v) = \deg^+(v)$.

PROOF.—The proof is elementary, but it provides an algorithm to get a Eulerian circuit. Start from any vertex v_0 . Choose an edge starting in this vertex. Repeat the procedure from the reached vertex: choose an edge among the edges that are still available (i.e. not yet chosen during a previous step). Since the graph is finite and since, for all vertices $v \in V$, $\deg^-(v) = \deg^+(v)$, after a finite number of choices, we are back to v_0 . If the set of edges that have been already chosen is equal to E, we have obtained an Eulerian circuit. Otherwise, we extend the closed trail as follows. Pick in that trail a vertex v_1 such that there exists an edge with origin v_1 among the set of unchosen edges (such an edge exists because the graph is connected). Repeat the procedure from v_1 and get a new closed trail going through v_1 and merge in an appropriate way this closed trail with the first one to get a longer closed trail: start the trail from v_0 , when reaching v_1 complete the second closed trail coming back to v_1 , then finish the initial trail leading back to v_0 . Repeat the procedure if there are edges left. The algorithm terminates because of the finiteness of the graph.

COROLLARY 1.43.— A weakly connected (finite) directed multigraph G = (V, E) has a Eulerian trail from u to v if and only if, $\deg^-(u) + 1 = \deg^+(u)$, $\deg^-(v) = \deg^+(v) + 1$ and, for all vertices $w \in V \setminus \{u, v\}$, $\deg^-(w) = \deg^+(w)$.

PROOF.— If we add an edge (v,u) to the directed multigraph, then we are back to the previous lemma.

We can directly reformulate the result in the unoriented case.

COROLLARY 1.44.— A connected (finite) multigraph G = (V, E) is Eulerian if and only if all vertices have even degree. A connected (finite) multigraph

G = (V, E) has an Eulerian trail from u to v if and only if u and v are of odd degree and all other vertices have even degree.

This result gives the solution to the historical problem solved by Euler about the seven bridges of Königsberg: seven bridges were situated across the Pregolya River and the people living in Königsberg (now Kaliningrad) wanted to go for a walk on these bridges; however, their stroll should not use the same bridge twice. In other words, they were looking for what we call a Eulerian circuit. They were unsuccessful but Euler showed that, indeed, there is no such circuit (see Figure 1.18).

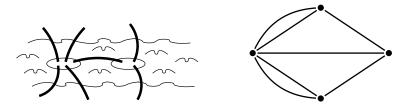


Figure 1.18. The seven bridges, the borders of the river and two isles are represented by the four vertices

Fleury's algorithm given in Table 1.3 connects two notions encountered so far: Eulerian graphs and bridges. But it has a drawback. To implement this method, we have to detect bridges efficiently 14 . Graph traversal and the detection of bridges leads to an algorithm whose running time is quadratic in #E. The idea is to postpone the crossing of a bridge as much as possible. Indeed, when we cross a bridge, there is no way to go back to the component we were in without taking it a second time, which is not permitted. Thus that component must have been completely visited first (see the comments in section 1.7). Recall that $\omega(v)$ is the set of edges adjacent to v. Note in line 6 that the graph is updated. So we are looking for bridges in the subgraph restricted unvisited edges.

The output of Fleury's algorithm is a sequence of edges. Either the length of this sequence is equal to #E and we have found a Eulerian circuit or a Eulerian trail, or if we have less than #E edges in the sequence, then the graph is not Eulerian. To find an algorithm with a better performance, search for Hierholzer's algorithm on the web. Applying Fleury's algorithm to the graph

¹⁴ For instance, see Tarjan's Bridge-finding algorithm [TAR 74].

depicted in Figure 1.19, one possible output is represented (the edges have been ordered with respect to the output sequence of the algorithm). Note that after selecting the first three edges, the edge numbered 8 is a bridge of the remaining graph. Thus, we cannot choose that one at this step of the algorithm. Nevertheless, we could have chosen either edge 4 or edge 7 to pursue. The proof of the exactness of Fleury's algorithm is left as an exercise.

```
FLEURY(G, v_0) where G = (V, E) is a multigraph and v_0 \in V
1
    i \leftarrow 1;
2
    repeat
3
              if \omega(v_{i-1}) contains an edge that is not a bridge
                then pick such an edge e_i = \{v_{i-1}, v_i\} \in E;
4
5
                else pick a bridge e_i = \{v_{i-1}, v_i\} \in E;
              G \leftarrow G - e_i; i \leftarrow i + 1;
6
7
       until i > \#E
8
    return (e_1, e_2, ...);
```

Table 1.3. Fleury's algorithm [FLE 83]

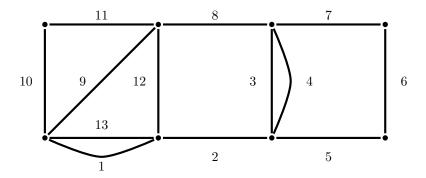


Figure 1.19. An application of Fleury's algorithm (starting with lower-left vertex)

1.4. Defining Hamiltonian graphs

A notion dual to Eulerian graphs (vertices versus edges) is the following one. In a digraph, a path is *Hamiltonian* if it visits all the vertices. In

Figure 1.13, the path visiting the vertices 2, 1, 3, 4, 5, 6, 7, 9, 8 is the unique Hamiltonian path for this graph.

As in the Eulerian case where we have first defined an Eulerian trail, then a Eulerian graph, a digraph is **Hamiltonian** if there exists a cycle starting and ending in the same vertex and going exactly once through all the vertices. This cycle is a *Hamiltonian circuit*. If we can answer the question of whether or not a digraph is Hamiltonian, then we can also trivially answer the question if we allow multiple edges. So we can consider simple digraphs. Analogous definitions can be given in the unoriented case.

Example 1.45.— A trivial example is given by K_n , $n \geq 3$, where every permutation of the n vertices gives a Hamiltonian circuit. Hence, K_n has n! distinct Hamiltonian circuits. Another example is depicted in Figure 1.20 where we have to find a circuit for a Knight on a chessboard in such a way that every square is visited once. So here, we have an underlying graph with 64 vertices and there is an edge between two vertices if there is a legal Knight's move between these two squares.

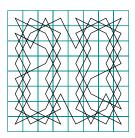


Figure 1.20. A Knight's tour on a chessboard

It turns out that finding a Hamiltonian circuit seems to be much more difficult than the Eulerian counterpart (lemma 1.42 and corollary 1.44). Indeed, deciding (using a generic algorithm) whether or not a graph is Hamiltonian is well known to be an NP-complete problem [GAR 79]. In Chapter 2, we make precise the latter notion. Chapter 3 will present necessary or sufficient conditions for a graph to be Hamiltonian.

1.5. Distance and shortest path

In this section, in great detail we present Dijkstra's algorithm computing one shortest path 15 from a vertex v_1 (single source) to every other vertex in the graph. We will consider simple weighted digraphs. Indeed, if several edges are connecting two vertices, we can simply consider the one of smallest weight. We can also disregard loops that will increase the total weight. Note that the ideas developed for Dijkstra's algorithm are similar to those found in Prim's algorithm for minimum spanning trees (see remark 4.8).

Let G=(V,E) be a simple (finite) digraph and $\mathbf{w}:E\to\mathbb{R}_{\geq 0}$ be a weight function. If there is no weight function attached to G, we may assume that every edge has a weight equal to one (thus we will count the length of the corresponding walk and this notion is compatible with the distance discussed in remark 1.31). If (e_1,\ldots,e_k) is a walk joining u and v, then the weight of this walk is

$$\sum_{j=1}^k \mathsf{w}(e_j) \, .$$

If we are interested in walks of minimal weight, we can restrict ourselves to paths from u to v. We also extend w to $V \times V$ with values in $\mathbb{R}_{\geq 0} \cup \{+\infty\}$ by setting $\mathrm{w}(u,v) = +\infty$ when $(u,v) \not\in E$. As usual, $r+\infty = +\infty$ for all real numbers r. If ℓ is a list and x is an element, $\mathrm{concat}(\ell,x)$ is the list obtained by appending x to ℓ .

A set X is initialized with $\{v_1\}$ and the idea is roughly to let this set grow until it is equal to V. At each step, one vertex is added to X. We choose the "best" candidate (see line 8). Then, we decide if we gain something for the remaining vertices using this new vertex (lines 10–13). It is remarkable that local decisions lead to a global solution.

Example 1.46.— To grasp the idea behind Dijkstra's algorithm given in Table 1.4, we first run it on a small example. Consider the weighted graph depicted in Figure 1.21. The first row in Table 1.5 corresponds to the initialization of the variables in lines 1–6 of the algorithm. For every vertex u, the variable T(u) stores the value of the smallest path found so far and C(u) is a sequence of vertices starting with v_1 realizing such a path from v_1 to v. In

¹⁵ We write "one" shortest path and not "the" shortest path because several paths with minimal weight may exist.

line 8, we choose a vertex v having a minimal T value among the unchosen vertices. Then in lines 10–13, we update the variable T and C for the remaining unchosen vertices by determining if there is a benefit (line 11) using the vertex v.

```
DIJKSTRA(G, w, v_1) where G = (V, E) is a simple digraph, w a weight function and v_1 \in V
```

```
1
      for all v \in V \setminus \{v_1\},
 2
             do T(v) \leftarrow \mathsf{w}(v_1, v);
 3
                  if T(v) \neq +\infty
 4
                     then C(v) \leftarrow (v_1, v)
 5
                     else C(v) \leftarrow ();
 6
      X \leftarrow \{v_1\};
 7
      while X \neq V
 8
             do pick v \in V \setminus X s.t. \forall y \in V \setminus X, T(v) \leq T(y);
 9
                  X \leftarrow X \cup \{v\};
10
                  for all y \in V \setminus X,
                       do if T(y) > T(v) + w(v, y)
11
12
                               then T(y) \leftarrow T(v) + w(v, y);
13
                                       C(y) \leftarrow \mathtt{concat}(C(v), y);
```

Table 1.4. Dijkstra's algorithm

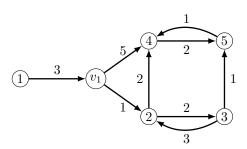


Figure 1.21. A weighted (simple) digraph

We now give a proof of the exactness of the algorithm. It is clear that the algorithm terminates when starting with a finite graph: on line 5, we consider each time a new vertex and the algorithm stops when all the vertices have been considered. We essentially follow the lines of [GIB 85] for the proof.

nth		T(1)	T(2)	T(3)	T(4)	T(5)
iteration	X	C(1)	C(2)	C(3)	C(4)	C(5)
1	$\{v_1\}$	$+\infty$	1	$+\infty$	5	$+\infty$
		()	$(v_1, 2)$	()	$(v_1, 4)$	()
2	$\{v_1, 2\}$	$+\infty$	1	3	3	$+\infty$
		()	$(v_1, 2)$	$(v_1, 2, 3)$	$(v_1, 2, 4)$	()
3	$\{v_1, 2, 4\}$	$+\infty$	1	3	3	5
		()	$(v_1, 2)$	$(v_1, 2, 3)$	$(v_1, 2, 4)$	$(v_1, 2, 4, 5)$
4	$\{v_1, 2, 4, 3\}$	$+\infty$	1	3	3	4
		()	$(v_1, 2)$	$(v_1, 2, 3)$	$(v_1, 2, 4)$	$(v_1, 2, 3, 5)$
5	$\{v_1, 2, 4, 3, 5\}$	$+\infty$	1	3	3	4
		()	$(v_1, 2)$	$(v_1, 2, 3)$	$(v_1, 2, 4)$	$(v_1, 2, 3, 5)$
6	$\{v_1, 2, 4, 3, 5, 1\}$	$+\infty$	1	3	3	4
		()	$(v_1, 2)$	$(v_1, 2, 3)$	$(v_1, 2, 4)$	$(v_1, 2, 3, 5)$

Table 1.5. In bold face is indicated the choice made at line 8

PROOF.— Since the variables X and T(y) are evolving during the execution of the algorithm, we let X_n (respectively, $T_n(y)$) denote the set X (respectively, the value T(y)) during the nth iteration. In particular, $X_1 = \{v_1\}$ and $\#X_n = n$ for all $n \leq \#V$. We let v_{n+1} denote the unique vertex in $X_{n+1} \setminus X_n$ selected at line 8. From lines 11–12, observe that either there is no update or there is an update of T(y) and it is replaced by a smaller value. Thus, for all n and all vertices y,

$$T_{n+1}(y) \le T_n(y).$$
 [1.2]

We will show by induction on n that

- i) for all $v \in X_n \setminus \{v_1\}$, $T_n(v)$ is the smallest weight of *all* the paths joining v_1 to v;
- ii) for all $v \in V \setminus X_n$, $T_n(v)$ is the smallest weight of the paths joining v_1 to v and visiting only vertices in X_n before reaching v.

Hence, we will get the expected result when n=#V. We do not take into account the variables C(y) that are simply used to store a path achieving the smallest weight given by T(y).

When n=1, then (i) and (ii) hold from lines 1–5. Assume that (i) and (ii) hold for $1 \le n < \#V$. We will show that (i) and (ii) hold for $X_{n+1} = X_n \cup \{v_{n+1}\}$.

Proceed by contradiction and assume that (i) does not hold for X_{n+1} . Since (i) holds for X_n this means that (i) does not hold exactly for v_{n+1} : there exists a path \mathfrak{p} joining v_1 to v_{n+1} of weight w less that $T_{n+1}(v_{n+1})$.

But we also know from (ii) that $T_n(v_{n+1})$ is the smallest weight among the paths joining v_1 to v_{n+1} and visiting only vertices in X_n before reaching v_{n+1} .

From [1.2], we have $w < T_{n+1}(v_{n+1}) \le T_n(v_{n+1})$, thus we deduce that \mathfrak{p} is visiting a vertex $u \notin X_n \cup \{v_{n+1}\}$. Let u be the first vertex of \mathfrak{p} encountered outside of X_n . Note that the first section \mathfrak{p}' of \mathfrak{p} from v_1 to u has weight at most w (the weight of the full path \mathfrak{p}).

Using (ii), we get $T_n(u) \leq w$ because $T_n(u)$ is the minimal weight of all paths joining v_1 to u and visiting only vertices in X_n except for the last one and \mathfrak{p}' is a path of this form.

We obtain that $T_n(u) \le w < T_{n+1}(v_{n+1}) \le T_n(v_{n+1})$ and thus

$$T_n(u) < T_n(v_{n+1})$$

contradicting the choice of v_{n+1} in line 8 of the algorithm.

We still have to prove (ii) for the (n+1)st iteration. How is $T_n(y)$ updated for $y \notin X_{n+1}$ when moving from X_n to X_{n+1} ? Consider all paths joining v_1 to y and visiting only vertices in X_{n+1} before reaching y. There are those not going through v_{n+1} and those going through v_{n+1} . For the latter ones, we need only to consider those ending in v_{n+1} because of (i). The conclusion follows from lines 10–12 of the algorithm.

1.6. A few applications

In the previous sections, we already have mentioned several applications, e.g. Google's PageRank, graphs associated with social networks like Facebook or Twitter, collaboration graphs and computing shortest path for a GPS device. Of course, graphs occur in many other practical situations: transportation or

flow networks¹⁶, e.g. electrical distribution systems, water running in a series of pipes of different diameters with various capacities and computer networks and distributed resources. We can also think about quivers¹⁷ occurring in the study of friezes in algebraic combinatorics [BER 16, Chapter 10].

Let us present six more examples.

EXAMPLE 1.47 (Group Theory).— Let \mathbb{G} be a finitely generated group and g_1, \ldots, g_k be generators of \mathbb{G} , i.e. every element of \mathbb{G} is a finite product of the g_i 's and their inverses. The corresponding **Cayley graph** of \mathbb{G} is defined as follows: the set of vertices is \mathbb{G} and, for each g_i , there is a directed edge from x to y if and only if $x.g_i = y$. Hence, the outdegree of every vertex is k. In particular, we have an example of an infinite graph whenever \mathbb{G} is infinite. In Figure 1.22, we have represented the Cayley graph of the group of permutations over four elements. This group has 24 elements. We have considered the two cycles $(1\ 2\ 4)$ and $(3\ 4)$ as generators.

For instance, the label of any closed walk is a word over the generators and their inverses, which is equal to the identity element of the group; taking an edge backward corresponds to multiplication by the inverse of a generator. More generally, the labels of two walks between any two vertices are two representations of the same element of the group. The multiplication by the cycle $(1\ 2\ 4)$ (respectively, $(3\ 4)$) is represented by a gray (respectively, black) edge. The identity permutation is the vertex 1.

EXAMPLE 1.48 (Combinatorics on words).— In combinatorics on words, we are interested in properties of infinite words, i.e. maps \mathbf{w} from \mathbb{N} to a finite set A called alphabet. In particular, we can search for the set of factors made up of n consecutive symbols

$$\mathsf{Fact}_{\mathbf{w}}(n) := \{ \mathbf{w}(i) \cdots \mathbf{w}(i+n-1) \mid i \ge 0 \}$$

that may occur in w. The celebrated Thue-Morse word [ALL 99] starts with

 $01101001100101101001011001101001 \cdots$

¹⁶ In this book, we will not discuss this important topic; for a few pointers make a search about Ford–Fulkerson algorithm or max-flow min-cut theorem.

¹⁷ This terminology simply refers to a directed multigraph and can be encountered in category theory and representation theory.

¹⁸ Such a graph can be easily obtained using Mathematica with a built-in function CayleyGraph or other softwares like SAGE.

and does not contain any cube, i.e. a factor of the form uuu. Thus, the factors of length 3 occurring in this word are 001, 010, 011, 100, 101, 110. A Rauzy graph is a handy tool to study the structure of these factors. The set of vertices of the Rauzy graph of order n>1 is $\operatorname{Fact}_{\mathbf{w}}(n)$ and there is an edge labeled by b from u to v if u=ax and v=xb where a,b are symbols and x is a word of length n-1 such that axb is a factor occurring in \mathbf{w} . Thus, we learn from the Rauzy graph some information about the sequencing of the factors of length n within \mathbf{w} . More about these graphs are presented in section 3.6. We will see that a Rauzy graph is a subgraph of a de Bruijn graph. In Figure 1.23, we have depicted the Rauzy graph of order 3 of the Thue-Morse word.

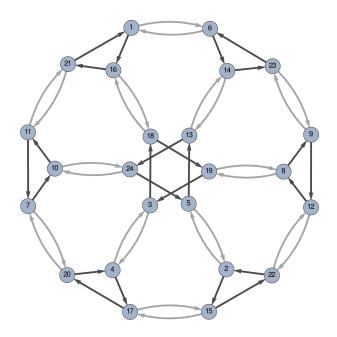


Figure 1.22. A Cayley graph for S_4

EXAMPLE 1.49 (Chemistry).— Several molecules may have the same formula but distinct molecular structures. They are called isomers: they have the same number of atoms but with different arrangements so they can have different properties. We can ask which configurations are possible from a combinatorial point of view (see [PÓL 87, TEM 96]).

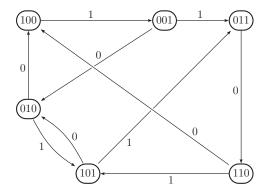


Figure 1.23. The Rauzy graph of order 3 for the Thue-Morse word

EXAMPLE 1.50 (Assigning IP Addresses).— The assignment of IP addresses to nodes in a network takes into account the natural hierarchy of the network and its division into subnetworks. Assignment of addresses then follows a simple rule inside these subnetworks. The goal is to minimize the sizes of routing tables on the nodes and packets are forwarded using a longest prefix matching.

For a related (but quite unrealistic) example, we may assign addresses to the vertices of a simple graph G in such a way that the Hamming distance¹⁹ between two addresses is equal to the distance between the two vertices if and only if [DJO 73]:

- G is a connected bipartite graph;

-for every edge $\{a,b\}$ of G, if for all vertices x,y,z such that $\mathsf{d}(a,x) < \mathsf{d}(b,x)$, $\mathsf{d}(a,y) < \mathsf{d}(b,y)$, $\mathsf{d}(x,z) + \mathsf{d}(z,y) = \mathsf{d}(x,y)$, then $\mathsf{d}(a,z) < \mathsf{d}(b,z)$.

EXAMPLE 1.51 (Coloring).— Here is an application of the notion of proper coloring introduced in example 2.10. Consider a train transporting several chemical products. In case of a train accident, it is important that some of these products do not mix because it would lead to producing toxic or explosive reactions. The chemist tells us which products may or may not mix. It is the task of the organizer to put products that may not mix in different wagons. But from an economical point of view, we also want to minimize the

¹⁹ The Hamming distance between two finite sequences $u, v \in \{0, 1\}^k$ is the total number of the indices i such that $u_i \neq v_i$.

number of wagons. Assume that we are transporting products P_1, P_2, \ldots, P_9 . The products are the vertices of the graph depicted in Figure 1.24. There is an edge between two products if they may not be mixed. Chapter 7 presents some results on colorings. Here, three wagons are needed because of the cycle of length 3. These wagons are enough: a first wagon for P_5, P_7, P_8 , a second wagon for P_1, P_2, P_3, P_6 and a third wagon for P_4 and P_9 . Every wagon is made up of a set of pairwise independent vertices. This is not the only solution. Of course, you can also think of extra constraints depending on the quantities to be carried.

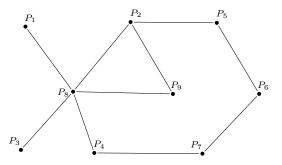


Figure 1.24. Chemical products that may not be mixed

EXAMPLE 1.52 (Detecting communities in large graphs).— The question of community detection is to find a partition of a network into "communities" of densely connected nodes, with the nodes belonging to different communities being only sparsely connected. I agree that this is a non-rigorous definition. There are several algorithms that give partitions of this form. The quality of the resulting communities can, for instance, be measured by its modularity, a real number in [-1,1] defined by

$$\frac{1}{2M} \sum_{i,j} \left[A_{ij} - \frac{k_i k_j}{2M} \right] \delta(c_i, c_j)$$

where A_{ij} is the weight between the vertices i and j (weights can express stronger links between some vertices, for instance the number of coauthored publications in a collaboration graph), $k_i = \sum_j A_{ij}$, c_i is the community to which vertex i is assigned by the algorithm and $M = \frac{1}{2} \sum_{ij} A_{ij}$. As usual $\delta(x,y) = 1$ if x = y and 0 otherwise. To give a few pointers, see [BLO 08] and also [NEW 06, NEW 04, PON 11, PON 06].

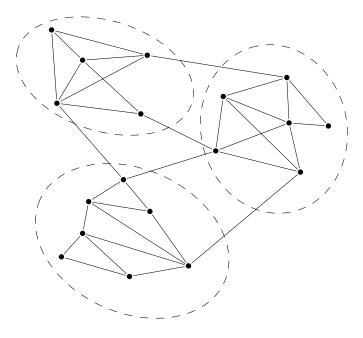


Figure 1.25. Three communities in a graph

1.7. Comments

We give some comments or remarks in chronological order of appearance within the text.

Generalizations of multisets have been proposed, for instance, fuzzy multisets [YAG 87] or real-valued multisets [BLI 89].

A generalization of a graph is given by a *hypergraph* H = (V, E) where V is, as usual, the set of vertices and E is the set of *hyperedges*, i.e. a subset of the set of non-empty subsets of V. We can therefore model other types of relations occurring between more than two vertices. Several variants exist (see [BER 89]).

For some general references on graph theory, see [DIE 10] or [BON 08]. In particular, the first reference gives more details on infinite graphs.

About ranking and rating techniques discussed in example 1.6, we will study the basics of the PageRank algorithm in Chapter 10. For a pleasant and comprehensive introduction to the subject, see [LAN 12].

The road coloring problem mentioned in example 1.15 can be stated as follows: given a k-regular irreducible aperiodic²⁰ digraph, is it possible to color the edges in such a way that there exists a synchronizing sequence \mathfrak{s} , i.e. there exists a vertex v such that, for all vertices u, following a path of label \mathfrak{s} from u leads to v. This problem was first considered by Adler, Goodwyn and Weiss [ADL 77] and solved by Trahtman [TRA 09]. This problem has applications in data storage [LIN 95], automated design [EPP 90] or communication protocols [AHO 95] (see the chapter by Béal and Perrin in [BER 16]).

In a *small world*, everyone on earth is supposedly connected to everyone else by a chain of at most six "friends". The famous psychologist Milgram and his collaborators started to examine this phenomenon with people asked to send letters across the United States, see [EAS 10, p. 31]. Graph theoretic models may also explain other social phenomena such as homophily and the *glass ceiling effect* that keeps women from reaching highest positions in companies [AVI 15]. *Homophily* is the tendency for people to stay "close" to other people sharing the same characteristics (e.g. gender, ethnicity and cultural tastes), see again [EAS 10] and Schelling's mathematical model of segregation in sociology [SCH 71, ZHA 04].

Concerning *Eulerian graphs*, when a multigraph is not Eulerian we can try to find a closed walk of minimal length that visits every edge at least once. This problem is known as the *Chinese postman problem*. The number of Eulerian circuits in a connected Eulerian digraph (the situation is more difficult in the unoriented case) is given by the so-called BEST theorem named after Ehrenfest and de Bruijn [VAN 51], Tutte and Smith [TUT 41]

$$t_w(G) \prod_{v \in V(G)} \left(\mathsf{deg}^+(v) - 1 \right)!$$

where we recall that for an Eulerian digraph $\deg^+(v) = \deg^-(v)$ for all v (see corollary 1.43) and $t_w(G)$ denotes the number of arborescences rooted at the vertex w. An arborescence rooted at w is a digraph where, for every vertex v, there is exactly one path from w to v. We will see in section 8.6 (and more

²⁰ Aperiodicity will be discussed in Chapter 9.

precisely, with the concluding corollary 8.44) that $t_w(G)$ does not depend on the choice of w. As an example, consider the graph depicted in Figure 1.26, we can check that it contains three Eulerian circuits. We have also depicted the three arborescences rooted at the bottom left vertex. Applying the above formula yields

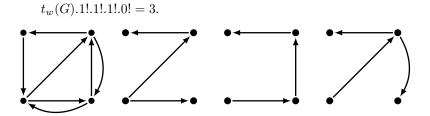


Figure 1.26. Number of Eulerian circuits and arborescences

Domination (definition 1.23) in graph is an important topic of its own. See, for instance, [HEN 13] for more on the subject. For general graphs, the determination of the total domination number is an NP-complete problem [PFA 83] (see also example 2.12).

For important practical issues and implementation of Dijkstra's algorithm, several refinements have been considered. For details and discussions about the average-case analysis of this algorithm, see, for instance, [MEH 08].

Connected to Cayley graphs, the *word problem for groups* is a well-known question arising in abstract algebra: given any two words written over an alphabet of generators and their inverses, can we algorithmically decide whether these two words represent the same element of the group? In full generality, Novikov showed that this problem is undecidable [NOV 55]. For special families of groups, e.g. automatic groups, the problem is decidable.

1.8. Exercises

- 1) Can we find a group of 11 people such that each member of the group exactly knows three other people belonging to the group? Same question but with a group of eight people. In case of a positive answer, draw a graph illustrating the situation. Is such a graph always connected?
- 2) In a meeting with at least two persons, people who know each other shake hands (and no one else). Prove that there are two persons who shaked exactly the same number of hands.

- 3) n couples are invited to a party. Some guests shake hands, but nobody shake hands with his/her partner. One of the guests, Mr. G., asks all guests how many hands they have shaken. He gets 2n-1 different answers. How many hands has the wife of Mr. G. shaken?
- 4) Prove that there is no simple graph that is 3-regular and has seven vertices. Prove that there is no graph with an odd number of vertices and all vertices of odd degree.
- 5) Let G be a simple graph whose vertices have degree at least 2. Prove that G has a cycle.
- 6) Let G = (V, E) be a connected graph. We make use of the notion of distance (remark 1.31). The *eccentricity* of a vertex u is defined by

$$\epsilon(u) := \max_{v \in V} \mathsf{d}(u, v).$$

As usual in a metric space, the *diameter* of G (also see definition 8.32) is

$$\mathsf{diam}(G) := \max_{u \in V} \epsilon(u).$$

The radius of G is defined as

$$\mathsf{rad}(G) = \min_{u \in V} \epsilon(u) = \min_{u \in V} \max_{v \in V} \mathsf{d}(u,v).$$

Prove that

$$\operatorname{rad}(G) \leq \operatorname{diam}(G) \leq 2\operatorname{rad}(G).$$

For which graphs do we have rad(G) = diam(G)? Same question with $diam(G) = 2 \, rad(G)$.

7) Let G=(V,E) be a connected graph. Let $k=\max_{v\in V}\deg(v).$ If $k\geq 3,$ prove that

$$\#V \le \frac{k(k-1)^{\mathsf{rad}(G)}}{k-2}.$$

- 8) Prove that a minimum vertex cover of the Petersen has size 6, see Figure 1.8.
 - 9) Give an example of a Hamiltonian graph that is not Eulerian.

- 10) Prove that the Petersen graph (depicted in Figure 1.8) is not Hamiltonian, but find a Hamiltonian path.
- 11) Prove that the complete bipartite graph $K_{m,n}$ is Hamiltonian if and only if m = n.
- 12) Let $n \ge 1$. The *n*-cube Q_n is the graph defined below. First the graphs Q_1 , Q_2 and Q_3 have been represented in Figure 1.27.

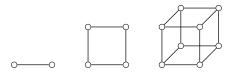


Figure 1.27. The graphs Q_1 , Q_2 and Q_3

For all $n \ge 1$, we get Q_{n+1} by considering two disjoint copies of Q_n and adding an edge for every pair of vertices that correspond to each other in the two copies of Q_n . A representation of Q_4 is given in Figure 1.28.

- a) In terms of n, how many vertices and edges do Q_n have? What is the degree of every vertex in Q_n ?
- b) For which values of n, is the n-cube Hamiltonian?
- c) For which values of n, is the n-cube Eulerian?

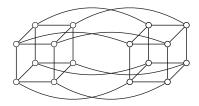


Figure 1.28. A representation of Q_4

13) Let $n \ge 1$. Define the graph where the vertices are 2^n strings of length n over $\{0,1\}$ and two vertices are connected if and only if their Hamming distance (see example 1.50) is one. Compare this graph with the n-cube introduced above.

- 14) For the *n*-cube, determine its edge-connectivity $\lambda(Q_n)$.
- 15) Prove that a (multi)graph G is bipartite if and only if every circuit in G has an even length.
- 16) Find all values a,b,c with $1 \le a \le b \le c$ such that the complete tripartite graph $K_{a,b,c}$ has a Eulerian trail but no Eulerian circuit.
- 17) Give examples of simple graphs such that $\lambda(G) = i$ for i = 1, 2, 3, 4. Same question with vertex-connectivity $\kappa(G)$.
- 18) Use Menger's theorem to derive a polynomial time algorithm computing the vertex-connectivity of a graph.
- 19) Prove that if $F \subset E(G)$ is a minimal cut-set of a connected graph G, i.e. for all $f \in F$, $F \setminus \{f\}$ is not a cut-set, then the number of connected components of G F is exactly 2.
 - 20) Prove that a 3-regular graph has a cut-vertex if and only if it has a bridge.
- 21) Let G be a simple graph with m edges e_1, \ldots, e_m . We define the **line graph** L(G) as the graph with m vertices v_1, \ldots, v_m and the edge $\{v_i, v_j\}$ belongs to L(G) if and only if the edges e_i and e_j of G are adjacent (i.e. they share an endpoint).
- a) represent the line graph of the complete graph K_4 , the bipartite complete graph $K_{2,3}$ and a cycle with six vertices,
 - b) show that $K_{1,3}$ and K_3 have the same line graph,
- c) express the number of edges in ${\cal L}(G)$ in terms of the degrees of the vertices of G,
- d) show that if G is a simple k-regular graph (i.e. each vertex has degree k), then L(G) is (2k-2)-regular.
- 22) Build a simple 3-regular graph that has a cut-edge. Determine the minimal number of vertices that such a graph has.
 - 23) Work out a proof of the exactness of Fleury's algorithm.
- 24) Prove the following [BON 69]. Let G be a graph with n vertices ordered by increasing degree $\deg(u_1) \leq \deg(u_2) \leq \cdots \leq \deg(u_n)$. This sequence is called the *degree sequence*. If there exists $k \in \{0,\ldots,n\}$ such that $\deg(u_j) \geq j+k-1$ for $j=1,\ldots,n-1-\deg(u_{n-k+1})$, then G is k-connected (i.e. k-vertex connected).
- 25) With the notation of definition 1.38, prove the following [CHA 68]. Let $G \neq K_n$ be a graph with n vertices. Then, $\kappa(G) \geq 2 \min_{v \in V(G)} \deg(v) + 2 n$.

26) Consider the Roy–Warshall algorithm described in Table 1.6. The input is a simple digraph with n vertices $\{1,\ldots,n\}$ given by its adjacency matrix $\mathbf{A}(G)$. In the last line of the algorithm, the evaluation $\mathbf{M}_{i,j}$ or $(\mathbf{M}_{i,k}$ and $\mathbf{M}_{k,j})$ returns 1 if $\mathbf{M}_{i,j}=1$ or if both $\mathbf{M}_{i,k}=1$ and $\mathbf{M}_{k,j}=1$. Recall that we write $u\to v$ if u is connected to v. Prove that this cubic-time algorithm (with respect to n) returns a matrix \mathbf{M} where $\mathbf{M}_{u,v}=1$ if and only if $u\to v$. Hence, this matrix provides the connectivity relation within G. An application of the algorithm is depicted in Figures 1.29 and 1.30.

```
\begin{aligned} & \text{ROY-WARSHALL}(\mathbf{A}(G)) \\ & 1 \quad \mathbf{M} \leftarrow \mathbf{A}(G); \\ & 2 \quad \text{for } i = 1 \text{ to } n \\ & 3 \quad \quad \text{do } \mathbf{M}_{i,i} \leftarrow 1 \\ & 4 \quad \text{for } k = 1 \text{ to } n \\ & 5 \quad \quad \text{do for } i = 1 \text{ to } n \\ & 6 \quad \quad \quad \text{do for } j = 1 \text{ to } n \\ & 7 \quad \quad \quad \quad \text{do } \mathbf{M}_{i,j} \leftarrow \mathbf{M}_{i,j} \text{ or } (\mathbf{M}_{i,k} \text{ and } \mathbf{M}_{k,j}) \end{aligned}
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Table 1.6. Roy-Warshall algorithm for connectivity

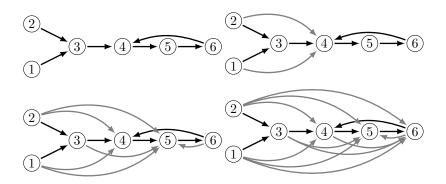


Figure 1.29. Application of Roy–Warshall algorithm for k = 3, 4, 5

27) What can be said about an infinite word w whose Rauzy graph (see example 1.48) of order n is reduced to a cycle? What can be said about Rauzy graphs of order n for ultimately periodic infinite words, i.e. words of the form $uvvv\cdots$ where u, v are finite non-empty words. Sturmian words are

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infinite words ${\bf w}$ characterized by $\#{\sf Fact}_{\bf w}(n)=n+1$ for all $n\geq 0$. Can you characterize Sturmian words using Rauzy graphs?

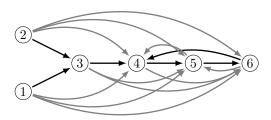


Figure 1.30. Final application of Roy–Warshall algorithm for k=6

A Glimpse at Complexity Theory

Many problems in graph theory are considered as "hard" from an algorithmic point of view. In this chapter, we present the minimal theoretical background necessary to understand the usual classification of "hard" problems (from the point of view of a "worst-case scenario"). In the last section of this chapter, we introduce the reader to a few of these problems.

2.1. Some complexity classes

Turing machines are a useful model of computation providing a formal definition for algorithms. We will not present this model but we will assume that the reader has a reasonable understanding of what an algorithm is ¹. Our aim is to give a rough presentation of what are the classes P, NP and what are NP-hard and NP-complete decision problems. For references, see, for instance, [SUD 06, ARO 09].

A **decision problem** can be formulated as a general question depending on some input parameters for which the answer is either yes or no. An *instance* of a decision problem is the specific values given to the parameters. As an example, given any integer n>1, decide whether n is prime. Or given any digraph G, decide whether G is Hamiltonian. The instances for which the answer is yes (respectively, no) are the *positive instances* (respectively, the *negative* ones). Consider a convenient coding that contains all the relevant

¹ We thus rely on the Church–Turing thesis. Roughly, if you have a function from \mathbb{N}^k to \mathbb{N} that you can "compute" in any "reasonable" way, then it is computable by a Turing machine.

information about an instance, i.e. a finite description of the input parameters using prescribed rules. We assume that such a coding always exists – we can always provide the data to be processed by an algorithm. We usually make no distinction between a decision problem and the set of codings of all its positive instances. The task is to distinguish codings of positive instances from any other input. Consider base-2 expansions, the first few elements in the set of codings of prime numbers are

$$10, 11, 101, 111, 1011, \ldots$$

So the problem is transformed into the following one: given any finite string made up of 0's and 1's, decide whether this string is the base-2 expansion of a prime number. In the same way, the adjacency list of a graph (see page 4) can be seen as a finite description of a graph. Using delimiters: a semicolon specifies an end of line in the adjacency list and commas are used as separators, a list can thus be coded as a finite string. As an example, the string

contains the same information as given in Table 1.1. Of course, we can devise other equivalent codings. To encode a graph, we can also use its adjacency matrix (see section 8.2). If x is the coding of an instance, we let |x| denote its length, i.e. the number of bits or characters of x. For a directed multigraph G=(V,E), the length of such a coding is proportional to #V+#E.

A decision problem is *decidable*, if there exists an algorithm that, given any instance, correctly determines in a finite number of steps whether or not this instance is positive.

DEFINITION 2.1 (P Class).— A decision problem belongs to the complexity class P of polynomial time problems, if there exist a polynomial Q and an algorithm (formally a deterministic Turing machine) that, given any² input x, answers whether or not x is the coding of a positive instance of the problem in a number of steps (i.e. number of elementary operations) bounded by Q(|x|).

² It is important to note that we are discussing what is called the worst case (time) complexity. Indeed, the definition asks that the algorithm runs in polynomial time for all inputs. Maybe, you can have an algorithm that behaves "well" on average, i.e. the time complexity is polynomial for most entries, but has an exponential complexity for a minority of entries. Such a situation is useful in practice because we will be able to solve most instances of a problem. Nevertheless, this is not covered by the notions presented here.

In practice, we are lucky enough that problems of interest belonging to P may usually be solved by algorithms whose complexity is bounded by a polynomial of small degree (and manageable coefficients) and can thus most of the time be used in real-life applications. Nevertheless, working with large graphs having billions of vertices, it could be unsatisfying to have an algorithm in cubic or even quadratic running time.

Deciding if a connected multigraph is Eulerian is a decidable problem belonging to P. Using corollary 1.44, we simply have to determine the degree of every vertex in G. Thus, we can derive an algorithm where the number of required operations is proportional to the number of edges of G. Not every problem has such a simple solution and we need some more definitions to define what is a "difficult" problem.

DEFINITION 2.2 (NP Class).— A decision problem belongs to the complexity class NP if it is decidable and there exist an algorithm \mathcal{A} and polynomials R, S such that for every <u>positive</u> instance coded by x, there exists an extra piece of information C_x , depending on x, (usually called a certificate) such that

- the length of C_x is bounded by R(|x|);
- given x and C_x as input, the algorithm A checks/proves that x is a positive instance and A runs in a number of steps bounded by S(|x|).

Let us make two observations about problems belonging to NP. Maybe the only available known algorithms run very slowly but, at least, if we have unlimited computing power, we can theoretically solve any problem in NP. Second, if a certificate is provided with a positive instance, there is a polynomial time verification algorithm that checks positiveness of this instance. Two examples (composite numbers and Hamiltonian graphs) are given in the following.

REMARK 2.3.— With the previous two definitions, we directly have $P \subseteq NP$.

Deciding if an integer n is composite (i.e. not a prime number) is a problem that belongs to NP. First, testing all possible divisors up to \sqrt{n} , this problem is clearly decidable. Second, given a composite number n, i.e. a positive instance of the problem, if we provide a possible factorization of n into two factors $n_1, n_2 > 1$, then to check that n is indeed composite, it is enough to compute the product $n_1 \cdot n_2$ and compare it to n. So the certificate for n is given by the two numbers n_1 and n_2 . If n is written in base-2, its length is $\lfloor \log_2(n) \rfloor + 1$ thus the lengths of n_1 and n_2 written in base-2 are similar and it is well known that multiplying two numbers whose base-2 expansions are of length

at most ℓ requires $\mathcal{O}(\ell^2)$ steps using elementary schoolbook multiplication. (Faster methods exist but this one already runs in polynomial time.) We have thus the two items of definition 2.2: the certificate has a length proportional to $2\lfloor\log_2(n)\rfloor$ and the verification algorithm runs in a quadratic number of steps with respect to $\lfloor\log_2(n)\rfloor$.

REMARK 2.4.— Deciding if a number is prime, also is a decidable problem belonging to P [AGR 04].

Deciding if a graph is Hamiltonian is also a problem belonging to NP. First, trying all the permutations³ of the vertices to find a candidate for a Hamiltonian circuit shows that this problem is decidable. Second, given a Hamiltonian graph G, if we also provide a candidate for a Hamiltonian circuit, it is easy to check that the graph is indeed Hamiltonian. The size of the certificate is less than the size of the graph: a circuit is a subgraph of G. We can easily produce a verification algorithm to check Hamiltonicity of the given circuit: is the provided list of edges a circuit? Is every vertex of the graph visited exactly once? These questions have to be answered positively.

In view of this example, if a problem belongs to NP, it seems maybe challenging – or at least computationally challenging – to decide whether an instance is positive. But given a positive instance and an extra piece of information, it is "easy" to check that the instance is indeed positive.

2.2. Polynomial reductions

We would like to compare problems. To that end, we introduce a preorder relation (a reflexive and transitive binary relation).

DEFINITION 2.5.— Let \mathcal{P}_1 and \mathcal{P}_2 be two decision problems. We say that \mathcal{P}_1 polynomially reduces to \mathcal{P}_2 if there exist a polynomial Q and a function f that maps every coding x of an instance (positive or negative) of \mathcal{P}_1 to some coding of an instance of \mathcal{P}_2 in such a way that

1) x is the coding of a positive instance of the first problem if and only if f(x) is the coding of a positive instance of the second problem, i.e. the answer for x on \mathcal{P}_1 and the answer for f(x) on \mathcal{P}_2 are the same,

³ Being decidable does not require to find an efficient algorithm. Indeed, this one could need to search through (#V)! permutations and this cannot be done in practice.

2) f(x) can be computed in a number of steps bounded by Q(|x|), in particular |f(x)| is bounded by Q(|x|).

We write $\mathcal{P}_1 \leq \mathcal{P}_2$.

REMARK 2.6.— It is easy to see that if \mathcal{P}_1 polynomially reduces to \mathcal{P}_2 and \mathcal{P}_2 belongs to P, then \mathcal{P}_1 belongs to P. This is because composing two polynomials yields a polynomial. This shows that \leq is transitive.

How "difficult" a decision problem can be?

DEFINITION 2.7 (NP-Hard Problem).— A decision problem \mathcal{P} is NP-hard if $Q \leq \mathcal{P}$, for all problems Q in NP. Roughly, this means that \mathcal{P} is at least "as hard" as any problem in NP. Indeed, if one NP-hard problem can be solved in polynomial time, then this would imply that NP \subseteq P. Finally, a decision problem is NP-complete if it belongs to NP and is NP-hard.

EXAMPLE 2.8.— Deciding if a digraph is Hamiltonian or, deciding if a digraph has a Hamiltonian path or deciding if a simple graph is Hamiltonian are known to be NP-complete problems [GAR 79]. The latter problem will be denoted by HC.

EXAMPLE 2.9.— Consider a traveling salesman who wants to visit cities at a limited cost. Given a weighted complete graph where values on the edges represent travel time or expense, find a Hamiltonian circuit of minimal weight. Expressed like this, it is not a decision problem. So we reformulate the problem by adding an extra parameter k. TSP: Given a weighted complete graph, is there a Hamiltonian circuit of weight less than k? Trying all the possible circuits, this problem is decidable. Given a positive instance of the problem and a circuit satisfying the constraints, the verification is easy. So TSP \in NP. We will show that

and thus, the traveling salesman will be NP-complete. Indeed, we know that HC is NP-complete from example 2.8. Thus, for all $\mathcal{P} \in \text{NP}$, $\mathcal{P} \leq \text{HC}$. Since the polynomial reduction relation \leq is transitive, we conclude that, for all $\mathcal{P} \in \text{NP}$, $\mathcal{P} \leq \text{TSP}$.

What is this polynomial reduction from HC to TSP? Given a simple graph G = (V, E), we replace it with the complete graph $K_{\#V}$ and we define weights as follows: if $\{u, v\} \in E$ (respectively, $\notin E$), then the weight is set to 1

(respectively, 2). We ask whether the new graph has a Hamiltonian circuit of weight at most #V (see Figure 2.1). The codings of the graph G and the weighted graph $K_{\#V}$ have similar size of order $(\#V)^2$. We can derive the weighted graph $K_{\#V}$ in polynomial time from G. Finally, G is Hamiltonian if and only if the corresponding graph has a Hamiltonian circuit of weight at most #V. From the assignments of the weights, the only possibility is to have a Hamiltonian circuit of weight exactly #V.

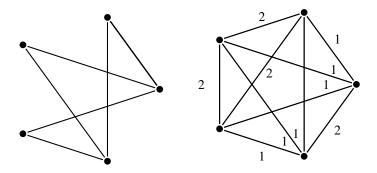


Figure 2.1. A polynomial reduction from HC to TSP

This example shows that we transform the set of instances of HC into a strict subset of the set of instances of TSP.

EXAMPLE 2.10 (Coloring).— Let $k \geq 3$. Given a graph, does there exist a map $c: V \to \{1,\ldots,k\}$, i.e. a coloring (see definition 7.12) of the vertices, such that for any two adjacent vertices $u,v,c(u)\neq c(v)$? If such a map exists, it is called a proper coloring. The problem is decidable and in NP, since there are $k^{\#V}$ colorings of V. Given a positive instance of the problem and a proper coloring as a certificate, the verification is easily carried on in polynomial time with respect to the size of the graph. The k-coloring problem is another example of an NP-complete problem [GAR 79].

Even in the restricted case where k=3, the problem remains NP-complete, see [GAR 76]. We can even restrict the class of considered graphs [DAI 80]: the 3-coloring problem remains NP-complete on planar graphs (see Chapter 6) of degree 4.

To determine, or at least make some progress, about the exact relations existing between NP and P is one of the most challenging open problems in theoretical computer science. It is also one of the seven Millennium Problems

listed by the Clay Mathematics Institute⁴ whose solution has an award of one million dollars. Many researchers are inclined to think that $P \subseteq NP$. Thousands of decision problems are known to be NP-complete. Because of remark 2.6, it would suffice to find a polynomial time algorithm to solve just one of them to prove P = NP.

If you are pragmatic and encounter an NP-complete problem, then do not look for a polynomial time algorithm to solve it. In the best case, look for some heuristic or some approximated solution (e.g. when looking for a Hamiltonian circuit, you would already be happy to have a circuit visiting 90% of the vertices). Also recall that NP-completeness is about worst-case analysis. It is possible that there is a polynomial time algorithm solving "most" instances of the problem.

Also, we can wonder if every problem in P can be solved efficiently. Indeed, the formal definition does not say anything about the degree of the polynomial bounding the complexity. We could imagine that we may face problems in the class P such that the best known algorithms would have polynomial complexity with a too high degree. Nevertheless, this theoretical complexity class turns out to be practical. Surprisingly, almost all problems that can be proven to be in P have a complexity bounded by a polynomial of a small degree like 3 or 4.

2.3. More hard problems in graph theory

Many problems in graph theory are computationally hard. Classical textbooks [GAR 79] present graph problems that are NP-complete: the appendix of Garey and Johnson's book contains a list with 65 problems from graph theory and pursues with related problems about networks, cuts or connectedness. We simply list a few of those that are related to notions that we will soon encounter. If you are facing a new problem that seems algorithmically challenging, you should first search the literature, then think about a possible reduction to a well-known NP-complete problem (see definition 2.5).

EXAMPLE 2.11 (Vertex Cover).— Finding a minimum vertex cover (recall definition 1.23) is an NP-complete problem [GAR 79, GT2, p. 190; PFA 83]. To turn it into a decision problem, consider the question given a graph G and an integer k, does G have a vertex cover of cardinality k?

⁴ www.claymath.org/.

EXAMPLE 2.12 (Dominating Set).— As mentioned in section 1.7, the total domination number is an NP-complete problem [GAR 79, GT2 – p.190] or [PFA 83], i.e. given a graph G and an integer k, does G have a dominating set of size k?

EXAMPLE 2.13 (1-Planarity).— Given a multigraph G, deciding whether or not G is planar is in P (see Chapter 6 for definitions and algorithms). Nevertheless, 1-planarity seems computationally harder, unless P = NP. A multigraph G is 1-planar if there exists an embedding of G on \mathbb{R}^2 such that each edge is crossed at most once (by a single edge). Deciding 1-planarity is NP-complete (see [GRI 07]). A characterization of 1-planar complete n-partite graphs is given in [CZA 12]. As an example, $K_{n,3}$ is 1-planar if and only if $n \leq 6$.

EXAMPLE 2.14 (Clique).— Given a graph G and an integer k, the clique problem (see example 1.21) is NP-complete: decide whether or not G contains a clique of size k. This problem was already presented in Karp's paper [KAR 72] giving polynomial reductions between many combinatorial problems.

Example 2.15 (Independent Set).— Very similar to the previous example, given a graph G and an integer k, deciding whether or not G=(V,E) contains k independent vertices is NP-complete (see definition 1.1). Take the complement G^c of G where adjacent vertices are replaced with independent ones and conversely, see definition 5.6: the set of edges of G^c is $\{\{u,v\}\mid u\neq v \text{ and } \{u,v\}\not\in E\}$. Clearly, there exist k-independent vertices in G if and only if there is a clique of size k in G^c .

EXAMPLE 2.16 (Graph Homomorphism).— Given two graphs G and H, deciding whether there exists a homomorphism (see definition 7.1) from G to H is NP-complete [GAR 79, GT52 – p. 202].

EXAMPLE 2.17 (Degree-Bounded Connected Subgraph).— Given a graph G and two integers k, d, deciding whether or not there exists a connected subgraph of G with at least k edges and every vertex of the subgraph has degree less than d is NP-complete (see [GAR 79, GT26 – p. 196]).

EXAMPLE 2.18 (Degree-Constrained Spanning Tree).— Given a graph G and an integer k, deciding whether or not G contains a spanning tree (see definition 4.5) whose vertices all have degree less than k is NP-complete (see [GAR 79, ND1 – p. 206]).

EXAMPLE 2.19 (Monochromatic Triangle).— The next problem can be related to Ramsey numbers (see section 7.5). Given a simple graph, deciding whether there exists a coloring of the edges such that there is no blue triangle nor red triangle (i.e. a monochromatic copy of K_3) is NP-complete (see [GAR 79, GT6-p.~191]).

Hamiltonian Graphs

In this chapter, we will only consider simple graphs. So we are dealing with the unoriented case and since we are searching for a circuit visiting once every vertex of the graph, there is no need to consider loops or multiple edges.

Recall that a simple graph is *Hamiltonian* (section 1.4) if there exists a cycle going through all the vertices: a *Hamiltonian circuit*.

In contrast with the Eulerian case (see corollary 1.44), it is a much more delicate task to handle the Hamiltonian situation (see example 2.8 about the NP-completeness of the problem). Therefore, unless P = NP, it is unlikely to get an "easy" characterization of Hamiltonian graphs. For pedagogical reasons (the arguments are easier to grasp), we first present a sufficient condition for Hamiltonicity given by Dirac, but this first result can be derived from stronger results that we present later on.

3.1. A necessary condition

The next result can be used to prove that some graphs are not Hamiltonian.

THEOREM 3.1.— If a simple graph G is Hamiltonian, then for every subset X of vertices, the number of connected components of the graph induced by $V(G) \setminus X$ is less than or equal to the cardinality of X.

If we remove n (well-chosen) vertices and we get strictly more than n connected components in the resulting induced graph, then the original graph is not Hamiltonian. Consider the graph depicted in Figure 3.2 and remove the two vertices u and v, we get three connected components and conclude that the graph is not Hamiltonian.

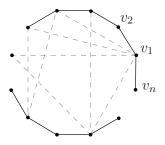


Figure 3.1. Illustrating the proof of theorem 3.1

PROOF.— Assume that G is a graph with a Hamiltonian circuit (v_1,\ldots,v_n,v_1) going through all the n vertices of G. It is enough to make our reasoning by only considering the edges along this circuit. If we delete one vertex from the graph, let us say v_i , the resulting graph remains connected: we still have the path $(v_{i+1},\ldots,v_n,v_1,v_2,\ldots,v_{i-1})$ connecting all the n-1 vertices.

If we remove an extra vertex, the path could either split into two paths (or a path and a single vertex), or we keep a path if the removed vertex is v_{i-1} or v_{i+1} . Each time we remove a vertex, the number of resulting paths (or isolated vertices) remains the same or increases by one. Only one of the paths can split into two.

After removing k vertices from the initial Hamiltonian circuit, we obtain at most k paths (and/or isolated vertices). So the number of connected components of the induced graph is at most k. If there exist other edges connecting vertices belonging to different paths, then this number is even smaller. The situation is illustrated in Figure 3.1 where the original Hamiltonian circuit is represented in black and several vertices have been removed. We have two paths and one isolated vertex. Some extra edges are suggested with dashed lines.

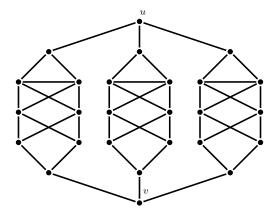


Figure 3.2. A non-Hamiltonian graph

3.2. A theorem of Dirac

The philosophy is that the more edges we have, the easier it is to have a Hamiltonian circuit.

THEOREM 3.2.— Let G be a simple graph with $n \ge 3$ vertices. If the degree of every vertex of G is greater than or equal to n/2, then G is Hamiltonian.

PROOF.— First, we claim that G is connected. Suppose to the contrary that G has at least two connected components. Thus, there exists one component having at most $\lfloor n/2 \rfloor$ vertices. By assumption, any vertex in that component should have at least $\lceil n/2 \rceil$ neighbors. So the component has at least $\lceil n/2 \rceil + 1$ vertices. This is a contradiction.

Let $\mathfrak{p}=(v_0,\ldots,v_k)$ be a path of maximum length k (among all the paths that can be found in G). In particular, all the v_i 's in this path are pairwise distinct and k < n. All the neighbors of v_0 are in $\{v_1,\ldots,v_k\}$ because, otherwise, we could extend the path \mathfrak{p} to a longer one, contradicting the choice of \mathfrak{p} . With the same reasoning, all the neighbors of v_k are in $\{v_0,\ldots,v_{k-1}\}$.

We claim that there exists i < k such that

$$\{v_0, v_{i+1}\} \in E(G)$$
 and $\{v_i, v_k\} \in E(G)$.

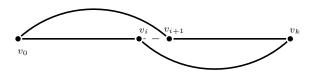


Figure 3.3. Illustration of Dirac's theorem

Proceed by contradiction. Let $I \subseteq \{0,\ldots,k-1\}$ be the set of indices i such that $\{v_0,v_{i+1}\} \in E(G)$. In particular, if $i \in I$, then $\{v_i,v_k\} \not\in E(G)$. Let $J \subseteq \{0,\ldots,k-1\}$ be the set of indices i such that $\{v_i,v_k\} \in E(G)$. In particular, if $i \in J$, then $\{v_0,v_{i+1}\} \not\in E(G)$. By assumption, $\#I \ge n/2$ and $\#J \ge n/2$. Since $I \cap J = \emptyset$, thus $\#(I \cup J) \ge n$. But I and J are subsets of $\{0,\ldots,k-1\}$, thus $\#(I \cup J) \le k < n$. As illustrated by Figure 3.3, we have a closed path going through the vertices v_0,\ldots,v_k .

To conclude with the proof, we have to show that this closed path is indeed a Hamiltonian circuit. We have to prove that it contains every vertex of G. Assume that there is one vertex u not occurring in this path. Since the graph is connected, there is a path $\mathfrak q$ from u to some v_j and visiting only vertices not in the path (except for v_j). This path $\mathfrak q$ followed by $(v_{j+1},\ldots,v_k,v_0,v_1,\ldots,v_{j-1})$ is a path strictly longer than $\mathfrak p$. This again contradicts the choice of $\mathfrak p$.

3.3. A theorem of Ore and the closure of a graph

The previous theorem was obtained by Dirac in 1952 [DIR 52]. Eight years later, Ore provided a weaker sufficient condition for Hamiltonicity (see remark 3.8). Its proof is quite similar to the previous one.

THEOREM 3.3.— Let G be a simple graph with $n \ge 3$ vertices. Let x, y be two vertices such that the sum of their degrees is greater than or equal to n. The graph G is Hamiltonian if and only if $G + \{x, y\}$ is Hamiltonian.

PROOF.— The case n=3 is clear. We will assume that $n\geq 4$. The only non-trivial part is when $\{x,y\}$ is not an edge in E(G) and $G+\{x,y\}$ has a Hamiltonian circuit $(x=v_1,v_2,\ldots,v_n=y,x)$ using explicitly the edge $\{x,y\}$. We have to derive from this circuit another Hamiltonian circuit not using this edge $\{x,y\}$. To that end, it is enough to prove that there exists an index i such that $3\leq i\leq n-1$ and

$$\{v_1, v_i\} \in E(G)$$
 and $\{v_{i-1}, v_n\} \in E(G)$. [3.1]

First note that v_1 has at least two neighbors in G: v_2 and another one in $\{v_3,\ldots,v_{n-1}\}$. Because otherwise, $\deg(v_1)=1$ and using the assumption, we get $\deg(v_n)\geq n-1$: v_n is adjacent to every vertex in G. So $\{x,y\}$ must belong to E(G) contradicting the initial assumption. Similarly, v_n has at least two neighbors: v_{n-1} and another one in $\{v_2,\ldots,v_{n-2}\}$.

Assume that [3.1] does not hold. Let $I\subseteq \{3,\ldots,n-1\}$ be the set of indices i such that $\{v_1,v_i\}\in E(G)$. In particular, if $i\in I$, then $\{v_{i-1},v_n\}\not\in E(G)$. Let $J\subseteq \{3,\ldots,n-1\}$ be the set of indices i such that $\{v_{i-1},v_n\}\in E(G)$. In particular, if $i\in J$, then $\{v_1,v_i\}\not\in E(G)$. By assumption, $\#I+\#J\geq n-2$ (we do not take the two edges $\{v_1,v_2\}$ and $\{v_{n-1},v_n\}$ into account). Since $I\cap J=\emptyset$, $\#(I\cup J)\geq n-2$. But I and J are subsets of $\{3,\ldots,n-1\}$, thus $\#(I\cup J)\leq n-3$.

DEFINITION 3.4.— Let $G = G_0$ be a simple graph with $n \geq 3$ vertices. Starting with G_0 , we build a finite sequence of graphs $(G_i)_{i\geq 0}$ such that G_{i+1} is the graph G_i where we add a new edge whose endpoints are non-adjacent vertices in G_i such that the sum of their degrees $(w.r.t.\ G_i)$ is greater than or equal to n. The construction stops when for all pairs of non-adjacent vertices, the sum of their degrees is less than n. There are usually several choices of edges to add, so the ordered sequence of graphs is not unique. But, since the degree of every vertex along such a sequence is non-decreasing, all the admissible sequences $(G_i)_{i\geq 0}$ have the same length and the process stops with a unique final graph that is called the **closure** of G and is denoted by C(G).

EXAMPLE 3.5.— In Figure 3.4, we have depicted a sequence of graphs leading to a complete closure, i.e. the closure of the graph is K_6 .

The next result was given by Bondy and Chvátal [BON 76].

THEOREM 3.6.— A simple graph G with $n \geq 3$ vertices is Hamiltonian if and only if its closure C(G) is Hamiltonian.

PROOF.— If $G = G_0, G_1, \ldots, G_k = \mathcal{C}(G)$ is a sequence of graphs leading to the closure of G, then we apply k times the previous theorem to G_i and G_{i+1} for $i = 0, \ldots, k-1$.

COROLLARY 3.7.— Let G be a simple graph with $n \ge 3$ vertices. If, for every pair of non-adjacent vertices, the sum of their degrees is greater than or equal to n, then G is Hamiltonian.

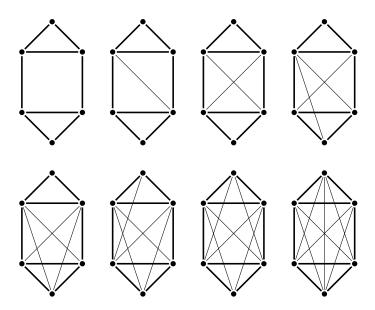


Figure 3.4. The closure of a simple graph

PROOF.— By assumption, the closure of G is the complete graph K_n , which is trivially Hamiltonian. By theorem 3.6, the graph G is Hamiltonian.

REMARK 3.8.— Note that the assumptions of Dirac's theorem are a special case of those of the latter corollary. So Ore's theorem directly implies Dirac's result.

Two years later, Pósa proved the following result [PÓS 62]. We will not prove this result, but it opens the way for the following section.

THEOREM 3.9.— Let G be a simple graph with $n \geq 3$ vertices. If for every k such that $1 \leq k < (n-1)/2$, the number of vertices of degree at most k is less than k and if the number of vertices of degree at most (n-1)/2 is less than or equal to (n-1)/2, then G is Hamiltonian.

REMARK 3.10.— If G has a complete closure, then G is clearly Hamiltonian. Note that the converse does not hold: there exists Hamiltonian graphs whose closure is not a complete graph. Take, for instance, a cycle of length $n \geq 5$. It is trivially Hamiltonian and equal to its closure.

3.4. Chvátal's condition on degrees

In this section, we present an elegant sufficient condition for a graph to be Hamiltonian. We have to check #V(G) inequalities about the degrees of the vertices of the graph. At the end of this section, we list (without proof) some other sufficient conditions about Hamiltonicity and give relevant bibliographic pointers.

DEFINITION 3.11.— The (vertex) degree sequence of a graph with n vertices is a non-decreasing sequence $d_1 \leq d_2 \leq \cdots \leq d_n$ of integers such that there exists an ordering, i.e. a map from $\{1,\ldots,n\}$ to V(G), of the vertices v_1,\ldots,v_n satisfying $\deg(v_i)=d_i$. Uniqueness of the degree sequence follows from the fact that it has been ordered.

Note that because of the handshaking formula [1.1], we have $\sum_i d_i = 2\#E(G)$. If we consider the graph of Belgian highways given in Figure 1.6, then its degree sequence is (3,3,3,4,4,4,5). In particular, the number of odd-degree vertices is even¹.

The following theorem is usually referred to as Bondy–Chvátal theorem because it relies on theorem 3.6 proved by these two authors. As for the theorem of Ore implying the theorem of Dirac, the sufficient condition given below is weaker than the one in Ore's result (see exercise 2).

THEOREM 3.12.— [CHV 72a]. Let G be a simple graph with $n \ge 3$ vertices and degree sequence (d_1, \ldots, d_n) . If, for every k < n/2, we have

$$d_k \le k \Rightarrow d_{n-k} \ge n - k$$

then G is Hamiltonian.

Prior to the proof, let us make a few observations:

- from a logical point of view, recall that if, for some k < n/2, we have $d_k > k$, then the implication $d_k \le k \Rightarrow d_{n-k} \ge n-k$ holds whatever the value of d_{n-k} is;
- as in remark 3.10, not every Hamiltonian graph satisfies the conditions. Take a cycle of length $n \geq 5$. Its degree sequence is $(2,\ldots,2)$. We have $d_2 \leq 2$ but $d_{n-2} = 2 < n-2$ and the implication is not satisfied;

¹ Did you try exercise 4 in section 1.8?

- the sequence (3,3,3,4,4,4,5) satisfies the conditions. Indeed, $d_1 > 1$, $d_2 > 2$ and $d_3 \le 3$. So we only have to check that $d_{7-3} = d_4 \ge 4$, which is the case. So the graph in Figure 1.6 is Hamiltonian;
- note that the result does not give any information about how to find a Hamiltonian circuit.

PROOF.— We shall prove that a graph satisfying the conditions has a complete closure and the conclusion thus follows from theorem 3.6.

Let (d_1, \ldots, d_n) be the degree sequence of G and (e_1, \ldots, e_n) be the degree sequence of $\mathcal{C}(G)$. We claim that (e_1, \ldots, e_n) still satisfies the conditions of Chvátal, i.e. for every k < n/2,

$$e_k \le k \Rightarrow e_{n-k} \ge n - k$$
.

Since $\mathcal{C}(G)$ is obtained by recursively adding edges to G, we just have to convince ourselves that if a graph satisfies Chvátal's condition, then adding one edge to this graph gives a new graph still satisfying the condition. Adding one edge will increase the value of two elements in the degree sequence. We even simplify the problem and just look at the effect of increasing one element of the sequence (one simply applies the argument twice). Let $1 \leq i \leq n$ and $t_1 \leq \cdots \leq t_i \leq \cdots \leq t_n$. Let $s_1 \leq \cdots \leq s_n$ be the sequence obtained after replacing t_i with $t_i + 1$ and reordering. It is enough to show that $s_k \geq t_k$ for all k:

– if $t_i+1 \leq t_{i+1}$, e.g. with $(3,3,\underline{3},4,4,4,5)$ and i=3, we replace the last 3 with 4 to get $(3,3,\underline{4},4,4,4,5)$. So no reordering of $(t_k)_{1\leq k\leq n}$ is required to get $(s_k)_{1\leq k\leq n}$. We have $s_k=t_k$ if $k\neq i, s_i=t_i+1\geq t_i$;

- if $t_i + 1 > t_{i+1} = \cdots = t_{i+\ell}$, e.g. with $(3, 3, 3, \underline{4}, 4, 4, 5)$ and i = 4, $\ell = 2$, a reordering is required: $s_{i+j} = t_{i+j+1} \ge t_{i+j}$ for $j \in \{0, \dots, \ell - 1\}$, $s_{i+\ell} = t_i + 1 > t_{i+\ell}$ and $s_k = t_k$ if $k \notin \{i, \dots, i + \ell\}$.

From the above discussion, we may assume that G is a graph equal to its closure and satisfies Chvátal's condition. Assume that G is not complete. There exist two non-adjacent vertices u,v in G. Among all the pairs of non-adjacent vertices, we may choose u,v such that $\deg(u)+\deg(v)$ is maximal. Without loss of generality, we assume that $\deg(u)\leq \deg(v)$. Note that since $G=\mathcal{C}(G)$, we have $\deg(u)+\deg(v)< n$ because otherwise, the edge would have been added to the closure.

Let $i = \deg(u)$. We have i < n/2, otherwise $\deg(u) + \deg(v) \ge n$. Let $A_v := \{w \in V(G) \mid \{w,v\} \not\in E(G) \text{ and } w \ne v\} = V(G) \setminus \mathbb{N}[v]$.

In particular, u belongs to A_v . By our choice of u,v, every vertex $w \in A_v$ is such that $\deg(w) \leq \deg(u)$. This set A_v contains all the vertices not equal to v and non-adjacent to v, so $\#A_v = (n-1) - \deg(v) \geq \deg(u) = i$. So there are at least i vertices of degree $\leq i$. If (d_1,\ldots,d_n) is the degree sequence of G, this means that $d_i \leq i$. Since i < n/2 and $d_i \leq i$, the assumption about Chvátal's condition implies that we must have $d_{n-i} \geq n-i$.

We pursue with a quite similar argument. Let

$$A_u := \{ w \in V(G) \mid \{u, w\} \not\in E(G) \text{ and } w \neq u \} = V(G) \setminus \mathsf{N}[u].$$

In particular, v belongs to A_u . By our choice of u,v, every vertex $w \in A_u$ is such that $\deg(w) \leq \deg(v) < n-i$. Moreover, we have $\#A_u = (n-1) - \deg(u) = n-i-1$. We have found n-i-1 vertices of degree < n-i. Furthermore, the vertex u has degree i, which is < n-i (because $i < n - \deg(v)$ and $\deg(v) \geq i$). So there are at least n-i vertices of degree < n-i. This means that $d_{n-i} < n-i$, which is a contradiction. We conclude that G is complete.

About other results generalizing the ones discussed so far in this chapter, see the survey paper [LI 13]. The papers [BRO 00] and [STA 05] are also of interest. As an example, let us mention the following two results.

THEOREM 3.13 (Nash–Williams).— [LOV 07]. Every k-regular graph with 2k + 1 vertices is Hamiltonian.

THEOREM 3.14.— [FAN 84] Let G be a simple graph with $n \ge 3$ vertices and degree sequence (d_1, \ldots, d_n) satisfying

$$d_i = \begin{cases} r - t, & \text{if } 1 \le i < r; \\ n - r + t - 1, & \text{if } r < i \le n; \end{cases}$$

where r,t are integers such that $2 \le 2t < r < (n+2t)/3$. Then, G is Hamiltonian.

² Sometimes, this argument is difficult to grasp. If you know that a graph has at least five vertices of degree at most 3, what do you know about d_1, \ldots, d_5 ? Maybe there are other vertices of smaller degrees, but at the very least, we know that $d_5 \leq 3$.

For results generalizing Ore's theorem, see [LIC 13]. For other extensions to the directed case, see the surveys [KÜH 12] and [KÜH 10].

THEOREM 3.15 (Chvátal–Erdős).– [CHV 72b]. Let G be a simple graph with $n \geq 3$ vertices. If the vertex connectivity of G (see definition 1.38) is greater than or equal to the maximal number of pairwise independent vertices, then G is Hamiltonian.

3.5. Partition of K_n into Hamiltonian circuits

A traveling salesman wants to visit n cities, several times, using Hamiltonian circuits and trying not to be bored by repeated travels. He wants to find as many Hamiltonian circuits as possible not using twice the same connection between two cities. So the question is to use all the edges of the complete graph K_n to build Hamiltonian circuits not using the same edge twice. This is what we call a *partition*: every edge belongs to one of the circuits of the partition.

In itself, the result presented in this section might not seem really surprising. Nevertheless, the embedding into a geometrical setting provides us with new arguments³. First observe that a regular n-gon has angles measuring $(n-2)\pi/n$. Indeed, a convex n-gon can be triangulated with n-2 triangles whose angles sum up to π (see Figure 3.5).

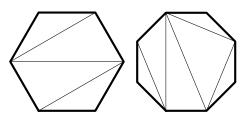


Figure 3.5. Triangulation of a n-gon

³ More geometrical applications will be discussed in section 6.3. I was not able to trace the origins of the proof I present here. It can be found in several references, such as [AGA 09].

LEMMA 3.16.— Let $n \ge 4$ be an even number. The complete graph K_n can be partitioned into n/2 Hamiltonian paths, i.e. any two such paths do not share any common edge and every edge in K_n belongs to one path of the partition.

PROOF. – Note that a Hamiltonian path has n-1 edges and K_n contains n(n-1)1)/2 edges. So we can find at most n/2 Hamiltonian paths that do not share any common edge. Now we exhibit a way to construct such paths. We work with a geometrical representation of K_n where its vertices define a regular ngon centered at the origin of the plane. Moreover, we assume that this n-gon has the x-axis as a symmetry axis. In Figure 3.6, we have represented the cases of a hexagon and an octagon. To prove that the same edge does not occur in two paths, our argument relies on the slope of the edges. We consider a first path with all the horizontal edges (zero slope) and all the edges parallel to the one starting from the bottom-left vertex to the right one on the upper level. It is easy to see that these latter edges have slope π/n . Now proceed to a rotation centered at the origin of angle $2\pi/n$. Under this rotation, every vertex is sent to another vertex and thus every edge is sent to an edge. Applying this rotation once gives edges of slope $2\pi/n$ and $3\pi/n$. So there are distinct from those of slope 0 and π/n . Applying again this rotation gives edges of slope $4\pi/n$ and $5\pi/n$. We can rotate the initial path n/2-1 times (see Figure 3.7). Each time, we get edges of different slopes: $0, \pi/n, 2\pi/n, 3\pi/n, \dots, \pi-2\pi/n, \pi-\pi/n$. This proves that we have defined n/2 Hamiltonian paths that do not share any common edge.

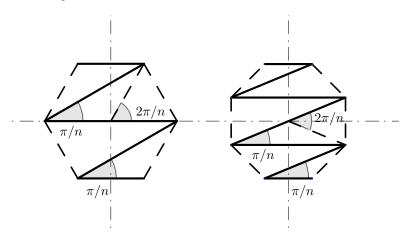


Figure 3.6. Definition of a Hamiltonian path

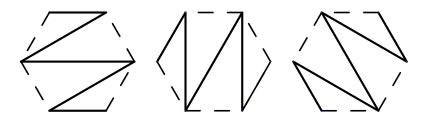


Figure 3.7. Applying rotations twice

COROLLARY 3.17.— Let $n \ge 5$ be an odd number. The complete graph K_n can be partitioned into (n-1)/2 Hamiltonian circuits, i.e. any two such circuits do not share any common edge and every edge in K_n belongs to one circuit of the partition, if and only if K_{n-1} can be partitioned into (n-1)/2 Hamiltonian paths.

PROOF.— Suppressing one vertex of K_n gives K_{n-1} and each Hamiltonian circuit of K_n thus corresponds to a Hamiltonian path of K_{n-1} . Conversely, adding one vertex to K_{n-1} and n-1 edges from this vertex to the n-1 other vertices gives K_n and every Hamiltonian path of K_{n-1} thus corresponds to a Hamiltonian circuit of K_n . Note that all the Hamiltonian paths of the partition of K_{n-1} have distinct endpoints (because otherwise, this contradicts the fact that we have a partition⁴), so we indeed get a partition of K_n in Hamiltonian circuits.

PROPOSITION 3.18.— The complete graph K_n can be partitioned into Hamiltonian circuits, i.e. any two such circuits do not share any common edge and every edge in K_n belongs to one circuit of the partition, if and only n is odd.

PROOF.— If n is odd, then we can use the previous corollary and lemma 3.16. If n is even, we claim that there is no such partition. The graph K_n is (n-1)-regular and each circuit going through one vertex consumes two edges adjacent to it. So, if n is even, at most (n-2)/2 circuits using pairwise distinct edges can go through one vertex, leaving one edge adjacent to it. These remaining edges do not form a circuit and we do not have a partition of K_n .

⁴ Argue on the parity: in K_{n-1} , all vertices have odd degree. They must each be endpoint of at least one Hamiltonian path, thus exactly once.

3.6. De Bruijn graphs and magic tricks

Rauzy graphs were quickly introduced in example 1.48. Recall that an *alphabet* is a finite set and a *word* is a finite sequence of symbols belonging to the alphabet.

DEFINITION 3.19.— Let A be a finite alphabet. Let $n \ge 1$ be an integer. The de Bruijn⁵ graph of order n over A is a digraph whose set of vertices is A^n . Let v, w be words of length n. There is an edge from v to w if there exist symbols $a, b \in A$ such that vb = aw. We take the convention that the label of this edge will be b (but depending on the situation, we can similarly construct a graph whose labeling is given by a). Note that such a graph is always strongly connected.

Example 3.20.— Consider a binary alphabet $A = \{0,1\}$. The de Bruijn graph of order 3 over A is depicted in Figure 3.8.

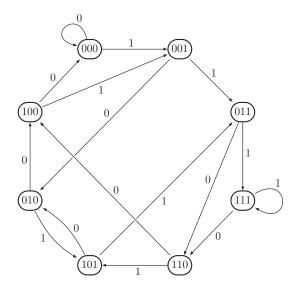


Figure 3.8. The de Bruijn graph of order 3 for a 2-symbol alphabet

⁵ Nicolaas Govert de Bruijn (1918–2012) acknowledged [BRU 75] that C. Flye Sainte-Marie has the priority about what we call nowadays de Bruijn graphs [FLY 94]. See [ALL 03, p. 343].

THEOREM 3.21.— The de Bruijn graph of order $n \ge 1$ over an alphabet A is both Eulerian and Hamiltonian.

PROOF.— It is clear from the definition that the out-degree of every vertex in the de Bruijn graph G_n of order $n \geq 1$ is exactly #A. For every word $u = u_1 \cdots u_n$, there is an edge of label u_n from $au_1 \cdots u_{n-1}$ for all $a \in A$. Hence the in-degree of every vertex in the de Bruijn graph G_n of order $n \geq 1$ is exactly #A. From lemma 1.42, we deduce that G_n is Eulerian.

The graph G_1 is trivially Hamiltonian. From an Eulerian circuit in G_n , we can deduce a Hamiltonian circuit in G_{n+1} . An edge with label a starting from a vertex v in G_n corresponds to the word va of length n+1, which is a vertex in G_{n+1} . Thus, there is a one-to-one correspondence between the edges of G_n and the vertices of G_{n+1} . From this correspondence, we deduce from any Eulerian circuit in G_n , a Hamiltonian circuit in G_{n+1} .

Let us make a final digression about the so-called *de Bruijn words* that will permit us to devise a nice magic trick.

DEFINITION 3.22.— Let $m \ge 1$ be an integer. We let $\mathbb{Z}/(m\mathbb{Z})$ denote the ring of integers modulo m. A circular word of length m over the alphabet A is a map $c: \mathbb{Z}/(m\mathbb{Z}) \to A$. Since $(m-1)+1 \equiv 0 \mod m$, we get the following definition for the factors of a circular word. Let c be a circular word of length m. Let i, j be integers such that $0 \le j - i < m$. The word

$$c(i \bmod m) \cdots c(j \bmod m)$$

is a factor of c. As an example, the word c= abba considered as a circular word of length 4 has the four factors abb, bba, baa, aab of length 3.

As a consequence of theorem 3.21, we obtain the following result.

COROLLARY 3.23 (de Bruijn Words).— [BRU 46]. Let $n \ge 1$ and A be an alphabet. There exists a circular word of length $(\#A)^n$ containing exactly once all the words in A^n as factors. Such a word is called a de Bruijn word.

As an example, the word 1111010010110000 can be seen as a circular word of length 16 containing the 16 distinct words in $\{0,1\}^4$ as factors.

PROOF.— Since the de Bruijn graph of order n is Hamiltonian, the label of a Hamiltonian circuit provides an expected circular word. Note that the $(\#A)^n$ vertices (i.e. words of length n over A) are visited exactly once. No shorter circular word can contain all the $(\#A)^n$ words.

This corollary permits us to devise a quite impressive magic trick (I did it more than 50 times and it always produces some effect on the audience). I saw for the first time this trick as an introduction to a research seminar given by Raphaël Jungers who himself held the trick from another mathematician Persi Diaconis. Based on the technique of the "chain", it is a beautiful application of combinatorics (on words).

The preparations consist of the magician in ordering his deck of cards. Let us say that he will proceed as in Table 3.1 (first from left to right and second, line by line).

Q♡	(Red)	$J\diamondsuit$	(Red)	7♦	(Red)	8 %	(Red)	$K \diamondsuit$	(Red)
7 .	(Black)	1.	(Black)	K♠	(Black)	1 🐥	(Black)	8♠	(Black)
9♡	(Red)	J♠	(Black)	Q♠	(Black)	10	(Black)	$Q\diamondsuit$	(Red)
7♡	(Red)	10	(Black)	J♣	(Black)	10♡	(Red)	9♠	(Black)
9\$	(Red)	K♣	(Black)	Q♣	(Black)	$8\diamondsuit$	(Red)	$J \heartsuit$	(Red)
1♡	(Red)	8♣	(Black)	$10\diamondsuit$	(Red)	9♣	(Black)	$K \heartsuit$	(Red)
1♦	(Red)	7♠	(Black)						

Table 3.1. A de Bruijn "chain"

Now proceed to the trick. The magician asks a spectator (or several spectators, this makes the trick even more spectacular) to cut the deck. Then each of six spectators picks one card, each time, the first of the heap without revealing anything to the magician. The first five announce aloud only the color (red or black) of their card. The magician then guesses the exact value of the sixth card. The magician can even find the exact value of the other five distributed cards.

How and why does it work? Look at the sequence of colors given by the arranged deck of cards:

RRRRRBBBBBRBBBRRBBRRBBRRRBRBRRB [3.2]

We claim that it is a de Bruijn word of order 5. Therefore, if we cut the deck, then we make a circular permutation of the cards but a de Bruijn word is a circular word. So it is not affected by this modification. Moreover, every factor of length 5 occurs exactly once so when the five spectators announce loudly the color of their card, the magician knows exactly where the deck was cut. He just has to memorize the sequence of 32 cards. When I do the trick, I use a little computer program that I call "my assistant" whose only task is to remember the sequence instead of me. To add some dramatic effect, the program displays

hundreds of cards but six of them appearing in some specific positions are relevant for me. For other similar tricks based on such a uniqueness property, see the useful book [DIA 12] where many mathemagical tricks are presented. See also [CHU 92, BLA 11] for more insight on the mathematical notion of *universal cycle*: this is again the idea that we know precisely a position in a given combinatorial structure $\mathbb S$ because some specific map provides different evaluations for distinct positions within $\mathbb S$. This question is also related to the notion of Gray code.

3.7. Exercises

- 1) Prove that the Petersen graph (Figure 1.8) is not Hamiltonian.
- 2) Prove that corollary 3.7 is a consequence of theorem 3.12.
- 3) Build a de Bruijn graph of order 5 over a 2-symbol alphabet and check that the word [3.2] is indeed a de Bruijn word.
- 4) Let G be a bipartite graph where V is partitioned into two subsets of different sizes. Prove that G is not Hamiltonian.
- 5) What is the maximal number of edges (in terms of the number n of vertices) that a simple graph G may have if $G \neq K_n$ and G is equal to its closure?
- 6) Let $n \geq 3$. What is the maximal number of edges (in terms of the number n of vertices) that a simple non-Hamiltonian graph may have?
- 7) Study the paper [BON 71] where Ore's theorem (corollary 3.7) is strengthened. Not only Hamiltonicity is considered but *pancyclicity*. A graph G is *pancyclic* if it contains cycles of all lengths in $\{3, \ldots, \#V(G)\}$.
- 8) This exercise is hard (*Lempel's conjecture*): Prove that the minimum number of vertices which, if removed from the de Bruijn graph of order n, will leave a graph with no cycles is

$$\frac{1}{n} \sum_{d|n} \varphi(\frac{n}{d}) \, 2^d$$

where φ is the Euler's totient function. This number is also the maximum number of vertex-disjoint cycles into which the graph can be decomposed [MYK 72].

Topological Sort and Graph Traversals

The main theme of this chapter is acyclicity. A connected graph with no cycle is a tree. There are several ways to visit the vertices of a tree. More generally, if a digraph has no cycle, then its vertices may be ordered in such a way that if (a,b) is an edge, then the index associated with a is less than the one associated with b. This ordering is called a topological sort.

4.1. Trees

In this section, we consider only unoriented graphs. Directed trees will only be considered in section 8.6. Trees are ubiquitous in computer science to manipulate various forms of data. As an example, when considering formal grammar, we associate with a string, a parse tree (or derivation tree) according to the rules of the grammar used to build the string.

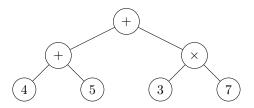


Figure 4.1. A parse tree associated with $4 + 5 + 3 \times 7$

The tree depicted in Figure 4.1 permits one to associate a value with an expression to be computed. To that end, we have to properly traverse the tree (see postorder traversal below).

DEFINITION 4.1 (Tree).— A tree is a simple connected acyclic graph. A simple graph whose connected components are trees l is a forest. A **rooted** tree is a pair (G, v_0) where G is a tree and v_0 is a vertex of G. In that case, a vertex u has level (or height) k when $d(v_0, u) = k$. This naturally induces an orientation of the edges from vertices of level ℓ to adjacent vertices of level $\ell+1$. With this induced orientation, we can thus speak of the successor of a vertex, usually called a child. If (G, v_0) is a rooted tree, a rooted subtree of G with root u is the subgraph induced by $succ^*(u)$ where we recall that $succ^*(v) := \{u \in V \mid v \to u\}$. A vertex of degree 1 in a tree is called a leaf.

REMARK 4.2.— An alternative recursive definition of trees is the following one. A single vertex is a tree. If $T_1, \ldots, T_k, k \geq 1$, are trees with disjoint sets of vertices and if v is a new vertex not in $V(T_1) \cup \cdots \cup V(T_k)$, then the graph obtained by adding k edges joining v to one vertex of each of the T_i 's is a tree. (Proof left as an exercise. You can even reduce the procedure to adding one new vertex attached with a new edge).

Let us make a few important observations about trees:

- 1) There is exactly one path between any two distinct vertices of a tree.
- 2) If we add an edge connecting two vertices of a tree, we create a cycle.
- 3) Note that all the edges of a tree are bridges. Conversely, a connected graph all of whose edges are bridges is a tree. Simply remember that a bridge does not belong to any cycle.

LEMMA 4.3.— A tree with at least two vertices contains at least one vertex of degree 1.

PROOF.— Assume that we have a connected graph where all vertices have a degree of at least 2. As in the proof of proposition 1.42, we conclude that the graph contains a closed trail and, in particular, a cycle. This contradicts the fact that we have a tree.

LEMMA 4.4.— If G = (V, E) is a tree, then 1 + #E = #V.

¹ You have to read a book entitled "advanced graph theory" to learn that a forest is made of trees.

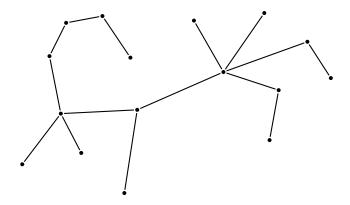


Figure 4.2. A tree

PROOF.—Proceed by induction on #V. The only tree with two vertices is K_2 and the result holds. Assume that G is a tree with at least three vertices. From the previous lemma, there exists a vertex v of degree 1. The graph G-v is still a tree with (#E)-1 edges and (#V)-1 vertices. The conclusion follows from the induction hypothesis applied to this tree.

We adapt definition 1.16.

DEFINITION 4.5 (Spanning Tree).— A tree H=(W,F) is a spanning tree of the multigraph G=(V,E) if W=V (and implicitly, $F\subseteq E$). In particular, since H is connected, for every vertex $v\in V$, there exists an edge $f\in F$ such that v is an endpoint of f.

As an example, assume that an electrical company wants to add a new type of connection on its network. The company provides electricity to the consumers but would also start a service of broadband Internet connection using optical fiber. Such a service is expensive (wire lines must be upgraded and expenses have to be taken into account). Therefore, only some part of the existing network will be upgraded. Since every consumer wants access to the new service, the company will be looking for a spanning tree of its network.

In network protocol design, we can also mention the spanning tree protocol for Ethernet networks.

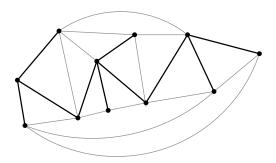


Figure 4.3. A spanning tree in a graph

PROPOSITION 4.6.— A graph is connected if and only if it contains a spanning tree.

PROOF.— Let G=(V,E) be a connected graph. Consider any connected spanning subgraph H of G having a minimal number of edges, meaning that removing any single edge of H leads to a graph that is not a connected spanning subgraph of G.

Note that since G is connected, such a subgraph H always exists: start with the graph G and remove as many edges as possible.

We claim that H is a tree. By minimality of H, every edge of H is a bridge.

Combining this proposition and lemma 4.4 yields to the following result.

COROLLARY 4.7.— If G = (V, E) is a connected graph, then #E > #V - 1.

To find a spanning tree of a graph, we can adapt the procedure $\mathsf{TRANSITIVECLOSURESUCC}(G,v)$ given in Table 1.2. The strategy is to start with one vertex v and add its neighbors, i.e. vertices at distance one, then add vertices at distance 2 of v and continue until all the vertices have been visited. This type of exploration of a graph is called a **breadth-first-search**. If the graph is rooted at v, this means that vertices are listed by increasing level. Note that the choice made at lines 8 and 9 ensures that we do not create any cycle. Recall that $\mathsf{N}(u)$ stands for the open neighborhood of u.

REMARK 4.8 (Minimum Spanning Tree).— The input is a weighted connected graph. It is natural to search for a minimum spanning tree: a

spanning tree whose sum of the weights of the edges is minimum among all the spanning trees. Many algorithms can be found. See, for instance, Prim's algorithm whose philosophy is very similar to the one of Dijkstra's algorithm for shortest paths: start with one vertex (it does not matter, every vertex belongs to the spanning tree), grow a tree by choosing a best possible edge that connects to a new vertex not yet in the tree and now that a new vertex has been added, see if there is some benefit of using an edge connecting this vertex to vertices already in the tree and modify accordingly. In its basic form, its time complexity is in $\mathcal{O}((\#V)^2)$. Also see Kruskal's algorithm. Many pointers and more efficient algorithms can easily be found on the web [GRA 85].

```
SPANNINGTREE(G)
```

```
1
     Choose a vertex v;
 2
     Component \leftarrow \{v\}; New \leftarrow \{v\}; Edges \leftarrow \emptyset;
 3
     while New \neq \emptyset,
 4
           do Neighbors \leftarrow \emptyset;
 5
               for all u \in New,
 6
                   do Neighbors \leftarrow Neighbors \cup N(u);
 7
               New \leftarrow Neighbors \setminus Component;
 8
               for all v \in New,
 9
                   do find an edge \{u, v\} with u \in Component;
10
                       Edges \leftarrow Edges \cup \{\{u,v\}\};
               Component \leftarrow Component \cup New;
11
12
     if Component \neq V(G)
13
        then return 'Error: G is not connected';
14
        else return (Component, Edges);
```

Table 4.1. Algorithm returning a spanning tree of G

We conclude this section with classical tree traversals. Let T=(V,E) be a rooted tree. We assume that the successors of every vertex have been ordered. For instance, for every level of the tree, the vertices have pairwise distinct indices. In Figure 4.4, we assume that successors are ordered from left to right. The prefixes "pre", "post" and "in" suggest when the root is processed.

Preorder traversal: first output the root, then recursively proceed to a preorder traversal of each subtree rooted at the successors of the root (if any) respecting the given ordering (from left to right) of the successors. For the tree in Figure 4.4, the traversal is 1, 2, 4, 8, 9, 5, 3, 6, 10, 11, 7, 12.

Postorder traversal: first recursively proceed to a postorder traversal of the subtrees rooted at the ordered successors of the root (if any), then output the root. For the tree in Figure 4.4, the traversal is 8, 9, 4, 5, 2, 10, 11, 6, 12, 7, 3, 1.

For **in-order traversal**, we assume that we have a binary rooted tree (each vertex has at most two successors). Proceed recursively to an in-order traversal of the subtree rooted at the first successor, then output the root, finally recursively proceed to an in-order traversal of the subtree rooted at the second successor of the root (if any). For the tree in Figure 4.4, the traversal is 8, 4, 9, 2, 5, 1, 10, 6, 11, 3, 12, 7.

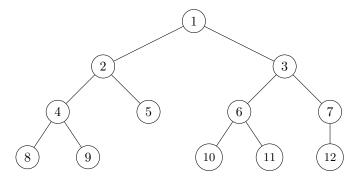


Figure 4.4. A rooted binary tree

There is one last way to search a tree. The philosophy of a **depth-first traversal** is to start from a vertex v_1 then go as far as possible visiting an unvisited neighbor from the most recently visited vertex. When the possible options only consist of previously visited vertices (line 6), go backward a minimal number of steps to find, among the options, a vertex not yet visited and proceed again from that one (lines 7–8). For the pseudo-code given in Table 4.2, the variable Component is an ordered list (v_1, v_2, \ldots) recording the visited vertices. For a practical implementation, we could also use a table. We have access to the length of this list, its last element, its *i*th element denoted by Component[[i]]. We can append an element v to a list (v_1, \ldots, v_k) to get the list (v_1, \ldots, v_k, v) . The algorithm is initialized with the empty list ().

For the tree in Figure 4.4, a depth-first traversal is 1, 2, 4, 8, 9, 5, 3, 6, 10, 11, 7, 12, when picking in line 8 of Table 4.2 an element of X we have chosen the smallest one. Depth-first traversal is useful when considering backtracking methods. Looking for a solution of a combinatorial problem

(e.g. completing a Sudoku grid, putting eight queens on a chessboard so that no queen may take any other), we start with a candidate partial solution satisfying the constraints of the problem and try to build a larger candidate. If the partial candidate does not satisfy the constraint, we come back to an earlier stage and try an alternative.

```
DEPTHFIRSTTRAVERSAL(T, v_1)
1
    Component \leftarrow ();
2
    append v_1 to Component
3
    while length(Component) \neq \#V(T),
         do i \leftarrow length(Component);
4
5
             X \leftarrow \mathsf{succ}(Component[[i]]) \setminus Component;
6
             while X = \emptyset,
7
                  do i \leftarrow i - 1;
8
                      X \leftarrow \mathsf{succ}(Component[[i]]) \setminus Component;
9
             append an element of X to Component;
```

Table 4.2. Depth first search of T starting with v_1

REMARK 4.9.— A depth-first traversal can be applied to trees but also to other graphs.

Example 4.10.— We can apply tree traversals to get out of a maze². Indeed, a maze can be seen as a tree, see Figure 4.5, where vertices correspond to the entrance 1, the exit 8, the dead-ends 3,4,5,7 and positions where a choice may occur 2,6. Choices have been ordered from left to right. With a preorder traversal, it corresponds to sticking close to the left wall: 1,2,3,6,8 because of our ordering of the possible choices.

Example 4.11 (Formal Language Theory).— Here, we will give an example of an infinite tree. An alphabet A is a finite set, e.g. $\{a,b\}$. A (finite) word over A is a finite sequence of elements in A. A language is a set of finite words. Usually, a language is infinite, e.g. the set of words over $\{a,b\}$ having a prime number of a and an even number of b. Consider the infinite binary tree T_A whose set of vertices is A^* , the set of words over a. The root is the empty word a corresponding to the null sequence. There is an edge from the vertex a to

² If you like to be lost in mazes in a fun fair, do not read this example. It will spoil all the fun (when I was a kid, I liked it) – maybe use the trick to rescue your own children.

ua for all $a \in A$. The levels of this tree correspond exactly to the length of vertices. There are exactly $(\#A)^{\ell}$ vertices of level ℓ .

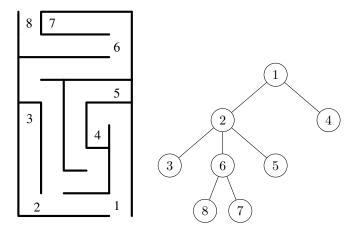


Figure 4.5. A maze and a tree representation

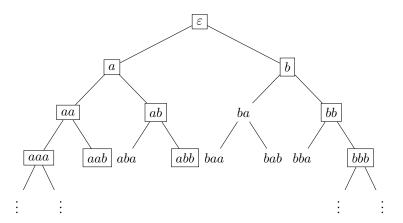


Figure 4.6. A tree associated with a language

Now, for a given language L, as a characteristic function, we color the vertices of this tree. A vertex u has color 1 if $u \in L$; and 0 otherwise. In Figure 4.6, we have considered the language of the words starting with an

arbitrary number of a (possibly 0) followed by an arbitrary number of b. Words in the language have been represented inside a box. In an equivalent way, these are the words without any factor ba.

Here is an appetizer for Chapter 7. In formal language theory, a language is said to be regular if the associated colored tree has only finitely many subtrees counted up to isomorphism. The notion of isomorphism will be discussed in definition 7.4 and section 7.2. In Figure 4.6, the reader can check that there are exactly three non-isomorphic subtrees: the ones rooted at ε , b and ba. For instance, the trees rooted at ε , a or an are isomorphic (see, for instance, [SUD 06]).

Comparing a graph with a tree can be useful. Measuring how close a graph is from a tree can be done by introducing the tree width. More can be found in [DIE 10, Chapter 12.3].

DEFINITION 4.12.— Let G = (V, E) be a graph. A tree decomposition of G is a tree T = (X, F) where the vertices of T are subsets X_1, \ldots, X_n of V, i.e. $X = \{X_1, \ldots, X_n\}$, such that

- 1) (vertex coverage) $\bigcup_{i=1}^{n} X_i = V \colon X_1, \dots, X_n$ are covering V;
- 2) (edge coverage) if $\{u, v\} \in E$, then there exists some i such that $u, v \in X_i$;
- 3) (coherence) the set F of edges satisfies the following. If X_k belongs to the (unique) path between X_i and X_j , then $X_i \cap X_j \subseteq X_k$.

The width of (X, F) is equal to $(\max_i \# X_i) - 1$. Since G may have several tree decompositions, the **tree width** of G is the minimum of the width among all the tree decompositions of G. A k-tree is a maximal graph of tree width k: adding an edge would increase its tree width.

EXAMPLE 4.13.— In Figure 4.7, we have depicted a connected graph. In Figure 4.8, we have represented a tree decomposition of this graph. This shows that the tree width of the graph is at most 3.

PROPOSITION 4.14.— Let G be a graph. The tree width of any subgraph of G is less than or equal to the tree width of G.

PROOF.- Left as an exercise.

THEOREM 4.15.— A connected graph has a tree width equal to one if and only if it is a tree.

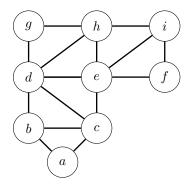


Figure 4.7. A graph to be decomposed

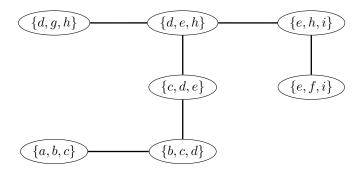


Figure 4.8. A tree decomposition of the graph in Figure 4.7

PROOF.— Left as an exercise. Consider a tree decomposition where each set X_i is reduced to an edge of the given tree.

PROPOSITION 4.16.— A graph has a tree width of at most k if and only if all its connected components have a tree width of at most k.

PROOF.- Left as an exercise.

Computation of the tree width is computationally challenging.

EXAMPLE 4.17 (Tree Width).— Given a graph G and an integer k, it is NP-complete to determine whether or not G has a tree width of at most k [ARN 87].

4.2. Acyclic graphs

In this section³, we are interested in digraphs (it will rapidly become clear that one can restrict oneself to simple digraphs). A directed multigraph G = (V, E) with n vertices has a **topological sort**, if there exists an *enumeration* $t: V \to \{1, \ldots, n\}$ of the n vertices of G such that

if
$$(a, b) \in E$$
, then $t(a) < t(b)$.

A typical example is given by a list of tasks to be achieved in some prescribed order. For instance, a student has to follow a series of courses to achieve his/her curriculum but some courses are prerequisite to other ones. The aim is to provide, if it exists, an ordered sequence of courses without any incompatibility: prerequisite courses are listed prior to the other ones. An example of such an enumeration is depicted in Figure 1.3. The ordering has a visual interpretation: all the edges are represented with the same direction "from left to right".

A necessary condition for the existence of a topological sort is obviously that the digraph does not contain any cycle (nor loop). The aim of this section is to show that such a condition is also sufficient (corollary 4.21).

LEMMA 4.18.— Let G be a directed (finite) multigraph without any cycle. Then, G has a source⁴ (respectively, a sink).

PROOF.— Since the graph is finite, the notion of (simple) path of maximal length is well defined. Let (v_1,\ldots,v_k) be such a path. We claim that v_1 is a source. Assume to the contrary that $\deg^-(v_1)>0$ and there exists an edge $(u,v_1)\in E(G)$. If u is in $\{v_1,\ldots,v_k\}$, then there is a cycle in G. If u is not in $\{v_1,\ldots,v_k\}$, then we can find a (simple) path (u,v_1,\ldots,v_k) longer than a maximal path. In both cases, we get a contradiction. The same argument applies to show that v_k is a sink.

PROPOSITION 4.19.— Let G be a directed (finite) multigraph. The multigraph has no cycle if and only if there exists a source and, for all sources v of G, G-v has no cycle.

PROOF.— The fact that the condition is necessary follows from the previous lemma. Assume that v is a source in G and that G - v has no cycle. Add the

³ Preparing this part, we were inspired by the lectures of V. Bouchitté, ENS Lyon, France.

⁴ For the definition, see page 7.

vertex v (and the corresponding edges attached to v) to build the whole graph G. We have to prove that G has no cycle. By contradiction assume that G has a cycle. Since G-v has no cycle, any cycle in G should visit v and thus the indegree of v in G is non-zero. This contradicts the fact that v is a source.

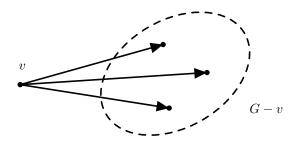


Figure 4.9. Illustration of the proof of proposition 4.19

A similar result can of course be stated in terms of sinks. We can derive an algorithm to test whether or not a digraph has a cycle. In the worst case, we have to visit all the vertices of the graph at each step of the loop, thus the time complexity⁵ of this method is quadratic in #E(G) + #V(G).

```
TESTINGCYCLICITY(G)
```

```
1 while there exists v such that deg^-(v) = 0,

2 do G \leftarrow G - v;

3 if G = \emptyset

4 then return G has no cycle;

6 else return G has a cycle;
```

Table 4.3. Algorithm determining whether *G* has a cycle

⁵ There exist better algorithms than the one described here. We can be a bit more clever than suppressing a vertex and then searching all the graph again. Indeed, simply maintain a list of the sources of the graph and when a vertex is suppressed, determine if new sources have been created in the resulting graph and add them to the list (see [KAH 62]).

THEOREM 4.20.— Let G = (V, E) be a directed (finite) multigraph. The multigraph has no cycle if and only if there exists an enumeration $t: V \to \{1, \dots, \#V\}$ of the vertices for which, for all $j \leq \#V$, v_j denotes the unique vertex v such that t(v) = j, and the indegree of v_i in the subgraph induced by $V \setminus \{v_1, \dots, v_{i-1}\}$ is zero for all $i \leq \#V$.

PROOF.— If the multigraph has no cycle, then an enumeration with the required properties is provided by proposition 4.19 (or the algorithm in Table 4.3).

Let n = #V. Now assume that we have an enumeration of the vertices v_1, \ldots, v_n following the requirements of the statement. For $i \leq n$, we let G_i denote the subgraph induced by

$$V \setminus \{v_1, \dots, v_{i-1}\} = \{v_i, \dots, v_n\}.$$

We proceed by induction on $i=n,n-1,\ldots,1$. The result is clear for i=n: the graph is reduced to a single vertex v_n and obviously has no cycle. Assume that G_i has no cycle. We have to prove that G_{i-1} has no cycle. The reasoning is exactly the same as in the proof of proposition 4.19 and is depicted in Figure 4.9. If G_{i-1} contains a cycle, this cycle should visit v_{i-1} but, by assumption, the indegree of v_{i-1} in G_{i-1} is zero.

COROLLARY 4.21.— A directed finite multigraph has a topological sort if and only if it has no cycle.

PROOF.— This is a direct consequence of the previous theorem. A topological sort is given by the enumeration t. Indeed, notice that every edge (v_i, v_j) is such that i < j.

A directed acyclic graph is usually shortened as DAG.

REMARK 4.22.— Note that in general a topological sort is not unique. Let G be a directed multigraph and

$$S(G)=\{v\in V(G)\mid \deg^-(v)=0\}$$

be the set of sources of G. The set T(G) of topological sorts of G is given recursively by

$$T(G) = \bigcup_{v \in S(G)} \{ \texttt{concat}(v,t) \mid t \in T(G-v) \}$$

where concat corresponds to appending a sequence t after a first element v.

Let G be a tree rooted at v_0 . We have seen in definition 4.1 that a fixed root induces an orientation of the edges of G. This digraph has no cycle. The vertices of G can thus be ordered using a topological sort. The preorder traversal of a rooted tree is clearly a topological sort.

4.3. Exercises

- 1) Enumerate, up to isomorphism (see definition 7.4), all trees with 6 (respectively, 7, 8) vertices. How many trees, up to isomorphism, have exactly n vertices and a diameter equal to 2 (respectively, 3)?
- 2) Build two non-isomorphic trees with 12 vertices where exactly three vertices have degree 3 and a unique vertex has degree 2.
- 3) Generalizing lemma 4.4, prove that a forest with n vertices and k connected components has n-k edges.
- 4) Prove that a tree with at least two vertices has at least two vertices of degree 1 (i.e. two leaves).
 - 5) Prove that the number of leaves of a tree T with $n \ge 2$ vertices is

$$2 + \sum_{\substack{v \in V(T) \\ \deg(v) \geq 3}} (\deg(v) - 2).$$

- 6) Prove that in every tree, any two paths of maximal length have a common vertex.
- 7) Let G be a connected graph where each vertex has degree either 1 or 4. Let k be the number of vertices of degree 4. Prove that G is a tree if and only if the number of vertices of degree 1 is 2k + 2.
 - 8) Build a graph with a tree width equal to two.
 - 9) Work out a proof for propositions 4.14 and 4.16 and theorem 4.15.
 - 10) Build a digraph having two topological sorts.
- 11) Devise an algorithm for a topological sort of a digraph based on a depth-first traversal of the graph (see page 74).
- 12) Prove that if a DAG has a Hamiltonian path, then the topological sort is unique. Conversely, prove that if a topological sort of a DAG is not a Hamiltonian path, then the topological sort is not unique. As a consequence of this exercise, either a DAG has several topological sorts or a Hamiltonian path. Even though deciding the existence of a Hamiltonian path is a NP-complete

problem for a general instance (see example 2.8), this problem belongs to P when restricted to DAG.

- 13) Given a DAG G=(V,E), we can define a partial order \prec on V by $u \prec v$ if there exists a path from u to v in G. Recall that a **partial order** is a binary relation over V which is reflexive $(u \prec u)$, antisymmetric (if $u \prec v$ and $v \prec u$, then u=v) and transitive (if $u \prec v$ and $v \prec w$, then $u \prec w$). This is simply a reformulation of $u \to v$. Give an example of two DAGs on the same set V corresponding to the same partial order \prec on V. Show that there exists a DAG on V with a minimal number of edges corresponding to this partial order. It is called the *transitive reduction* of G.
- 14) For an application to string algorithms, have a look at a directed acyclic word graph [CRO 97b, CRO 97a]. It is an efficient data structure used in the analysis of repetitions in a text, e.g. DNA sequences.
- 15) For a digraph G=(V,E), we define a *kernel* of G as a subset W of independent vertices, i.e. for all $v,w\in W, (v,w)\not\in E$, which is absorbing: for all $u\not\in W$, there exists $w\in W$ such that $(u,w)\in E$.
 - a) prove that the cycle of length 4 has two kernels;
 - b) build a digraph with no kernel;
- c) prove that an acyclic digraph has a kernel. If the DAG is finite, what about the uniqueness of the kernel?
- d) if E is symmetric, i.e. G is an undirected simple graph, then prove that G has a kernel.

Building New Graphs from Old Ones

5.1. Some natural transformations

We have already seen (induced) subgraphs in definition 1.16. With this process, we build a new graph from another one by deleting some edges and vertices. In this chapter, we present various constructions of graphs. Some resulting graphs will have fewer vertices and edges but for products, we will build larger graphs. At first, since V(G) and E(G) are sets (or multisets), Boolean operations may be applied to these sets. As an example, assume that two graphs G_1 and G_2 are defined over the same set of vertices. We could consider the set of edges $E(G_1) \cup E(G_2)$, $E(G_1) \cap E(G_2)$, etc. We can also consider the disjoint union of graphs where it is assumed that $V(G_1)$ and $V(G_2)$ are disjoint and the set of edges is the union $E(G_1) \cup E(G_2)$.

Let us start with the special case of a subgraph induced by the vertices at distance at most k from a given vertex. In Figure 5.1, we have represented the so-called Watkins snark¹ and the subgraph made up of the vertices at a distance at most four from the leftmost vertex in the representation.

For the next construction, it is useful to recall the reflexive and transitive closure discussed in section 1.2.1.

¹ It is a connected, bridgeless 3-regular graph. There is a proper coloring of the edges with four colors (it is the dual notion of a proper coloring of the vertices discussed in example 2.10). The term *snark* is due to Martin Gardner. For a complete definition, see, for instance, [CAV 98].

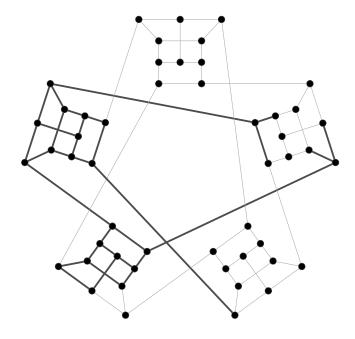


Figure 5.1. A subgraph of the Watkins snark

DEFINITION 5.1.— Let G=(V,E) be a digraph. The transitive closure is the smallest digraph G'=(V,E') having G as a subgraph such that if there is a path from u to v in G, then $(u,v)\in E'$, i.e. E is a subset of E' and no strict subset of E' has this property.

The closure depicted in Figure 5.2 has been computed using the Roy–Warshall algorithm described in Chapter 1. Compare this notion with the transitive reduction introduced in exercise 13 in section 4.3.

There are several non-equivalent definitions for the *power* of a graph (related to algebraic graph theory discussed in Chapter 8 and, in particular, what we will use in theorem 9.12 is not quite what we define here).

DEFINITION 5.2.— Let G = (V, E) be a digraph. The nth power (respectively, strict nth power) of a digraph is the smallest graph G' = (V, E') having G as a subgraph such that if there is a path from u to v of length at most n (respectively, exactly n) in G, then $(u, v) \in E'$.

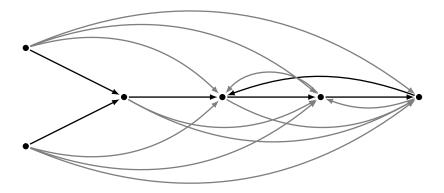


Figure 5.2. Transitive closure of a digraph (added edges in gray)

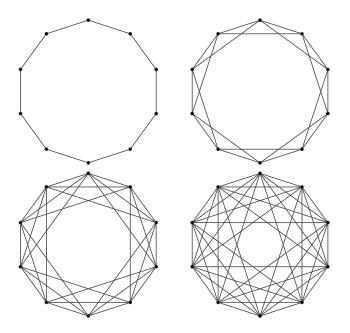


Figure 5.3. The first few powers of a cycle of length 10

DEFINITION 5.3 (Edge contraction).— In a multigraph, the edge contraction of an edge $\{u,v\}$ where $u\neq v$ consists of deleting this edge and then merging the two vertices u,v into a new one w. All the remaining edges that were incident to u or v are replaced with edges incident to w, i.e. every edge $\{x,u\}$ or $\{x,v\}$ is replaced with an edge $\{x,w\}$. In particular, $k\geq 0$ loops on u and $\ell\geq 0$ loops on v are replaced with $k+\ell$ loops on w. If for some vertex $y\neq u,v$, $r\geq 0$ edges $\{y,u\}$ and $s\geq 0$ edges $\{y,v\}$ exist, then the resulting graph will have r+s edges between y and y. So edge contraction in a simple graph usually leads to a multigraph. Starting with a multigraph, if there are y0 edges between y1 and y2 on one of these edges is contracted, the resulting graph will have y1 loops attached to the new vertex y2 not counting the possible loops initially on y3 or y4. We will make use of this construction in section 5.4.

Some authors consider after this edge contraction the underlying simple graph as discussed below. So be careful when using various resources.

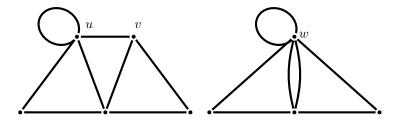


Figure 5.4. Contracting the edge $\{u, v\}$

There are several natural transformations that can be applied to a graph:

- replacing a directed multigraph with its **underlying digraph** where multiple edges (or loops) have been replaced with single edges (or loops), i.e. the non-zero multiplicities of the elements in the multiset E(G) are set to one;
- replacing a digraph with its **underlying simple digraph**, i.e. loops are deleted:
- reversing the edges of a directed multigraph, i.e. each edge (u,v) is replaced with (v,u) according to the multiplicity. In particular, for each vertex, indegree and outdegree are exchanged;
- finally, we can replace a digraph with its **unoriented version**, i.e. a minimal number of edges are added so that the set E(G) is symmetric.

In Figure 5.5, we have represented a directed multigraph, then from left to right, the underlying digraph and simple digraph and finally the reversed version of the original multigraph.

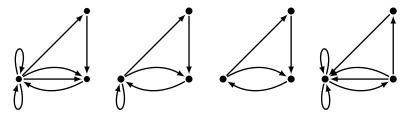


Figure 5.5. Starting with a directed multigraph...

The next notion will be useful in section 6.6 when dealing with (topological) minors.

DEFINITION 5.4.— An elementary subdivision of a multigraph G is a new graph with an extra edge and an extra vertex added in the following way. One edge $\{u,v\}$ (or a loop when u=v) is replaced with two new edges $\{u,w\}$ and $\{w,v\}$ where w is a newly created vertex. A multigraph H is a **subdivision** (also known as an expansion) of G if it can be obtained after applying finitely many elementary subdivisions starting with G.

Two multigraphs G, G' are **homeomorphic**² if there exists one multigraph H such that H is a subdivision of both G and G'.

REMARK 5.5.— When an elementary subdivision is applied and an edge e is divided into two edges e_1 and e_2 , it is useful to observe that contracting the edge e_1 (or equivalently e_2) gives back the original graph.

The three graphs in Figure 5.6 are subdivisions of the graph depicted in Figure 5.7.

DEFINITION 5.6.— The complement of a digraph G=(V,E) is the digraph $G^c=(V,V\times V\setminus E)$. We usually consider the underlying simple digraph (without loops). This definition applies naturally to undirected graphs.

² Indeed, homeomorphism is a fundamental notion in topology. The name is well-chosen because, as we will explain in section 6.1, this notion has the same topological meaning when a graph is considered as a topological space.

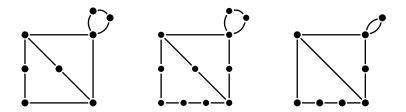


Figure 5.6. From left to right, three graphs G, H, G' where G and G' are homeomorphic (H is a subdivision of both)

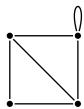


Figure 5.7. A graph to be subdivided

5.2. Products

We conclude this chapter by presenting two usual product constructions. A motivation to define these products is to build new graphs with prescribed properties about their spectrum, their connectivity, their group of automorphisms, etc.

Let $G_1=(V_1,E_1)$ and $G_2=(V_2,E_2)$ be two digraphs. For the two products, the set of vertices will be the Cartesian product $V_1\times V_2$ of the two sets of vertices.

The **direct product** (also known as cross product, conjunction or tensor product) of G_1 and G_2 is denoted $G_1 \times G_2$ and the set of edges is given by

$$E(G_1 \times G_2) := \{((x_1, x_2), (y_1, y_2)) \mid (x_1, y_1) \in E_1, (x_2, y_2) \in E_2\}.$$

The Cartesian product of G_1 and G_2 is denoted $G_1 \square G_2$ and

$$E(G_1 \square G_2) := \{((x, z), (y, z)) \mid (x, y) \in E_1, \ z \in V_2\}$$
$$\cup \{((x, y), (x, z)) \mid (y, z) \in E_2, \ x \in V_1\}.$$

Taking multiplicities into account, these constructions can be extended to directed multigraphs. In Figure 5.8, we have depicted these two products.

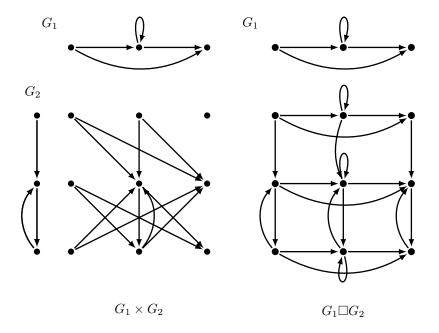


Figure 5.8. Direct product and Cartesian product of two digraphs

As a possible application, when we will be dealing in Chapter 8 with the eigenvalues of a directed multigraph G, it is easy to see that the Cartesian product of a directed acyclic graph with G has the same eigenvalues but the algebraic multiplicities are multiplied by the number of vertices of the DAG (left as an easy exercise). Another example is to consider the total domination number of the Cartesian product of two graphs.

If you search a little on the web, you will find many other products of graphs such as: *lexicographic product* [GEL 75], *zig-zag product*, *rooted product* where a rooted copy of G_2 is "inserted" at every vertex in G_1 , *corona product* [FRU 70], or, the *strong product* of graphs where the set of edges is given by $E(G_1 \times G_2) \cup E(G_1 \square G_2)$.

5.3. Quotients

Let us mention the notion of *quotient* of a digraph G=(V,E). Let B_1,\ldots,B_k forming a partition P of V. We assume that G is finite, but the definition can be extended to infinite graphs. In particular, if \sim is an equivalence relation over V, then V is partitioned into equivalence classes for \sim . The quotient of V by \sim is the set of these equivalence classes and is denoted by V/\sim . For instance, \leftrightarrow is an equivalence relation and if vertices have a color, then "having the same color" is another equivalence relation over V. We will also introduce another equivalence relation over V in definition 9.31.

DEFINITION 5.7.— The quotient graph induced by the partition P is the digraph whose set of vertices is P and there is an edge from B_i to B_j , $i \neq j$, if there exist $u \in B_i$, $v \in B_j$ such that $(u, v) \in E$.

We will use this quotient to reduce a digraph to its strongly connected components (SCCs), see section 9.4.1. Indeed, we may partition V into its SCCs as depicted in the following example.

EXAMPLE 5.8.— Consider the digraph depicted in Figure 1.13. It has four SCCs and the vertices have been ordered accordingly. The quotient graph with respect to \leftrightarrow is depicted in Figure 5.9.

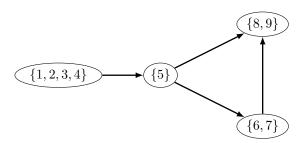


Figure 5.9. Quotient of a graph for ↔

Note that this reduced graph is acyclic. The SCCs can thus be topologically sorted.

5.4. Counting spanning trees

As an application (but to be honest, this one is not efficient), we present a recursive formula counting the number of spanning trees of a connected multigraph G. The definition of a spanning subtree was given in definition 4.5. We let $\tau(G)$ denote the number of spanning trees of G. We are NOT counting trees up to isomorphism³: if two trees have the same shape but do not share exactly the same edges, then they are counted twice. In Figure 5.10, the trees made up of the edges 1, 2, 3 or 2, 3, 4 are isomorphic but they are not made up of the same set of edges. They are both counted. Consider the graph depicted in Figure 5.10. It has eight distinct spanning trees⁴



Figure 5.10. How many spanning trees?

For the oriented case, see section 8.6.

PROPOSITION 5.9 (Contraction/deletion formula).— Let G be a multigraph and e be an edge that is not a loop. We have

$$\tau(G) = \tau(G - e) + \tau(G \cdot e)$$

where G-e (respectively, $G \cdot e$) is the multigraph obtained by erasing (respectively, contracting) the edge e.

One can apply this formula recursively for every resulting graph and for every edge e that is not a loop and such that G-e remains connected. Thus we apply this formula until we get trees or trees with extra loops. An example is given in Figure 5.11 where we highlight the chosen vertex when the formula is applied. We got eight trees (or trees with loops). This means that $\tau(G)=8$.

³ This notion will be given in definition 7.4.

⁴ They are built from the vertices: 123, 234, 341, 412, 153, 254, 125, 345.

PROOF.—The edge e is fixed. The set of the spanning trees of G is split into the trees containing e and those that do not contain e. In the latter case, the number of trees spanning G and not using e is equal to $\tau(G-e)$.

Observe that there is a one-to-one correspondence between the set of trees spanning G and containing e and the set of trees spanning $G \cdot e$. Indeed, every tree in G using e, when contracting this edge, yields a tree in $G \cdot e$ and conversely.

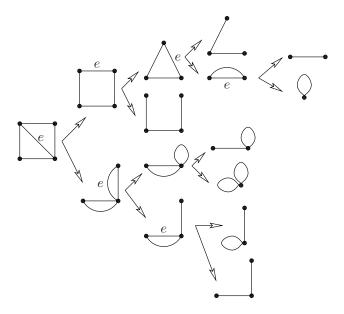


Figure 5.11. Recursive application of contraction/deletion formula

REMARK 5.10.— Applying the above contraction/deletion formula recursively is not efficient. Making use of algebra, we will see a much more direct way to compute $\tau(G)$ in corollary 8.44. We will also have a similar argument of contraction/deletion when dealing with colorings, see Proposition 7.26.

5.5. Unraveling

Let G = (V, E) be a (finite) digraph. We choose a vertex $v \in V$. The unraveling of G from v is an infinite tree (if G has at least a cycle) whose set of vertices is in one-to-one correspondence with the set of walks in G starting

from v. Thus, not only does this operation provides us with an infinite tree but we will discuss in depth walks in digraph in the second half of this book. In particular, we are interested in counting the number of walks of length n, i.e. the number of vertices on the nth level of the unrayeled tree.

EXAMPLE 5.11.— In Figure 5.13, we have represented the first few levels of the unraveling of the digraph depicted in Figure 5.12 from vertex v. Counting the number of vertices on each level of the tree, we see that there are exactly 1,1,2,3,5 walks of respective length 0,1,2,3,4 starting from v in the original graph.



Figure 5.12. A digraph to be unravelled

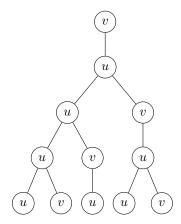


Figure 5.13. Unravelling from vertex v

By reading the sequence of labels in the vertices of the tree, we recover the walk considered in the original graph.

To conclude this chapter, let us mention that we will encounter another construction of graphs: the *dual* of a planar graph (see definition 6.8). We have also considered the notion of a *line graph* in exercise 21 in section 1.8.

5.6. Exercises

- 1) Reconsider the construction of the n-cube Q_n (exercise 12 in section 1.8) as a Cartesian product of graphs.
- 2) Let G be a graph and G^c be its complement (see definition 5.6). Prove that if G is not connected, then G^c is connected. Prove that if v is a cut-vertex of G, then v is not a cut-vertex of G^c .
- 3) A graph is *self-complementary* if G and G^c are isomorphic. Prove that there is no self-complementary graphs with three vertices. Find a self-complementary graph with four (respectively, 5) vertices.
- 4) Consider the direct product and Cartesian product of graphs. Is is true that if G and H are regular graphs, then $G \times H$ (respectively, $G \square H$) is a regular graph? Same question for bipartite graphs.
- 5) Cayley [CAY 89] proved that the number of trees spanning K_n is equal to $\tau(K_n) = n^{n-2}$. Prove this result by yourself or carry out a search. (It is also a direct application of the forthcoming theorem 8.41).
- 6) Prüfer⁵ proved Cayley's formula given in the previous exercise by devising a clever coding for trees. Let T be a tree with vertices labeled $\{1,\ldots,n\},\ n\geq 2$. We produce a sequence s(T) of n-2 integers by considering at each step i the leaf v (i.e. a vertex of degree 1) of smallest label. Output the degree of the unique neighbor of v, and then delete the vertex v. Repeat the procedure with the resulting tree until only two vertices remain. Figure 5.14 shows an application of this algorithm. It produces the sequence (4,2,3,2). For another example, the tree in Figure 4.4 is coded by the sequence (3,2,3,2,2,3,3,2,2,2). Prove that the set of trees with n vertices of label $\{1,\ldots,n\}$ is in one-to-one correspondence with the set of (n-2)-tuples of elements in $\{1,\ldots,n\}$. It is clear that each tree gives an (n-2)-tuples of elements in $\{1,\ldots,n\}$. The converse is not so obvious. Provide an algorithm that for a given sequence produces the corresponding tree.
 - 7) Which trees have a constant Prüfer coding?
- 8) Which trees have a Prüfer coding where all elements are pairwise distinct?
 - 9) Give all the spanning trees of K_4 and their Prüfer codings.
 - 10) Show that the Petersen graph has 2,000 spanning trees.

⁵ Heinz Prüfer (1896–1934) is mostly known for his contributions in group theory (e.g. Prüfer p-group).

11) The next result is more difficult, see [BER 89]. The number of trees with n vertices v_1, \ldots, v_n with respective degrees d_1, \ldots, d_n is equal to the multinomial coefficient

$$\binom{n-2}{d_1-1\cdots d_n-1} = \frac{(n-2)!}{(d_1-1)!\cdots (d_n-1)!}$$

provided that at least such a tree does exist.

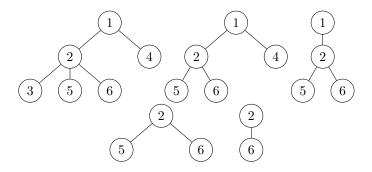


Figure 5.14. Suppressing vertices when computing the Prüfer coding of a tree

Planar Graphs

Roughly speaking a planar graph is a graph that one can represent (see remark 1.3) in the plane in such a way that no two edges intersect. Thus, if you think about wires connecting various electrical components, it is indeed desirable (when building a transistor, for instance) to prevent short circuits by avoiding crossings. In this chapter, orientation does not play any role. So, it is easier to think about unoriented multigraphs.

The first section is quite technical. It presents in a rigorous manner planarity that allows us to introduce the notion of a face. Then, we study the classical Euler's formula linking the number of faces, edges and vertices in a planar graph. To make a link with Euclidean geometry, we introduce Steinitz' theorem on convex polyhedra. Then, we color the faces of a planar graph with a minimal number of colors. Finally, Kuratowski's theorem allows us to introduce the famous theorem of Robertson–Seymour about forbidden minors.

6.1. Formal definitions

To give precise definitions¹ of the objects we will be dealing with (mostly planar graphs, faces and dual of a graph), we need to make use of topology (so we can play with continuous maps, interior, connected components, etc.). For classical textbooks, for instance, see [ARM 83, MOH 01]. If an informal presentation is enough, then proceed directly to the next section!

¹ This section is inspired by notes by C. de Verdière, also see [BEI 09].

A multigraph G=(V,E) can be seen as a topological space \mathcal{X}_G , hence we may define a continuous map from \mathcal{X}_G to another topological space such as \mathbb{R}^2 or the usual sphere \mathbb{S}^2 included in \mathbb{R}^3 . Each edge e is associated with a topological space \mathcal{X}_e homeomorphic² to [0,1].

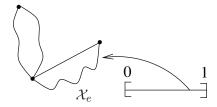


Figure 6.1. A graph seen as a topological space

 \mathcal{X}_G is the disjoint union of the \mathcal{X}_e 's, $e \in E$. If two edges e and e' have a common vertex, then the corresponding endpoints in \mathcal{X}_e and $\mathcal{X}_{e'}$ are identified as the same element (formally, this identification is a quotient).

DEFINITION 6.1.— A multigraph G=(V,E) is planar if there exists an embedding of G on \mathbb{R}^2 , that is a continuous one-to-one map φ from \mathcal{X}_G to \mathbb{R}^2 , which maps distinct vertices in V to distinct points in \mathbb{R}^2 and edges in E to arcs (i.e. arcs of curves) of \mathbb{R}^2 such that:

- **P.1** for every edge e, the endpoints of the arc $\varphi(e)$ are the images by φ of the endpoints of e;
- **P.2** for every edge e, except possibly at its endpoints, $\varphi(e)$ is a simple path given by a continuous one-to-one map ν from [0,1] to $\varphi(e)$: the restriction of ν to the open interval (0,1) is one-to-one the relative interior of $\varphi(e)$ has no multiple points;
- **P.3** for every two distinct edges e, e', the relative interiors of $\varphi(e)$ and $\varphi(e')$ are disjoint;
- **P.4** for each edge e and each vertex v, $\varphi(v)$ does not belong to the relative interior of $\varphi(e)$.

² A homeomorphism $h:A\to B$ between two topological spaces A and B is a continuous one-to-one correspondence between A and B such that h^{-1} is also continuous.

Roughly speaking, P.2 means that when drawing an edge of G, we do not allow self-intersection. P.3 means that two distinct edges do not intersect and, finally, P.4 means that an edge cannot pass through some vertex.

For simple planar graphs, the next result is known as Fáry's theorem [FÁR 48]. Note that obviously loops and multiple edges cannot be represented with straight line segments only.

THEOREM 6.2.— A simple planar graph can be embedded on \mathbb{R}^2 using only straight line segments for drawing edges.

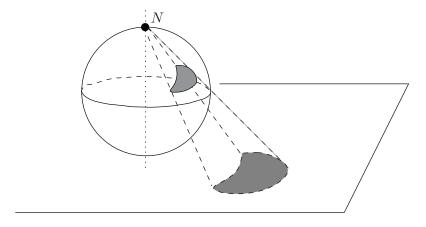


Figure 6.2. A stereographic projection

REMARK 6.3.— Using what is called a stereographic projection, see Figure 6.2, the plane \mathbb{R}^2 is homeomorphic to the sphere \mathbb{S}^2 where a point (that we call north pole) has been removed. Hence, a graph is planar if and only if there exists an embedding of G on \mathbb{S}^2 . Note that the closer a point is to the north pole N, the further it is from the origin of the plane (that coincides with the south pole of the sphere).

We are now ready to define the faces of a planar graph. In the next definition, we will clearly mention that we should formally speak of the faces of a graph embedding, but quickly enough, we will make no distinction between the graph and one of its embedding and freely speak of the faces of a graph. In particular, the number of faces is independent of the planar embedding (see remark 6.11).

Said otherwise, when speaking of a planar graph, we should think of one of its embeddings in the plane.

DEFINITION 6.4.— Let G be a planar graph. The **faces** of a planar embedding of G, or simply, the faces of G are the connected components³ of the complement in \mathbb{R}^2 of the image of the vertices and edges of the graph.

In Figure 6.3, we have a planar embedding with nine faces.

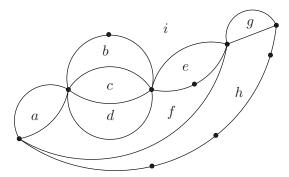


Figure 6.3. A graph with nine faces

The next results are classical in topology. See, for instance, [ARM 83, section 5.6]. Also see [HAL 07].

THEOREM 6.5 (Jordan theorem).— Let C be a Jordan curve⁴ in the plane \mathbb{R}^2 . Its complement, $\mathbb{R}^2 \setminus C$, consists of exactly two connected components. One is bounded and the other is unbounded. The curve C is the frontier of each component.

Let us mention a related result on the sphere, see [THO 92]. Sometimes, it is more convenient to work on the sphere because all faces are bounded. Recall that \mathbb{S}^1 (respectively, \mathbb{S}^2) denotes the usual circle in \mathbb{R}^2 (respectively, sphere in \mathbb{R}^3).

³ In the topological sense.

⁴ A *Jordan curve* is the image of a one-to-one continuous map of the circle \mathbb{S}^1 into the plane. Think of it as a "nice" deformation of a circle with no self-crossing.

Theorem 6.6 (Jordan–Schönflies theorem).— Let $f: \mathbb{S}^1 \to \mathbb{S}^2$ be a one-to-one continuous map. Then, the set $\mathbb{S}^2 \setminus f(\mathbb{S}^1)$ is homeomorphic to two disjoint open disks.

Let G be a planar graph. We can make use of Jordan theorem to define the **infinite face** or *outer face* of G, which is the unique unbounded face of the graph (when embedded on \mathbb{R}^2). In the representation in Figure 6.3, the infinite face is denoted by i.

Since a face is a subset of \mathbb{R}^2 , we can speak of the **frontier** of a face.

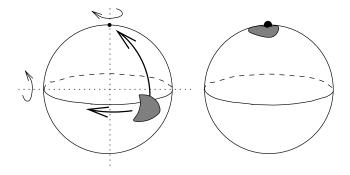


Figure 6.4. Choosing the outer face

Because of the remark 6.3, we can "choose" which face will be the infinite face in a representation. Considering an embedding of G on \mathbb{S}^2 , the infinite face is the one containing the "north pole" of \mathbb{S}^2 . Moving continuously the embedding of G (for instance, by rotations on the sphere along two axis), we can choose which face contains the north pole, see Figure 6.4. Then, if we apply a stereographic projection, we get a different embedding on \mathbb{R}^2 .

DEFINITION 6.7.— A planar graph G is cellularly embedded (on the sphere \mathbb{S}^2) if its faces are (homeomorphic to) open disks. This is clearly the case if and only if G is connected. In that case, we speak of a cellular embedding.

DEFINITION 6.8.— The dual of a cellular embedding of the graph G=(V,E) on \mathbb{S}^2 is a graph embedding G^* defined as follows: put one vertex f^* of G^* in the interior of each face f of G; for each edge e of G, create an edge e^* in G^* crossing e and no other edge of G (if e separates faces f_1 and f_2 , then e^* connects f_1^* and f_2^*).

In Figure 6.5, we have represented a cellular graph with black vertices and edges. The dual of this graph has white vertices and dashed edges.

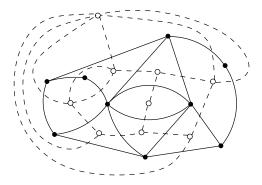


Figure 6.5. Dual of a graph

It is not difficult to see that the dual of G^* is G itself. Making use of the dual of a planar graph, the problems of coloring faces or vertices turn out to be equivalent.

6.2. Euler's formula

The next formula will be useful to prove the non-planarity of graphs.

THEOREM 6.9.— Let G = (V, E) be a planar connected finite multigraph. Let #V (respectively, #E, #F) be the number of vertices (respectively, edges, faces) in G. Then,

$$\#V - \#E + \#F = 2.$$

PROOF.—We proceed by induction on #F. If #F=1, G has only the infinite face. Hence, G has no cycle and is connected. It is a tree. From lemma 4.4, we note that #V=#E+1 and the formula holds.

Assume that the formula holds true for a graph with fewer than #F faces and prove it for a graph with $\#F \geq 2$ faces. Let x be an edge that belongs to the frontier of two faces F_1 and F_2 . Such an edge exists because the graph has at least two faces. If we remove this edge x, the resulting graph has #E-1 edges, the same number #V of vertices and #F-1 faces (because the two faces F_1

and F_2 are now a single face). By induction hypothesis, Euler's formula holds for this new graph:

$$\#V - (\#E - 1) + (\#F - 1) = 2$$

and the conclusion follows.

REMARK 6.10.— In Euler's formula, connectedness is needed. Take the graph made of two disjoint triangles. This graph is such that #V=6 and #E=6, but it has three faces: the triangles define two faces but there is also the infinite face. Think about an Euler's formula for planar unconnected finite graphs (exercise).

REMARK 6.11.— It is clear that all representations of a multigraph have the same number of vertices and edges. Nevertheless, one could think that the number of faces could depend on the chosen embedding of the planar graph on \mathbb{R}^2 or \mathbb{S}^2 . Euler's formula shows that the number of faces is invariant: it only depends on the number of vertices and edges. We repeat the message: when speaking of a planar graph, we always think about one of its embeddings.

This formula allows us to derive some interesting relations. As a first example, we consider a simple graph. The arguments are always of the same kind. We obtain inequalities between #V, #E and #F.

COROLLARY 6.12.— A simple planar graph has a vertex of degree at most 5.

PROOF.— Without loss of generality, we may assume that the graph is connected. If it is not the case, simply consider one of its connected components. We can also assume that every edge is used in the frontier of a face. Otherwise, there exists a vertex of degree zero or one (imagine a tree inside a face, see Figure 6.6) and such vertices can be removed iteratively⁵.

Since the graph is simple, a face is defined by at least three edges (there is no loop to define a face with a single edge, nor multiple edges defining a face with only two edges). We use two counting arguments. If we list the faces of the graph: each face is delimited by at least three edges (to estimate the number of edges, we could too quickly conclude that $\#E \geq 3 \#F$), but each

⁵ If we suppress, in a connected graph, the edges and vertices not defining a face, then we delete the same number of vertices and edges. So Euler's formula remains unchanged.

edge belongs to the frontier of two faces, thus:

$$3 \# F \le 2 \# E.$$
 [6.1]

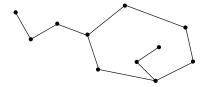


Figure 6.6. Suppressing edges and vertices not defining a face

Proceed by contradiction and assume that every vertex has degree of at least 6. If we list the vertices of the graph: each vertex is the endpoint of at least six edges (to estimate the number of edges, we could too quickly conclude that $\#E \geq 6 \, \#V$), but each edge has two vertices as endpoints, thus:

$$6 \# V \le 2 \# E$$
.

The graph is planar and connected, we may apply Euler's formula and use the above two inequalities:

$$2 = \#V - \#E + \#F \le \frac{\#E}{3} - \#E + \frac{2\#E}{3} = 0$$

which is a contraction.

As a corollary of Euler's formula, we get the easy part of the forthcoming Kuratowski's theorem characterizing planar graphs.

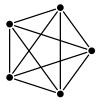


Figure 6.7. The complete graph K_5

PROPOSITION 6.13.— The complete graph K_5 is not planar.

PROOF.— Proceed by contradiction and assume that K_5 is planar. Since the graph K_5 is simple, we can make use of [6.1] and we get

$$2 \# E > 3 \# F = 6 + 3 \# E - 3 \# V$$

and thus:

$$\#E < 3 \#V - 6$$
.

But with K_5 , #E = 10 and #V = 5, contradicting the above inequality.

REMARK 6.14.— If we were interested in embeddings not on \mathbb{R}^2 but on the torus \mathbb{T}^2 , then K_5, K_6, K_7 can be embedded. But using a generalization of Euler's formula, one can show that K_8 cannot be embedded on \mathbb{T}^2 . Graphs that may be embedded on \mathbb{T}^2 are said to be toroidal.

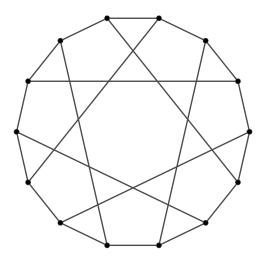


Figure 6.8. The Heawood graph is toroidal

PROPOSITION 6.15.— The complete bipartite graph $K_{3,3}$ is not planar.

PROOF.– Again we proceed by contradiction and assume that $K_{3,3}$ is planar. The graph $K_{3,3}$ is simple but we can strengthen [6.1] because it is bipartite:

•

the set of vertices is the disjoint union of V_1 and V_2 and every edge has one endpoint in V_1 and the other one in V_2 . The frontier of a face must contain at least four edges (in general, it is an even number of edges). Indeed, if there was a triangular face, then two vertices in the same subset V_1 or V_2 must be connected by an edge. Thus, [6.1] is replaced with

$$4 \# F \le 2 \# E$$

or $\#E \ge 2 \#F$. Using Euler's formula, we obtain

$$\#E = 2 \#E - \#E \le 2 \#E - 2 \#F = 2 \#V - 4.$$

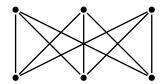


Figure 6.9. The complete bipartite graph $K_{3,3}$

But with $K_{3,3}$, #E = 9 and #V = 6, contradicting the above inequality.

It is obvious that if a multigraph G contains a non-planar subgraph, then G is non-planar. This observation holds true in particular when K_5 or $K_{3,3}$ is a subgraph of G. More generally, if G contains a subdivision (see definition 5.4) of K_5 or $K_{3,3}$, then G is not planar. What is striking is that the converse holds: if a multigraph G does not contain any subdivision of K_5 or $K_{3,3}$, then G is planar.

As a summary, we have an avoidance/forbidden graph characterization for planar graphs. The original proof can be found in [KUR 30]. See [THO 81] for proofs and survey.

THEOREM 6.16 (Kuratowski's theorem).— A multigraph is planar if and only if it does not contain a subgraph which is a subdivision of K_5 or $K_{3,3}$.

Another terminology can also be found.

DEFINITION 6.17.– A subdivision of K_5 or $K_{3,3}$ is sometimes called a Kuratowski graph.

Given a non-planar graph G, a Kuratowski subgraph of G can be found in linear time with respect to the size of G [WIL 84].

6.3. Steinitz' theorem

In this short section, we mention another connection between graph theory and geometry of polytopes. We use definition 1.38 about vertex connectivity. A polyhedron is a three-dimensional object made of polygonal faces, vertices and straight edges. We can thus define a graph whose vertices (respectively, edges) are the vertices (respectively, the edges) of this polyhedron. This graph is called the *skeleton* (or 1-skeleton) of the polyhedron.

We state Steinitz' theorem⁶ [STE 22], leading to the definition of *polyhedral graphs*, that is those satisfying Steinitz' theorem. See, for instance, [ZIE 95, Chapter 4]. A general resource is [GRÜ 07].

THEOREM 6.18.— A graph G is the skeleton of a convex polyhedron if and only if G is planar and 3-vertex connected.

In geometry, the embedding of such a planar graph on \mathbb{R}^2 is called a *Schlegel diagram* (such a projection may be defined for k-dimensional polytopes). In particular, we may thus apply Euler's formula to three-dimensional convex polyhedra to recover the *Platonic solids* depicted in Figure 6.10.

PROPOSITION 6.19.— There are exactly five regular convex polyhedra, that is all faces are identical regular polygons.

PROOF.—Let $n \geq 3$ be the number of edges of a face, that is we are considering a polyhedron made up of regular n-gons. Similarly to [6.1], if we list faces and count the number of edges (not forgetting that each edge belongs to two faces), we obtain

$$n \# F = 2 \# E.$$
 [6.2]

⁶ This is the same Ernst Steinitz (1871–1928) known by every student learning basic linear algebra and *Steinitz exchange lemma* implying that all basis of a finite dimensional vector space have the same number of elements.

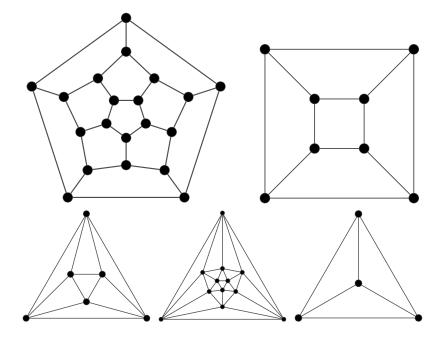


Figure 6.10. Skeletons of a dodecahedron, a cube (or hexahedron), a octahedron, an icosahedron and a tetrahedron

Let $d \geq 3$ be the degree of each vertex. If we list the vertices and count the number of edges (not forgetting that each edge has two endpoints), we obtain

$$d \# V = 2 \# E.$$
 [6.3]

If we plug these two relations into Euler's formula, we obtain

$$\frac{2\#E}{d} - \#E + \frac{2\#E}{n} = 2.$$

Dividing by 2 # E, since the number of edges is positive, we obtain

$$\frac{1}{d}-\frac{1}{2}+\frac{1}{n}>0$$

and

$$\frac{1}{d} > \frac{1}{2} - \frac{1}{n} \ge \frac{1}{2} - \frac{1}{3} = \frac{1}{6}.$$

Said otherwise, the degree d of each edge is either 3, 4 or 5. Similarly, we have

$$\frac{1}{n} > \frac{1}{2} - \frac{1}{d} \ge \frac{1}{2} - \frac{1}{3} = \frac{1}{6}$$

and n is either 3, 4 or 5.

If d = 5, then 1/n > 3/10, which implies n = 3. If d = 4, then 1/n > 1/4, which implies n = 3. If d = 3, then 1/n > 1/6, which implies $n \in \{3,4,5\}$. As a conclusion the possible pairs (d,n) are (3,3), (3,4), (3,5), (4,3), and (4,5).

d	\overline{n}	#V	#E	#F	
3	5	20	30	12	Dodecahedron
3	4	8	12	6	Cube
4	3	6	12	8	Octahedron
5	5	12	30	20	Icosahedron
3	3	4	6	4	tetrahedron

Table 6.1. The five platonic solids

To conclude with this proof, we just have to check that such polyhedra do exist. See Table 6.1.

If you are interested in regular polytopes, for instance, see [COX 73].

The next result is not really a corollary of what we have above. It is a pretext to work with Euler's formula. In particular, one could find other proofs relying on geometrical arguments.

COROLLARY 6.20.— There are exactly three regular tilings (or tesselations) of the plane, that is using only congruent regular polygons so that every side of each polygon is also the side of another polygon: triangles, squares and hexagons.

PROOF.— We use the same notation as in the previous proof: we are looking for a tesselation with n-gons and each vertex has degree d.

Assume that we have a tiling of a finite connected region of the plane with a finite number of n-gons, see Figure 6.11. Consider the region delimited by a disk of growing radius or a square of growing side. This tiling can be seen as a planar connected graph. Euler's formula and relations [6.2] and [6.3] apply

except for the outer face that is not an n-gon. We have to work a bit more. As usual, if we list all the faces and count the edges, each edge is counted twice. We let b denote the number of edges on the frontier of the outer face. Thus, the number of edges is

$$\frac{n}{2}(\#F-1) + \frac{b}{2}.$$

Now, if we list all the faces and count the vertices, each interior vertex not belonging to the frontier of the outer face is counted d times. The vertices of the frontier are counted at most d times. Thus, when dividing n#F by d, we make an error compensated by the introduction of c, which is less than the number of vertices on the frontier. Thus, the number of vertices is

$$\frac{n}{d} \# F + c.$$

An important argument is the comparison between perimeter and area. When our region of interest grows (e.g. a disk of growing radius), the number of faces inside this region grows quadratically, whereas the number of edges and vertices of the frontier of the outer face grow linearly. We conclude that the two quantities b and c are in $\mathcal{O}(\sqrt{\#F})$.

Euler's formula gives

$$\frac{n}{d}\#F + \#F = \frac{n}{2}\#F - \frac{n}{2} + \frac{b}{2} - c + 2.$$

We divide this relation by n#F and we let #F tend to infinity. It yields

$$\frac{1}{d} + \frac{1}{n} = \frac{1}{2}$$

because n is a constant and b/#F and c/#F tend to 0 when #F tends to infinity. Recall that d,n are integers greater than or equal to 3. If n=3 (respectively, 4, 6), then the only possible solution is d=6 (respectively, 4, 3). For n=5, there is no integer solution for d. If n is larger than 6, note that 1/7+1/3<0.48, then there is no pair (n,d), satisfying the above equation with n>6. As a conclusion, only three tesselations may exist and we note that they exist as seen in Figure 6.11.

In polyhedral combinatorics where one is interested in higher dimensional polytopes, we mention Balinski's theorem [BAL 61] (a four-page long paper) which generalizes one direction of Steinitz' theorem.

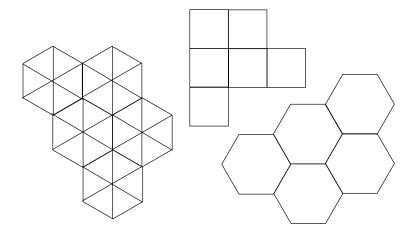


Figure 6.11. The three tesselations of the plane

THEOREM 6.21.— The skeleton made of the vertices and edges of any k-dimensional convex polytope is a k-vertex-connected graph.

6.4. About the four-color theorem

A general presentation of coloring problems will be given in Chapter 7. In the second part of this chapter, we limit ourselves to coloring faces of planar graphs.

We note that a planar multigraph has faces (including the infinite face). The question is to color the faces in such a way that adjacent faces (i.e. their frontiers have a common edge) get different colors. The four-color theorem states, as you can guess, that four colors suffice. It is not difficult to find a planar graph where four colors are needed (exercise). This result has a quite long and fascinating history. See [WIL 02] and [WIL 14] for a book version. In a letter from De Morgan to Hamilton (October 23, 1852), we can read:

A student of mine (Francis Guthrie) asked me today to give him reason for a fact which I did not know was a fact and do not yet. He says that if a figure be anyhow divided and the compartments differently colored, so that figures with any portion of common boundary line are differently colored – four colors may be wanted but no more.

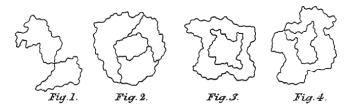


Figure 6.12. From Kempe's original paper [KEM 79]

The earliest attempts to answer this question have proven to have flaws, see, for instance Kempe's fallacious solution [KEM 79]. A first correct proof by Appel and Haken appeared in the late 1970s [APP 77a, APP 77b], more than a century after Guthrie's question. In this proof, one has to check some unavoidable set appearing in 1482 reducible configurations (whatever the precise meaning of this statement is). So, it requires extensive use of computers and raises a philosophical question about the nature of a proof (do we check or trust the processor inside a computer, the programming language, the compiler, etc.). Appel and Hanken wrote: "A person could easily check the part of the discharging procedure that did not involve reducibility computation in a month or two."

In the end of the last century, a refined proof was obtained but still requiring to check 633 configurations [ROB 96b]. As an ultimate step toward formalization, the four-color theorem was fully checked by the Coq formal proof assistant [GON 08].

In this book, we have decided to present a much simpler problem, namely we allow the use of a fifth color.

REMARK 6.22.— In topology, a connected surface S has genus g, if g is the maximum number of non-intersecting closed simple curves that can be drawn on S without disconnecting it. For instance, thanks to Jordan–Schönflies theorem 6.6, the sphere \mathbb{S}^2 has genus 0. The torus \mathbb{T}^2 has genus 1. If a multigraph can be embedded on a surface of genus g, then it can be colored with c_g colors where

$$c_g = \left[\frac{1}{2} (7 + \sqrt{1 + 48 \, g}) \right].$$

The first few values of c_g are given in Table 6.2. This expression, known as Heawood's formula, was conjectured at the end of the 19th Century. It had to

wait till 1968 to get a proof [RIN 68]. The only exception is for the Klein bottle that requires six colors even though it is a surface of genus 2. On the torus \mathbb{T}^2 , there is therefore a seven-color theorem. It is not an easy task to find a graph embedding on a surface of genus g where c_g colors are needed. An alternative to this formula exists in terms of Euler's characteristic.

g	0	1	2	3	4	5	6	7	8	9	10
c_g	4	7	8	9	10	11	12	12	13	13	14

Table 6.2. The first few values of c_q

Because of the notion of dual, it is equivalent to color faces of a planar graph G or vertices of G^* , adjacent faces in G are corresponding to adjacent vertices in G^* .

REMARK 6.23.— A quadratic-time algorithm for coloring planar graphs with four colors can be obtained. If we allow six or more colors, this can be done in linear time. See [ROB 96a]. With five colors, a linear-time algorithm also exists [THO 94].

Nevertheless, deciding whether or not a planar graph with vertices of degree at most 4 can be colored using three colors is an NP-complete problem [GAR 76].

For more on graph coloring problems, see [JEN 95].

6.5. The five-color theorem

We have decided to take an easier road and we will stick to the coloring of faces. The proof essentially follows the lines of Ore⁷ in [ORE 90]. Note that the proof that we will develop leads to a quadratic-time algorithm for coloring planar graphs with five colors (not being optimal, as discussed in remark 6.23).

DEFINITION 6.24.— Let k be an integer. We say that a planar multigraph G is k-colorable if the faces of G can be colored with (at most) k colors in such a way that any two adjacent faces get distinct colors.

⁷ Øystein Ore (1899–1968) is a Norwegian mathematician known for his work on graphs (and in particular, on the "four-color problem" which was not yet a theorem) and non-commutative algebra.

THEOREM 6.25.— Every planar multigraph is five-colorable.

PROOF.— In this proof, a *coloring* of G is map from the set of faces of G to $\{1, \ldots, 5\}$ such that it satisfies the proper coloring condition of definition 6.24: any two adjacent faces get distinct colors.

First, we may replace G with a 3-regular graph G' in such a way that if G' has a coloring, then we can deduce a coloring for G. Vertices of degree 1 can be deleted: they do not define any face (recall Figure 6.6). Vertices of degree 2 can also be suppressed: if $\deg(v)=2$ and $\{u,v\},\{v,w\}$ are the two edges having v as endpoint, then we replace these two edges with the single edge $\{u,w\}$. Now proceed with vertices of degree at least 4. The idea is to "inflate" these vertices as pictured in Figure 6.13. Observe that if there is a coloring of the resulting graph, then we clearly have a coloring of the original graph before "inflating" these vertices, just keep the coloring of the original faces. In some sense, coloring G' is more restrictive: there are more constraints to satisfy.

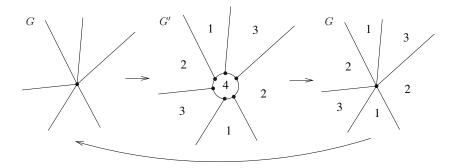


Figure 6.13. Get ridding of vertices of degree at least 4

From now on, we assume that G is a planar 3-regular graph. We let φ_i denote the number of faces of G whose frontier has exactly i edges. If we list all the faces and count the number of vertices on the frontier of a face, we obtain the following relation (each vertex belongs to three faces because the graph is 3-regular):

$$3 \# V = 2\varphi_2 + 3\varphi_3 + 4\varphi_4 + 5\varphi_5 + \cdots$$

The r.h.s. is a finite sum because the graph is finite. If we list all the faces and count the number of edges on the frontier of a face, we obtain the following relation (each edge belongs to the frontier of two faces):

$$2 \# E = 2\varphi_2 + 3\varphi_3 + 4\varphi_4 + 5\varphi_5 + \cdots$$

If we simply count the faces:

$$#F = \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 + \cdots$$

Euler's formula yields 12 = 6 #V - 6 #E + 6 #F and

$$12 = 4\varphi_2 + 3\varphi_3 + 2\varphi_4 + \varphi_5 - \varphi_7 - 2\varphi_8 - \cdots$$

Indeed, multiplying the first relation by 2, the second by 3 and the third by 6, the coefficients of φ_i is 2i-3i+6=6-i for all $i\geq 2$. But, for all $i\geq 2$, we note that $\varphi_i\geq 0$. Hence, we conclude that every planar 3-regular graph must contain a face delimited by at most five edges⁸.

The idea is the following one. Pick any face delimited by at most five edges. Delete at least one of these edges and modify slightly the graph. With two requirements: the resulting graph G' is still 3-regular and if G' has a coloring, then we can deduce a (valid) coloring for the initial graph.

If this double idea works, then we are done. If the construction preserves the 3-regularity, then we may apply it iteratively because we will again have a face delimited by at most five edges. Starting from $G = G_0$, we have a finite sequence of graphs G_1, \ldots, G_k with a decreasing number of faces. When we are left with five faces in G_k , there exists a trivial coloring of G_k .

$$G_0 \longrightarrow G_1 \longrightarrow \cdots \longrightarrow G_k$$

Figure 6.14. Decreasing the number of faces

Now proceed backwards, any coloring of G_{i+1} provides a coloring of its predecessor G_i and eventually yields a coloring of the initial graph G_0 .

$$G_0 \longleftarrow G_1 \longleftarrow \cdots \longleftarrow G_k$$

Figure 6.15. Propagating the coloring

⁸ An alternative is to use the dual G^* of the graph and apply corollary 6.12 (but one needs to check that G^* is simple).

We note that the graph has a face delimited by at most five edges.

Let us start with a face delimited by two edges as depicted in Figure 6.16 (we focus on a small portion of a potentially large graph G_i). Four edges are replaced with a single one (and two vertices are deleted), but this local surgery preserves the 3-regularity of the graph G_{i+1} . If the resulting graph G_{i+1} has a coloring, the face that has been deleted from G_i is surrounded by only two faces in G_i and we have three choices to color it: we deduce a coloring of the initial graph G_i from any coloring of the modified graph G_{i+1} . The only change is local and does not modify the constraint satisfied by the global coloring of G_{i+1} .

The construction is quite similar with a face delimited by three edges as depicted in Figure 6.17 (we again focus on a small portion of a potentially large graph G_i). Five edges are replaced with two (and two vertices are deleted). The 3-regularity of the resulting graph G_{i+1} is preserved and if G_{i+1} has a global coloring, then the face that has been deleted from G_i is surrounded by three faces in G_i and we have two choices to color it.

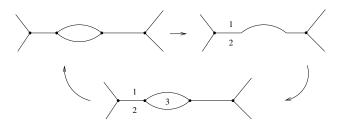


Figure 6.16. Suppressing a two-edge face

If we have a face F delimited by four edges, then it is surrounded by at least three different faces. We may encounter several cases as depicted in Figure 6.18, where we zoom on a zone of interest. In these situations, the faces B and D are distinct and have no common frontier. It is not possible that both A, C and B, D share a common frontier (or correspond to the same face). Otherwise, the graph K_5 would be planar contradicting proposition 6.13 (think about the dual of the graphs depicted in Figure 6.18, for the central graph we get K_5 with a single edge missing). There is no need to make reasoning on the figures. The point is that F always has two adjacent faces denoted by B and D with no common frontier. As usual, let us proceed to some surgery as depicted in Figure 6.19. Again, we keep a 3-regular graph G_{i+1} and a coloring of the initial graph G_i can easily be obtained from any

coloring of G_{i+1} . Observe that for the graph on the left, we will possibly (if colors 2 and 4 are distinct, because we have no control on the given global coloring of G_{i+1}) need five colors for G_i .

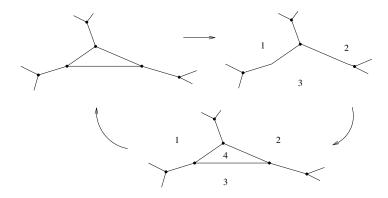


Figure 6.17. Suppressing a three-edge face

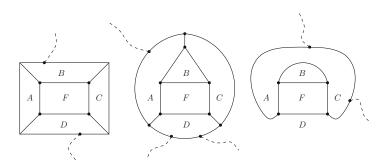


Figure 6.18. Suppressing a four-edge face *F*

The discussion with a five-edge face is similar. At least two faces have no common frontier and we proceed as in Figure 6.20.

REMARK 6.26.— An alternative argument is to use the dual of the graph. When a face has four or five adjacent faces, then in the dual graph, corresponding to that face, we have a vertex v of degree 4 or 5. In G^* , two neighbors of v are not adjacent because, otherwise G^* would contain a copy of K_5 and we note that G^* must be planar. This directly gives two faces with no common frontier in G.

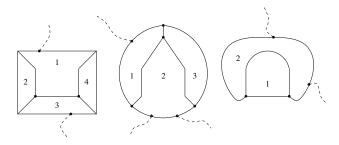


Figure 6.19. Surgery for suppressing a four-edge face

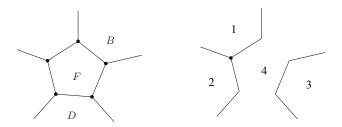


Figure 6.20. Suppressing a five-edge face F

6.6. From Kuratowski's theorem to minors

We give some complements on Kuratowski's theorem 6.16. We start with an equivalent formulation of Kuratowski's theorem.

DEFINITION 6.27.— If G contains a subdivision of H, then H is said to be a topological minor of G.

EXAMPLE 6.28.— For instance, $K_{3,3}$ is a topological minor of the Petersen graph seen, for the first time, in Figure 1.8. From left to right, in Figure 6.21, we have represented the Petersen graph, one of its subgraphs that is subdivision of $K_{3,3}$ where three edges have been divided. In particular, proposition 6.15 allows us to conclude that the Petersen graph is not planar.

With this definition, theorem 6.16 can be restated as follows.

THEOREM 6.29.— A multigraph is planar if and only if it does not have K_5 or $K_{3,3}$ as a topological minor.

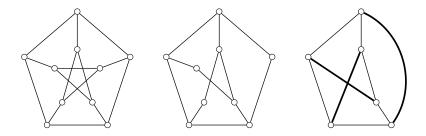


Figure 6.21. $K_{3,3}$ is a topological minor of the Petersen graph

There is another notion called minor of a graph that is more general. Edge contraction was given in definition 5.3.

DEFINITION 6.30.— If H can be obtained from G by a finite sequence of edge contractions and edge or vertex deletions, then H is a **minor** of G.

EXAMPLE 6.31.— For instance, K_5 is a minor of the Petersen graph. One has to contract the five edges between the inner and outer vertices in the representation given in Figure 6.21 (left).

A minor of a planar multigraph is again planar. A minor of a forest is again a forest (we need a forest and not simply a tree: a minor of a tree is not always connected). So, we can define a family of graphs closed under the operation of taking a minor.

PROPOSITION 6.32.— A topological minor H of G is a minor of G but the converse is not true.

PROOF.— Assume that G has a subgraph H' that is a subdivision of a graph H. To get H', some edges e_1, \ldots, e_k of H have been divided into two or more edges

$$e_{1,1}, e_{1,2}, \ldots, e_{1,d_1}, \ldots, e_{k,1}, e_{k,2}, \ldots, e_{k,d_k}$$

with $d_1, \ldots, d_k \geq 2$. Starting from G, we can delete some edges and/or vertices to obtain H'. As already observed in remark 5.5 (elementary division can be reversed by an edge contraction), if we contract the vertices $e_{i,j}$ for $i=1,\ldots,k$ and $j\geq 2$, then we get the graph H. This means that H is a minor of G.

Next, let us give an example of a minor that is not a topological minor. Consider the graphs Q_3 (seen in section 1.8) and H depicted in Figure 6.22. The graph H is not a topological minor of Q_3 because it has a vertex of degree 4 and Q_3 is 3-regular. Thus, any subdivision of any subgraph of Q_3 contains only vertices of degree at most 3. Clearly, we get H by contracting the four central edges in the representation of Q_3 .

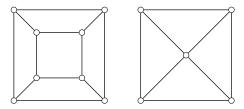


Figure 6.22. The graphs Q_3 and H H is a minor but not a topological minor of Q_3

Seven years after Kuratowski, Wagner⁹ obtained the following result [WAG 37].

THEOREM 6.33.— A multigraph G is planar if and only if does not have K_5 or $K_{3,3}$ as a minor.

This statement is a very special case of the so-called Robertson–Seymour theorem. Its proof is given by the "Graph minors project" in an impressive series of 20 papers entitled "Graph minors" that appear in *J. Combin. Theory* from 1983 to 2004. It implies that a forbidden minor characterization (e.g. not having K_5 or $K_{3,3}$ as a minor) exists for every property of graphs (not only planarity) that is preserved by edge/vertex deletions and edge contractions (e.g. the set of planar graphs is closed under these operations).

Wagner seems to have conjectured a similar characterization and Robertson-Seymour theorem is sometimes referred to as Wagner's conjecture. Let us quote Diestel [DIE 10]: "It seems that Wagner did indeed discuss this problem in the 1960s with his students. However, Wagner

⁹ Klaus Wagner (1910-2000).

apparently never conjectured a positive solution; he certainly rejected any credit for the conjecture when it had been proved."

Let \mathcal{F} be a family of graphs closed under the operation of taking a minor, for example the family of planar graphs, of forests, of graphs with tree-width¹⁰ bounded by a given constant. There exists a finite set $\mathcal{H}_{\mathcal{F}}$ (the elements in $\mathcal{H}_{\mathcal{F}}$ are called *excluded minors* or *minor minimal obstructions*) such that G belongs to \mathcal{F} if and only if G does not have an element in $\mathcal{H}_{\mathcal{F}}$ as a minor. But it could be challenging, for a given family \mathcal{F} , to determine the elements of $\mathcal{H}_{\mathcal{F}}$.

For survey papers on this result, see [BIE 95, FEL 89].

REMARK 6.34.— For every fixed graph H, one can decide in polynomial time [ROB 95] whether or not H is a minor of a given graph G. This implies that every graph property preserved by edge/vertex deletions and edge contractions may be recognized in polynomial time. In [KAW 12], testing for a fixed minor is shown to be carried out in $\mathcal{O}((\#V^2))$ time.

6.7. Exercises

- 1) Think about a Euler formula for planar unconnected finite multigraphs.
- 2) Prove that the Heawood graph depicted in Figure 6.8 is not planar. Is this graph 1-planar (see example 2.13)?
- 3) Consider a simple planar graph with six vertices. What is the maximal number of edges that such a graph may have? Give a planar representation of such a graph.
- 4) Can we assign pairwise distinct integer values between 1 and 12 to the edges of an octahedron in such a way that the sum of these values for edges incident to a vertex is independent of this vertex? Same question with a cube.
- 5) Consider a planar graph with 300 faces. All faces are triangular. How many vertices and edges does this graph have? Compare the sum of degrees of all vertices with the one of its dual. For such a planar graph, what is the largest n such that its dual has faces whose frontier is delimited by n edges.
- 6) A soccer ball is a convex polyhedron made up of hexagons and pentagons. Knowing that each vertex belongs to two hexagons and one

¹⁰ See definition 4.12 on page 77.

pentagon, determine the number of vertices, edges, hexagons and pentagons. (Check that it is a *truncated icosahedron*.)

- 7) Consider a convex polyhedron with six square faces and eight triangular faces. Each vertex belongs to c square faces and t triangular faces. Determine c, t, the number of vertices and edges. (Check that it is a *triangular orthobicupola*.)
- 8) Consider a planar graph where all faces are triangular with one vertex of degree 3 and two vertices of degree 6. Determine the number of vertices of degree 3 and 6, the number of edges and faces.
- 9) Consider a planar graph where all faces are pentagons and all faces of its dual are triangles. Determine the number of vertices, edges and faces of this graph. Same question if the faces of the dual are quadrilateral.
- 10) Consider a convex polyhedron with 32 faces either triangles, or pentagons. Each vertex belongs to t triangles and p pentagons. Determine t, p, the number of vertices and edges of this polyhedron. (Check that it is an icosidodecahedron.)
- 11) Do a bibliographic search for a proof of Kuratowski's theorem? Here are a few resources [TVE 89, KLO 89, MAK 97].
- 12) Prove that the relation "H is a minor of G" is a partial order (see section 4.3) on the set of all finite multigraphs.
- 13) See [WES 98] for a solution (and a definition) of the *Empire problem* where one has to color a map but taking also into account the existence of empires.
- 14) Have a look at a list [JEN 01] of 25 pretty graph coloring problems compiled by Jensen and Toft.

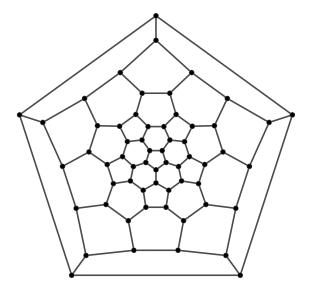


Figure 6.23. The skeleton of a soccer ball

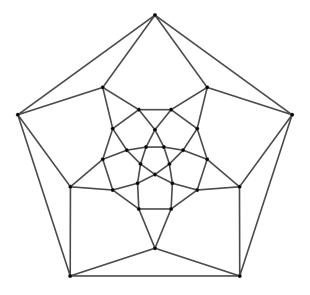


Figure 6.24. The skeleton of a icosidodecahedron

Colorings

In this chapter, we will be interested in coloring vertices of a graph in such a way that adjacent vertices receive distinct colors. This kind of coloring is a special case of homomorphisms of graphs. Hence, the first section briefly describes the latter notion. We conclude this chapter with the introduction of Ramsey numbers related to colorings of the edges of a complete graph.

7.1. Homomorphisms of graphs

The idea of a homomorphism from a digraph G to a digraph H is to consider a map f from V(G) to V(H) such that the image (f(u),f(v)) of every edge (u,v) in G by f is an edge in H. Recall that in the unoriented case, an edge $\{u,v\}$ corresponds to two directed edges (u,v) and (v,u).

DEFINITION 7.1.— Let G, H be two digraphs. A homomorphism from G to H is a map $f: V(G) \to V(H)$ such that, for all $u, v \in V(G)$, if $(u, v) \in E(G)$, then $(f(u), f(v)) \in E(H)$. For the particular case of undirected graphs, f is a homomorphism when for all $u, v \in V(G)$, if $\{u, v\} \in E(G)$, then $\{f(u), f(v)\} \in E(H)$.

Considering the homomorphism $1 \mapsto a$, $2 \mapsto b$, $3 \mapsto c$, $4 \mapsto c$ for the digraphs with $V(G) = \{1, 2, 3, 4\}$ and $V(H) = \{a, b, c, d\}$ depicted in Figure 7.1, we see that a homomorphism is not necessarily onto (surjective). If needed, we can restrict ourselves to the subgraph induced by the range of f (in our example, there is also a homomorphism from the first digraph to the subgraph induced by $\{a, b, c\}$.)

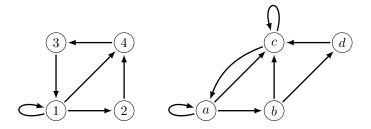


Figure 7.1. A homomorphism $1 \mapsto a, 2 \mapsto b, 3 \mapsto c, 4 \mapsto c$

We have mentioned in example 2.16 that given two graphs G and H, deciding whether there exists a homomorphism from G to H is NP-complete.

REMARK 7.2.— As seen in Figure 7.2, a homomorphism from G to H is not necessarily one-to-one (injective). The same observation can be done with the previous example of Figure 7.1.

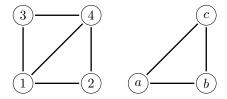


Figure 7.2. A homomorphism $1 \mapsto a$, $2 \mapsto b$, $3 \mapsto b$, $4 \mapsto c$

REMARK 7.3.— These definitions can be extended to (labeled) directed multigraphs. Let G, H be two directed multigraphs. Since E(G) and E(H) are multisets, we have to deal with multiple copies of the same edge. A homomorphism from G to H is a pair of maps (f_V, f_E) where $f_V: V(G) \rightarrow V(H)$ and $f_E: E(G) \rightarrow E(H)$ are such that, for all $e \in E(G)$, if e = (u, v), then $f_E(e) = (f_V(u), f_V(v))$ and $e, f_E(e)$ have the same label. The map f_E is required because we have multiple edges. Several multiple edges with the same label could be mapped to the same edge with the same label.

DEFINITION 7.4.— Let G, H be two digraphs. An **isomorphism** between G and H is a one-to-one correspondence $f: V(G) \to V(H)$ such that, for all $u, v \in V(G)$, $(u, v) \in E(G)$ if and only if $(f(u), f(v)) \in E(H)$. Otherwise

stated, both f and f^{-1} are graph homomorphisms. If there is an isomorphism between G and H, we say that G and H are isomorphic. The same definition applies for undirected graphs. An isomorphism from G to itself is an **automorphism** of G. Respecting multiplicities, the definition of isomorphism can be extended to directed multigraphs: $(u,v) \in E(G)$ and $(f(u),f(v)) \in E(H)$ have the same multiplicity.

In Figure 7.3, we have depicted three isomorphic graphs. For convenience, we have given the same labels to corresponding vertices.

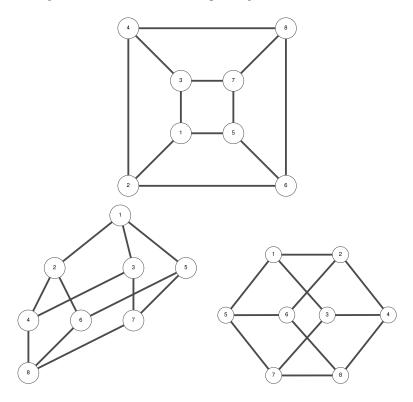


Figure 7.3. Three isomorphic graphs

If two digraphs are isomorphic, then they are the same up to a renaming of the vertices. An automorphism of a digraph is a one-to-one correspondence of the edges and the vertices that preserves the graph structure. If f is an automorphism of G = (V, E), then $\deg^+(u) = \deg^+(f(u))$,

 $\deg^-(u) = \deg^-(f(u))$, u,v belong to the same SCC if and only if f(u), f(v) belong to the same SCC and $\operatorname{d}(u,v) = \operatorname{d}(f(u),f(v))$ for all $u,v \in V$.

REMARK 7.5.— Given two digraphs G and H, deciding whether or not they are isomorphic is clearly in NP. A provided certificate can be checked in polynomial time. The status of the computational complexity of the problem is unknown: we do not know yet if the problem is in P or is NP-complete. Several families of graphs have an efficient solution. Very recently, Babai presented a possible breakthrough with a "quasipolynomial $(\exp((\log n)^{O(1)}))$ time" algorithm to solve the graph isomorphism problem in a 84-page long paper [BAB 15].

Since homomorphisms are maps, we can compose them as we do with functions. Observe that if f is an isomorphism between G and H, then f^{-1} is an isomorphism between H and G. In particular, if f is an automorphism of G, then so is f^{-1} .

PROPOSITION 7.6.— Let G, H, I be three digraphs. If f (respectively, g) is a homomorphism from G to H (respectively, from H to I), then $g \circ f : V(G) \to V(I)$ is a homomorphism from G to I. In particular, the set of automorphisms of G endowed with the composition of functions is a group denoted by Aut(G).

The proof is left as an (easy) exercise. The group Aut(G) is a subgroup of the group \mathcal{S}_V of permutations of the set vertices. Roughly, we can say that Aut(G) reflects the symmetries in G. As an example, for the Petersen graph P, Aut(P) contains 120 elements compared with 10! = 3,628,800. For the complete graph K_n , we trivially have $Aut(K_n) = \mathcal{S}_n$. Observe that, in general, the order (i.e. the number of elements) of Aut(G) divides (#V)!. The order of a subgroup divides the order of the group.

EXAMPLE 7.7.— With the graph depicted on the left in Figure 7.2, its group of automorphisms contains four elements: id, $(1\ 4)$, $(2\ 3)$ and $(1\ 4)$ $(2\ 3)$ where $(a\ b)$ denotes the permutation of a and b. With the skeleton of the cube depicted in Figure 7.3, its group of automorphisms has three generators $(2\ 3)\ (6\ 7)$, $(3\ 5)\ (4\ 6)$ and $(1\ 2)\ (3\ 4)\ (5\ 6)\ (7\ 8)$. It contains 48 elements.

DEFINITION 7.8.— An asymmetric graph is an undirected graph G such that $Aut(G) = \{id\}$ is trivial.

REMARK 7.9.— Every automorphism of a graph G can be described as a permutation matrix acting on the vertices of G.

For instance, the matrix associated with $(1 \ 4) (2 \ 3)$ is such that

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} = \begin{pmatrix} 4 \\ 3 \\ 2 \\ 1 \end{pmatrix}.$$

7.2. A digression: isomorphisms and labeled vertices

In this book, we have not much discussed infinite graphs. Here, we have an opportunity to discuss isomorphisms occurring in infinite trees and make a link with regular languages.

As in remark 7.3, homomorphisms or isomomorphisms can be extended to graphs with labeled vertices. Assume that G (respectively, H) is a digraph with a labeling of the vertices, i.e. a map from V(G) (respectively, V(H)) to a finite set $\{1,\ldots,k\}$. In this situation, an isomorphism f between G and H satisfies the same properties as in definition 7.4 and also, for all $u \in V(G)$, u and f(u) have the same label.

In formal language theory, we have seen in example 4.11 that we can associate a labeled tree with a language. The set A^* of all words over a finite alphabet A is infinite (countable), thus the associated tree has infinitely many vertices. We color vertices in black (respectively, white) if the corresponding word belongs (respectively, does not belong) to the language. In Figure 7.4, we have represented the first four levels of the tree associated with the language a^*b^* made up of words starting with an arbitrary number of a (possibly 0) followed by an arbitrary number of b. For instance, there is an isomorphism (respecting labels) between the full tree and the tree rooted at the first left child (corresponding to a). Up to isomorphism, the tree contains only three non-isomorphic subtrees: the full tree itself (1), a tree with a black right-most branch (2) and a white tree (3). Consider the subtrees rooted at ε , b and ba.

DEFINITION 7.10.— A language is regular if the associated colored tree has finitely many non-isomorphic subtrees.

This language a^*b^* is accepted by what is called a *deterministic finite* automaton (DFA). Such a computational model, as depicted in Figure 7.5, is

used to accept/reject in linear time words given as input. The machine reads the letters of the input one by one, from left to right. Starting from the initial state marked by an incoming arrow, the state is updated when reading a letter (we follow transitions in the graph). Accepted states are marked with outgoing arrows. The tree non-isomorphic subtrees correspond to the three states (vertices) of the DFA depicted in Figure 7.5.

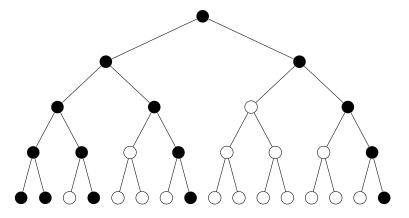


Figure 7.4. A prefix of the tree associated with the language a^*b^*

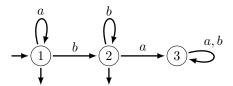


Figure 7.5. A deterministic finite automaton

There are non-regular languages too. Consider the language of words over $\{a,b\}$ having a prime number of a's. Recall that the first prime number is 2. The first few words in this language are aa, aaa, aab, aba, aba, aba, abab, abaa, abaa, abab, abaa, abaa,

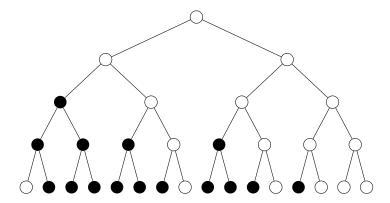


Figure 7.6. A prefix of the tree associated with the language of words having a prime number of a

With a number-theoretic flavor, there is another way to define infinite trees with colored vertices. Consider the tree having $\mathbb{N}_{\geq 1}$ as set of vertices, 1 as root and every vertex n has two children 2n and 2n+1. Let X be a subset of positive integers. We associate with X the following coloring of the vertices: n is black if and only if it belongs to X. In Figure 7.7, we have depicted the tree associated with the set of even numbers. This tree has two non-isomorphic subtrees: one rooted at a white vertex and one rooted at a black vertex. This construction is linked with base-2 expansions. If w is the base-2 expansion of the number associated with a vertex, then the expansion associated with its left (respectively, right) child is w0 (respectively, w1). Hence, we deduce that the language made up of the base 2-expansions of the numbers associated with the black vertices is a regular language if and only if the tree has a finite number of non-isomorphic subtrees. This construction can be extended to b-ary trees where each node n has b children: $bn, bn + 1, \ldots, bn + b - 1$.

DEFINITION 7.11.— Let $b \ge 2$ be an integer. A set X of integers is b-recognizable, if the language of the base-b expansions of the elements in X is regular.

The fact that a set of integers is b-recognizable depends on the choice of the base. This is the essence of Cobham's theorem. Let $b, c \geq 2$ be two integers such that $\log b/\log c$ is not rational¹. If X is simultaneously b-recognizable

¹ If two integers $b, c \ge 2$ are such that the only non-negative integers m, n satisfying $b^m = c^n$ are m = n = 0, then b and c are said to be *multiplicatively independent*.

and *c*-recognizable, then it is a finite union of arithmetic progressions along a finite set (see, for instance, [COB 69, ALL 03, RIG 14]).

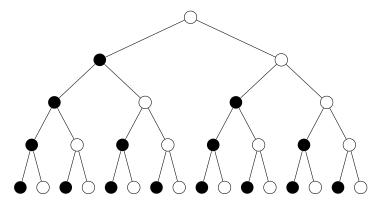


Figure 7.7. A prefix of the tree associated with the even numbers

7.3. Link with colorings

In the previous chapter, we were interested in coloring adjacent faces of a planar graph with distinct colors. It is an equivalent problem to properly color the vertices of the dual graph.

Thus, in general, we will be interested for planar, as well as for non-planar, graphs in coloring their vertices. We will limit ourselves to undirected graphs.

DEFINITION 7.12.— Let k be an integer. A k-coloring of a simple graph G = (V, E) is a map $c: V \to \{1, \ldots, k\}$ such that, if $\{u, v\}$ belongs to E, then $c(u) \neq c(v)$. A coloring satisfying this condition is usually said to be proper. If there exists a k-coloring of G, then G is said to be k-colorable. The least integer k such that G is k-colorable is the **chromatic number** of G and is denoted by $\chi(G)$.

As an example, for the complete graph, $\chi(K_k) = k$.

REMARK 7.13.— Having unoriented graphs with multiple edges does not modify the coloring problem. There is no restriction to consider k-coloring of multigraphs without loop. (It is clear that loops must be avoided.)

We can define a similar notion for digraphs with no opposite edges, i.e. if $(u, v) \in E$, then $(v, u) \notin E$. In that case, a proper coloring of such an oriented

graph is a map $c: V \to \{1, \ldots, k\}$ such that if $(u, v) \in E$, then $c(u) \neq c(v)$ and there is no edge $(x, y) \in E$ such that c(u) = c(y) and c(v) = c(x). This extra condition means that the coloring has to respect the orientation. If there is an edge from a blue vertex to a red vertex, there is no edge from a red one to a blue one. We can therefore define an oriented chromatic number (see [KOS 97]). For generalizations of graph coloring relying on homomorphisms, see [HEL 90, NEŠ 96, HEL 96a, HEL 96b].

If a graph is n-partite (see page 13), then $\chi(G) \leq n$. We may assign the same color to all the vertices of a component of the n-partition. In particular, a graph is bipartite if and only if it is 2-colorable.

PROPOSITION 7.14.— Let G, H be two simple graphs. If there exists a homomorphism from G to H, then $\chi(G) \leq \chi(H)$.

PROOF.— Let f be a homomorphism from G to H. For every $x \in V(H)$, $f^{-1}(x) = \{u \in V(G) \mid f(u) = x\}$ is a set of independent vertices (and can thus be assigned with the same color). Indeed, if u,v are such that $\{u,v\} \in E(G)$ and f(u) = f(v) = x, then x must have a loop but H is simple. If c is a proper coloring of H, then we can deduce a coloring d of G as follows: d(u) = c(f(u)) for all $u \in V$. This is clearly a proper coloring of G because if $\{u,v\} \in E(G)$, then $\{f(u),f(v)\} \in E(H)$. Hence, $c(f(u)) \neq c(f(v))$ and $d(u) \neq d(v)$.

REMARK 7.15.— In the previous proposition, we cannot hope for more than an inequality. Take a homomorphism $1\mapsto a, 2\mapsto c$ and $3, 4\mapsto b$ from a bipartite graph G to the complete graph K_3 as depicted in Figure 7.8. Then, $\chi(G)=2<\chi(K_3)$.

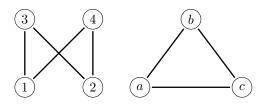


Figure 7.8. $\chi(G) = 2 < \chi(K_3)$

COROLLARY 7.16.— Let G be a simple graph and $k \ge 2$ be an integer. There exists a homomorphism from G to the complete graph K_k if and only if G is

k-colorable. Said otherwise, there exists a homomorphism from G to K_k and no homomorphism from G to K_{k-1} if and only if $\chi(G)=k$.

PROOF. Follows directly from proposition 7.14.

We have seen in example 2.10 that the k-coloring problem is NP-complete: Given a graph G and an integer $k \geq 3$, deciding whether $\chi(G) \leq k$ is NP-complete.

7.4. Chromatic number and chromatic polynomial

Formal power series can be seen as a way to encode and manipulate the terms of a sequence. Similarly, we will introduce a polynomial whose coefficients encode the number of proper colorings of a graph G with a given number of colors. Interestingly, we will see that the evaluation of this polynomial at j provides the number of proper colorings of G with at most j colors.

Let G be a simple graph with n vertices. We let $m_{k,G}$ denote the number of proper colorings of G using exactly k colors, i.e. each color is used by at least one vertex. By definition, we set $m_{k,G}=0$ for all k>n. It is not possible to use more than n colors with only n vertices.

We let $z^{\underline{k}}$ denote the *falling factorial power* [GRA 94, p. 48]

$$z^{\underline{k}} = z (z - 1) (z - 2) \cdots (z - k + 1).$$

Let $m, n \ge 1$ be integers. We have $m^{\underline{m}} = m!$ and $m^{\underline{n}} = 0$ if n > m.

DEFINITION 7.17.— The **chromatic polynomial** of a simple graph G with n vertices is the polynomial in $\mathbb{Z}[z]$ defined by

$$\pi_G(z) = \sum_{k=1}^n \frac{m_{k,G}}{k!} z^{\underline{k}}$$

where we recall that $m_{k,G}$ is the number of proper colorings of G using exactly k colors.

Here is a reformulation of the definition of $m_{k,G}$ showing that $\frac{m_{k,G}}{k!}$ are integers.

LEMMA 7.18.— Let G=(V,E) be a simple graph with n vertices. Let $k \in \{1,\ldots,n\}$. The number of partitions of V into k non-empty sets made of independent vertices is equal to $\frac{m_{k,G}}{k!}$.

PROOF.— Obvious.

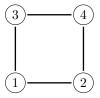


Figure 7.9. Determining the chromatic polynomial of a graph

EXAMPLE 7.19.— Consider the graph depicted in Figure 7.9. There is only one partition of V into two sets of independent vertices: $\{1,4\}$ and $\{2,3\}$. Also, $m_{2,G}=2$. We can assign the color blue (or red) to the vertices in the first subset and the other color to the vertices in the second subset. There are two partitions of V into three sets of independent vertices: either $\{1,4\}$, $\{2\}$ and $\{3\}$ or, $\{2,3\}$, $\{1\}$ and $\{4\}$. Hence, $m_{3,G}/3!=2$ and $m_{3,G}=12$. The graph has 12 different proper colorings using exactly three colors $\{r,g,b\}$ as given in the following table

Observe that for a n-vertex graph, $m_{n,G}=n!$ because every vertex receives a single color, thus each assignment of the n colors is a proper coloring.

EXAMPLE 7.20.— For the graph depicted in Figure 7.9, since $m_{1,G}=0$, $m_{2,G}=2$, $m_{3,G}=12$, $m_{4,G}=4!$, the chromatic polynomial of G is given by

$$z(z-1) + 2z(z-1)(z-2) + z(z-1)(z-2)(z-3)$$

or

$$z^4 - 4z^3 + 6z^2 - 3z.$$

EXAMPLE 7.21.— For small graphs, it is reasonable to compute the coefficients of the chromatic polynomial. For the cubic graph depicted in Figure 7.3, we find²

$$z^{8} - 12z^{7} + 66z^{6} - 214z^{5} + 441z^{4} - 572z^{3} + 423z^{2} - 133z$$
.

For the graph on the left in Figure 7.2, we find

$$z^4 - 5z^3 + 8z^2 - 4z$$
.

For the Petersen graph (depicted in Figure 1.8), we find

$$z^{10} - 15z^9 + 105z^8 - 455z^7 + 1,353z^6 -2,861z^5 + 4,275z^4 - 4,305z^3 + 2,606z^2 - 704z.$$

But things can become quite intricate. Consider the skeleton of a dodecahedron given in Figure 6.10. Its chromatic polynomial is given by

$$\begin{split} \pi(z) &= z^{20} - 30z^{19} + 435z^{18} - 4,060z^{17} + 27,393z^{16} - 142,194z^{15} \\ &+ 589,875z^{14} - 2,004,600z^{13} + 5,673,571z^{12} - 13,518,806z^{11} \\ &+ 27,292,965z^{10} - 46,805,540z^{9} + 68,090,965z^{8} \\ &- 83,530,946z^{7} + 85,371,335z^{6} - 71,159,652z^{5} + 46,655,060z^{4} \\ &- 22,594,964z^{3} + 7,171,160z^{2} - 1,111,968z. \end{split}$$

Let us collect a few easy observations.

PROPOSITION 7.22.— For simple graphs, the chromatic polynomial has the following properties.

- 1) For the complete graph, $\pi_{K_n}(z) = z^{\underline{n}}$.
- 2) If G has k connected components G_1, \ldots, G_k , then

$$\pi_G(z) = \prod_{i=1}^k \pi_{G_i}(z).$$

- 3) For all graphs G, $\pi_G(0) = 0$.
- 4) Let j be an integer, $\pi_G(j)$ is the number of proper colorings of G using at most j colors.

² This computation and the other ones were done using Mathematica and the instruction ChromaticPolynomial[GraphData["CubicalGraph"], z].

PROOF.— We only prove the last item.

Let n be the number of vertices of G. Let j be the number of available colors. There is no bound on j. The number of available colors is independent of n. We will count the number of proper colorings of G using exactly i colors. Note that we can limit ourselves to $i \leq n$ because we cannot color n vertices using more than n colors simultaneously. From lemma 7.18, for $i \in \{1,\ldots,n\}$, the number of partitions of V into i non-empty sets C_1,\ldots,C_i made up of independent vertices is $\frac{m_{i,G}}{i!}$. If $j \geq i$, then we choose one color out of j for the vertices in C_1 , one out of j-1 for the vertices in C_2,\ldots , one out of j-1 for the vertices in C_3,\ldots , one out of j-1 for the vertices in C_4,\ldots for every such partition, there are exactly j proper colorings of j using exactly j colors. If j if j

$$\frac{m_{i,G}}{i!}j^{\underline{i}}$$

colorings with exactly i colors out of j. Hence, the number of proper colorings using at most j colors is

$$\sum_{i=1}^{j} \frac{m_{i,G}}{i!} j^{\underline{i}} = \sum_{i=1}^{n} \frac{m_{i,G}}{i!} j^{\underline{i}}$$

which is equal to $\pi_G(j)$ because if $j \leq n$, then $j^{\underline{i}} = 0$ for $i = j + 1, \ldots, n$ and similarly, if j > n, then $m_{i,G} = 0$ for $i = n + 1, \ldots, j$.

COROLLARY 7.23.— The chromatic number of G is the smallest integer j such that $\pi_G(j)$ is non-zero.

EXAMPLE 7.24.— Let us reconsider example 1.51 with a train transporting several chemical products. For the graph depicted in Figure 1.24, its chromatic polynomial is given by

$$\pi_G(z) = z^9 - 10z^8 + 44z^7 - 112z^6 + 182z^5 - 195z^4 + 135z^3 - 55z^2 + 10z.$$

We have $\pi_G(1) = \pi_G(2) = 0$ and $\pi_G(3) = 264$. Hence, three wagons are needed to transport the chemical products and we know that we can safely arrange them in 264 different ways.

For some more examples (e.g. allocation of channels to television stations, construction of timetables) and properties of the chromatic polynomial, see [REA 68].

REMARK 7.25.— If the chromatic polynomial could be obtained in polynomial time from G, then the k-coloring problem would reduce to the evaluation of this polynomial at k and determining if the result is non-zero. Computing the coefficients of the chromatic polynomial or evaluating this polynomial is hard, more precisely it is #P-hard in the sense of Valiant's complexity class [VAL 79a, VAL 79b].

The next result is similar to the contraction/deletion formula discussed in proposition 5.9. Recall that $G \cdot e$ stands for the contraction of the edge e (definition 5.3). This result is useful when considering small graphs or graphs with a particular structure (reread remark 5.10).

PROPOSITION 7.26 (Contraction/Deletion Formula).— Let e be an edge in a simple graph G. We have

$$\pi_G(z) = \pi_{G-e}(z) - \pi_{G \cdot e}(z).$$

PROOF.— If we count all the proper colorings of G-e using exactly k colors, they are those assigning the same color to the endpoints of e and those assigning distinct colors. Those of the first (respectively, second) type are in one-to-one correspondence with the proper colorings of $G \cdot e$ (respectively, G) using exactly k colors. Said otherwise, the coefficients satisfy $m_{k,G-e} = m_{k,G\cdot e} + m_{k,G}$.

7.5. Ramsey numbers

We have colored faces of planar graphs, vertices of undirected graphs; now, we will color edges of complete graphs! So we will consider a map $c: E(K_n) \to \{1, \ldots, k\}$ coloring the edges of K_n with k possible colors. Here, we are not really interested in proper colorings. We will here speak of edge-coloring.

We will present Ramsey³ numbers but you have to know that this is only the beginning of a whole theory called *Ramsey theory*. Ramsey numbers have

³ Frank P. Ramsey (1903–1930) was a lecturer in mathematics at King's College. He made contributions in mathematical logic and decidability but also in philosophy and economics. The primary goal of Ramsey in his paper [RAM 30] from 1930 was related

applications [ROS 04] in many branches of mathematics: number theory, harmonic analysis, geometry, etc. For a survey, see Radziszowski's dynamic survey [RAD 94].

We start with a definition but at first glance, it is not at all clear that the quantity that we introduce does exist! Indeed, the fact that Ramsey numbers exist will follow from theorem 7.28.

DEFINITION 7.27 (Multicolor Ramsey numbers).— Let $k \geq 2$. Let $n_1, \ldots, n_k \geq 2$ be integers. The number $R(n_1, \ldots, n_k)$ is the smallest integer N such that, for every edge-coloring of K_N with k different colors, there exists i such that this edge-coloring of K_N contains a monochromatic complete subgraph K_{n_i} in color i.

An equivalent formulation is to say that for all $n < R(n_1, ..., n_k)$, there exists an edge-coloring of K_n that does not contain any monochromatic complete subgraph K_{n_i} in color i for each $i \in \{1, ..., k\}$.

We will first consider the case k=2 and R(s,t) with $s,t\geq 2$. The number R(s,t) is a *Ramsey number*. Instead of considering the colors 1 and 2, we will consider the colors red and blue. Ramsey theorem is an unavoidability result: for large enough n, all edge-colorings of K_n share a particular property.

THEOREM 7.28 (Ramsey theorem).— Let $s,t \geq 2$. There exists an integer R(s,t) such that, for all $n \geq R(s,t)$, every edge-coloring of K_n contains either a red K_s or a blue K_t as a subgraph.

Prior to the proof, let us make two observations. First, for all $s,t\geq 2,$ we have

$$R(s,t) = R(t,s).$$

Indeed, we consider the set C of all the edge-colorings of K_N and the map $\nu:C\to C$ that replaces an edge-coloring with its complement. Let $c:E(K_n)\to \{\text{red, blue}\}$ be an edge-coloring for all edges e of K_N , if c(e) is red (respectively, blue), then $\nu(c(e))$ is blue (respectively, red). The map ν is a one-to-one correspondence between C and itself, i.e. ν is a permutation over C and $C=\{\nu(c)\mid c\in C\}$. If an edge-coloring $c\in C$ of k0 has either a red

to a decision problem about logical formula. We quote his paper: "But in the course of this investigation it is necessary to use certain theorems on combinations which have an independent interest and are most conveniently set out by themselves beforehand."

 K_s or a blue K_t , then $\nu(c)$ is an edge-coloring such that K_N has either a blue K_s or a red K_t .

Also, for all s > 2,

$$R(s,2) = R(2,s) = s.$$

Every edge-coloring of K_s is either completely red or, contains at least a blue edge.

To get some intuition about these numbers, we may first observe that R(3,3) is at least 6. To prove that claim, it is enough to find edge-colorings of K_3 , K_4 and K_5 with no monochromatic triangles K_3 . Such edge-colorings are given in Figure 7.10 where we use plain and dashed edges to represent the two colors. Proving that $R(3,3) \leq 6$ was the second problem in Part I of the William Lowell Putnam Mathematical Competition⁴ held in March 1953.

For R(3,t) the first values for $t\geq 3$ are (Sloane's encyclopedia sequence A000791)

Then, R(4,4) = 18 and R(4,5) = 25. Not many exact values for other Ramsey numbers are known. Concerning the complexity of this problem, see example 2.19. For more precise statements, see [SCH 01] and [SCH 09].

The number of edge-colorings of K_n grows extremely rapidly. Without taking into account any symmetries (i.e. the edges have been numbered, we are not interested to count edge-colorings up to isomorphism), the total number of edge-colorings of K_n is the number of ways we can choose the color blue or red for each of the $\binom{n}{2}$ edges. The first values are given in Table 7.1.

LEMMA 7.29.— There is a one-to-one correspondence between the set of simple graphs with n vertices and the set of edge-colorings of K_n with two colors.

PROOF.— The n vertices are numbered $V = \{1, \ldots, n\}$. Consider the map μ defined as follows. For each simple graph G = (V, E), we consider the coloring $\mu(G)$ of K_n such that the edge $\{i, j\}$ in K_n is red if and only if

⁴ A renowed annual competetion of mathematics for undergraduate students in the U.S. and Canada.

 $\{i,j\}$ belongs to E. This is clearly a one-to-one correspondence: edges are associated with red edges in K_n and pairs of independent vertices are associated with blue edges in K_n . For instance, n independent vertices correspond to a monochromatic blue K_n .

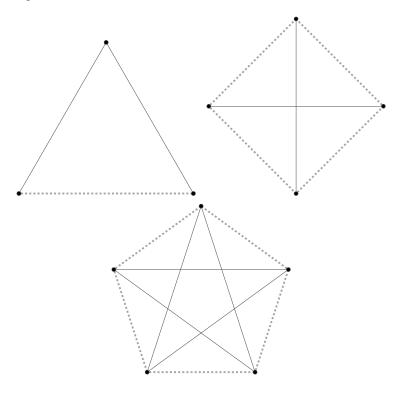


Figure 7.10. R(3,3) > 5

PROOF OF THEOREM 7.28.— We proceed by induction on s+t. We already know that the numbers $\mathsf{R}(2,t)$ and $\mathsf{R}(s,2)$ exist for all s,t. Hence, as a base case, $\mathsf{R}(s,t)$ exists if $4 \le s+t \le 5$ since $s,t \ge 2$, the only possible decompositions of 4 and 5 are 4=2+2, 5=2+3.

Let $N \ge 6$. Assume that R(s,t) exist for s+t < N. We will prove that R(s,t) exists for s+t = N. Moreover, we can also assume that $s,t \ge 3$.

More precisely, we will prove that every simple graph G with n vertices, where n = R(s-1,t) + R(s,t-1), has either a subgraph isomorphic to K_s or t

independent vertices. Because of lemma 7.29, this is an equivalent formulation. Note that by induction hypothesis, the numbers R(s-1,t), R(s,t-1) exist and thus n exists.

n	$2^{\binom{n}{2}}$
3	8
4	64
5	1024
6	32768
7	2097152
8	268435456
9	68719476736
10	35184372088832
11	36028797018963968
12	73786976294838206464
13	302231454903657293676544
14	2475880078570760549798248448

Table 7.1. Number of edge-colorings of K_n

Let v be a vertex of G. We define⁵ the set A_v made up of vertices that are not neighbors⁶ of v,

$$A_v = V \setminus (\mathsf{N}(v) \cup \{v\}).$$

If we count the number of vertices excluding v, we trivially have

$$\#(V \setminus \{v\}) = n - 1 = \mathsf{R}(s - 1, t) + \mathsf{R}(s, t - 1) - 1.$$

We claim that $\# N(v) \ge R(s-1,t)$ or $\# A_v \ge R(s,t-1)$. Indeed, if this was not the case, since N(v) and A_v make a partition of $V \setminus \{v\}$, we would have

$$\#(V \setminus \{v\}) = \#N(v) + \#A_v \le R(s-1,t) + R(s,t-1) - 2.$$

⁵ The reader may notice that it is exactly the same set as the one occurring in the proof of Theorem 3.12.

⁶ We could also have used the closed neighborhood N[v] of v.

If $\# N(v) \ge R(s-1,t)$, by definition of R(s-1,t), then the subgraph of G induced by N(v) has either a subgraph isomorphic to K_{s-1} or t independent vertices. Now if we consider the bigger graph G and, in particular, the vertex v, this vertex is adjacent to all the vertices in N(v). Hence, G has either a subgraph isomorphic to K_s or t independent vertices. Indeed, if we have independent vertices in the subgraph induced by $V' \subset V$, these vertices are also independent in the original graph.

If $\#A_v \geq \mathsf{R}(s,t-1)$, by definition of $\mathsf{R}(s,t-1)$, then the subgraph of G induced by A_v has either a subgraph isomorphic to K_s or t-1 independent vertices. Now if we consider the bigger graph G and, in particular, the vertex v, this vertex is independent to all the vertices in A_v . Hence, G has either a subgraph isomorphic to K_s or t independent vertices. This concludes the proof. We have shown that the Ramsey number $\mathsf{R}(s,t)$ exists and in fact, that

$$R(s,t) \le R(s-1,t) + R(s,t-1).$$
 [7.1]

COROLLARY 7.30.— Let $s, t \geq 2$. We have

$$\mathsf{R}(s,t) \leq \binom{s+t-2}{s-1}$$

and for all $s, t \geq 3$,

$$R(s,t) \le R(s-1,t) + R(s,t-1).$$

PROOF.— We proceed again on induction on s+t. For s=2, we have $t=R(2,t)=\binom{t}{1}$. Assume that $R(s,t)\leq \binom{s+t-2}{s-1}$ for all s,t such that s+t< N.

Assume that s + t = N with $s, t \ge 3$. From [7.1], we know that

$$\mathsf{R}(s,t) \leq \binom{s+t-3}{s-2} + \binom{s+t-3}{s-1}$$

and the conclusion follows from Pascal triangle formula.

Related to Ramsey theorem (in fact an application of it), let us also mention the following result (see, for instance, [GRA 02]).

THEOREM 7.31 (Erdős–Szekeres).— Let n be a positive integer. There exists a least integer N(n) such that every finite subset $X \subset \mathbb{R}^2$ of size N(n) made up of points in general positions (i.e. no three points in X are collinear) contains an n-tuple, which forms the vertices of a convex n-gon.

Only the first values of N(n) are known: $N(3)=3,\,N(4)=5,\,N(5)=9$ and N(6)=17.

We may move to colorings with three colors: red, blue and green. Let $n_1, n_2, n_3 \geq 2$ be three integers. We ask for a value of N such that every edge-coloring of K_N contains either a red K_{n_1} or a blue K_{n_2} or a green K_{n_3} . Every edge-coloring of the complete graph with $R(n_1, n_2)$ vertices contains a K_{n_1} red or a K_{n_2} blue. Now consider the number $N = R(R(n_1, n_2), n_3)$ and the two colors purple (which is a mix of red and blue) and green. As per theorem 7.28, every edge-coloring of K_N contains a purple $K_{R(n_1,n_2)}$ or a green K_{n_3} . Hence, every edge-coloring of K_N with three colors contains either, a green K_{n_3} or a subgraph $K_{R(n_1,n_2)}$ with edges colored in red or blue and we already know that such a complete graph has a K_{n_1} red or a K_{n_2} blue.

Proceeding by induction on the number of available colors, we have the following result.

COROLLARY 7.32.— Let $k \geq 2$. Let $n_1, \ldots, n_k \geq 2$ be integers. There exists a number $\mathsf{R}(n_1, \ldots, n_k)$ such that, for all $N \geq \mathsf{R}(n_1, \ldots, n_k)$, every edge-coloring of K_N with k different colors contains a monochromatic complete subgraph K_{n_i} in color i for some $i \in \{1, \ldots, k\}$.

Ramsey numbers can be extended as follows. Given two finite graphs H_1 and H_2 , there exists a number $\mathsf{R}(H_1,H_2)$ such that, for all $N \geq \mathsf{R}(H_1,H_2)$, every edge-coloring of K_n has either a monochromatic blue copy of H_1 or a monochromatic red copy of H_2 . Since H_1 and H_2 are subgraphs of a complete graph, these numbers $\mathsf{R}(H_1,H_2)$ exist.

REMARK 7.33.— Beyond our considerations on finite graphs, there are many extensions to infinite Ramsey theory (with countable and uncountable versions). Here is one possible version of this result. Color the subsets of size n of \mathbb{N} with k different colors. There exists an infinite subset S of \mathbb{N} such that all subsets of size n of S have the same color. For references, see [ERD 84].

7.6. Exercises

1) Determine all the automorphisms of the digraph depicted in Figure 7.11.

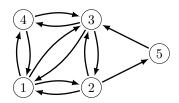


Figure 7.11. Determine Aut(G)

- 2) Give three simple pairwise non-isomorphic graphs that have exactly 20 automorphisms.
- 3) Let G (respectively, H) be a cycle graph of length m (respectively, n). For which values of m, n is there an homomorphism from G to H?
- 4) Work out a proof of the following theorem of Withney. Two connected graphs are isomorphic if and only if their line graphs (see page 40) are isomorphic, with a single exception: K_3 and $K_{1,3}$, which are not isomorphic but both have K_3 as their line graph.
- 5) A planar graph is *self-dual* if it is isomorphic to its dual. For which values of $n \geq 4$ can we build a self-dual planar connected graph with n vertices. Find a relation between the number of edges and vertices in a self-dual graph.
- 6) Let $d \geq 1$ be an integer. Given a finite labeled digraph G = (V, E, f) where $f: E \to \mathbb{Z}^d$ is a weight function, a periodic (infinite) d-dimensional graph $G^+ = (V^+, E^+)$ is defined by $V^+ = \{(z, v) \mid z \in \mathbb{Z}^d, v \in V\}$ and

$$E^{+} = \{((z, u), (z + f(u, v), v)) \mid (u, v) \in E\}.$$

Study the properties (connectedness, bipartiteness, etc.) of such graphs (see [COH 91]).

- 7) Determine the chromatic number of a few graphs such as K_5 , $K_{3,3}$, the Petersen graph and other graphs encountered in this book.
- 8) Consider the infinite grid $G(\mathbb{Z}^2)$ where the set of vertices is \mathbb{Z}^2 and for all $(x,y) \in \mathbb{Z}^2$, there is an edge from (x,y) to its four neighbors (x+1,y),

- (x,y+1), (x-1,y) and (x,y-1). A coloring (with two colors black/white) of the vertices is (t,i,j)-isotropic if every black (respectively, white) vertex has i (respectively, j) black vertices at distance at most t. Build a (2,8,10)-isotropic coloring of the grid. A coloring is *perfect* if, for all vertices v and all colors v, the number of vertices of color v and adjacent to v depends only on the color of v (for more detail, study the papers [AXE 03, PUZ 11]).
- 9) Build an infinite binary rooted tree with vertices colored black/white such that it has exactly n+1 non-isomorphic rooted subtrees of height n. Such a tree is said to be Sturmian (see [BER 10, KIM 15]).
- 10) Prove that for a (simple) path with n vertices, its chromatic polynomial is equal to $z(z-1)^n-1$.
- 11) Prove that for a tree with n vertices, its chromatic polynomial is equal to $z(z-1)^n-1$.
- 12) Prove that for a cycle with n vertices, its chromatic polynomial is equal to $(z-1)^n + (-1)^n(z-1)$.
- 13) A complete coloring with k colors $\{1,\ldots,k\}$ is a proper coloring of G such that for every two distinct colors $i\neq j$, there exist adjacent vertices colored with i and j. The largest k such that there exists such a complete coloring is called the *achromatic number* of G. Compute this value on small examples and study this notion, see [HEL 76, FAR 86].
 - 14) Prove that the diagonal Ramsey number R(s, s) satisfies

$$\mathsf{R}(s,s) \leq \frac{2^{2s-2}}{\sqrt{s}}.$$

- 15) Prove that R(3, 4) = 9.
- 16) From [BOL 98, p. 209], take the graph with vertex set \mathbb{Z}_{17} (the integers modulo 17) in which i is adjacent to j if and only if $i j \in \{\pm 1, \pm 2, \pm 4, \pm 8\}$ and show that R(4, 4) = 18.
 - 17) Make some search about the fact that R(3,3,3) = 17.
- 18) Given k directed graphs G_1, \ldots, G_k the Ramsey number $R(G_1, \ldots, G_k)$ is the smallest integer N such that for any partition (U_1, \ldots, U_k) of the edges of the complete symmetric directed graph K_N , there exists an integer i such that the partial graph induced by U_i contains G_i as a subgraph. Study this extension of Ramsey numbers (see [ERD 64] and [BER 74]).

- 19) With the same philosophy as Ramsey numbers, we can introduce Van der Waerden numbers. For any positive integers r and k there exists a positive integer W(k,r) such that, for all $n \geq W(k,r)$, if the integers $\{1,2,\ldots,n\}$ are colored with k colors, then there are at least r integers in arithmetic progression all of the same color: there exist $i \geq 1$, $d \geq 1$ such that $\{i+jd \mid j \in \{0,\ldots,r-1\}\}$ is monochromatic (see, for instance, [LUC 99]).
- 20) Make a search about Brooks' theorem [BRO 41]: Let G be a connected graph with $d = \max_{v \in V(G)} \deg(v)$. The chromatic number of G is at most d unless G is a complete graph or an odd cycle, in which case the chromatic number is d+1.
- 21) There are variants for coloring the vertices of a graph with prescribed non-repetitive properties (see, for instance, [GRY 11, CZE 07, GRY 07b, GRY 07a]). A coloring of a graph is *non-repetitive*, if there is no path (v_1,\ldots,v_{2r}) such that the first part (v_1,\ldots,v_r) has exactly the same sequence of colors as the second part (v_{r+1},\ldots,v_{2r}) . Work out some examples. For path graphs, this corresponds to the notion of avoidance in combinatorics on words. For instance.

RBBRBRRBBRRBRBBR

is a prefix of the Thue–Morse word (see example 1.48) and does not contain any square (i.e. repeated factor). The problem for cycles or trees is already more complicated (see, for instance, [CUR 02]).

22) We know that R(4,4)=18. Try to compute $R(C_4,C_4)$ which is the smallest N such that every edge-coloring of K_N with two colors contains a monochromatic cycle C_4 of length 4.

Algebraic Graph Theory

We are at a turning point of the book. In this chapter, we will discover that associating a matrix with a graph is a powerful concept because we can make use of all the machinery of linear algebra and matrix computations. In the following chapter, we will see that if the associated matrix has special properties (primitivity or irreducibility) then much more can be said about the corresponding graph. In particular, for Google's PageRank (see Chapter 10), one of the key points is to modify a graph to obtain a primitive matrix. For instance, we will soon learn the fact that a graph is bipartite is completely characterized by its spectrum, i.e. the set of eigenvalues of the associated matrix, or that the first coefficients of its characteristic polynomial have a combinatorial interpretation.

8.1. Prerequisites

We assume that the reader has a working knowledge of linear algebra. In this section, we fix notation and recap a few classical results that can be found in any textbook. In particular, matrices and row or column vectors will be denoted using boldface fonts. The set of $m \times n$ matrices with entries in the ring $\mathbb K$ will be denoted $\mathbb K^{m \times n}$, i.e. m (respectively, n) is the number of rows (respectively, columns). The *transpose* of the matrix $\mathbf M$ will be denoted by $\mathbf M^T$. Let $\mathbf A \in \mathbb C^{n \times n}$ and $\lambda \in \mathbb C$. If there exists a non-zero vector $\mathbf x \in \mathbb C^n$ such that $\mathbf A \mathbf x = \lambda \mathbf x$, then λ is an *eigenvalue* of $\mathbf A$. If λ is an eigenvalue of $\mathbf A$, every $\mathbf x \in \mathbb C^n$ such that $\mathbf A \mathbf x = \lambda \mathbf x$ is said to be an *eigenvector* of $\mathbf A$ associated with λ . Even though we will be dealing with matrices with integer entries, a matrix in $\mathbb N^{n \times n}$ or $\mathbb Q^{n \times n}$ may have complex (non-real) eigenvalues and eigenvectors.

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The field \mathbb{C} is algebraically closed but \mathbb{R} is not. We usually let \mathbf{I} denote the identity matrix (its dimension being clear from the context).

The **characteristic polynomial** of a matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ is the polynomial $p_{\mathbf{A}}(z) = \det(\mathbf{A} - z\mathbf{I})$ of degree n in the variable z. If \mathbf{A} belongs to \mathbb{K} , then $p_{\mathbf{A}}(z)$ belongs to $\mathbb{K}[z]$.

FACT 8.1.— The complex number λ is an eigenvalue of the matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ if and only if it is a root of the characteristic polynomial of \mathbf{A} .

Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. The algebraic multiplicity (respectively, geometric multiplicity) of an eigenvalue λ of \mathbf{A} is the multiplicity of λ as a root of $p_{\mathbf{A}}(z)$ (respectively, the dimension over \mathbb{C} of the eigenspace E_{λ} , which is the linear subspace $\{\mathbf{x} \in \mathbb{C}^n \mid \mathbf{A}\mathbf{x} = \lambda \mathbf{x}\}$). If $\lambda_1, \ldots, \lambda_p \in \mathbb{C}$ are the eigenvalues of \mathbf{A} , the **spectral radius** of \mathbf{A} is $\max\{|\lambda_1|, \ldots, |\lambda_p|\}$.

REMARK 8.2.— In general, the spectral radius of a matrix is not one of its eigenvalues.

FACT 8.3.— For each eigenvalue, its geometric multiplicity is less than or equal to its algebraic multiplicity.

FACT 8.4.— Let $P(z) = a_k z^k + \cdots + a_0$ be a polynomial in $\mathbb{C}[z]$ and **A** be a matrix in $\mathbb{C}^{n \times n}$ with $\lambda_1, \ldots, \lambda_p$ as eigenvalues. The eigenvalues of

$$P(\mathbf{A}) = a_k \, \mathbf{A}^k + \dots + a_0 \, \mathbf{I}$$

are exactly the complex numbers $P(\lambda_1), \ldots, P(\lambda_p)$. The algebraic multiplicity of an eigenvalue μ of $P(\mathbf{A})$ is the sum of the multiplicities of the eigenvalues λ_i of \mathbf{A} such that $P(\lambda_i) = \mu$. As an example, if 3 and -3 are eigenvalues of \mathbf{A} with multiplicity 2 and 3, then 9 is an eigenvalue of \mathbf{A}^2 with multiplicity 2+3=5.

FACT 8.5.— Non-zero eigenvectors associated with pairwise distinct eigenvalues are linearly independent.

A matrix **A** is *diagonalizable*, if there exists an invertible matrix **S** such that $S^{-1}AS$ is a diagonal matrix.

FACT 8.6.— A matrix \mathbf{A} is diagonalizable if and only if, for each eigenvalue, the corresponding algebraic and geometric multiplicities are the same. Otherwise stated, \mathbf{A} is diagonalizable if and only if there exists a basis of \mathbb{C}^n

made of up eigenvectors. In particular, for each eigenvalue α with algebraic multiplicity μ_{α} , every basis of E_{α} contains exactly μ_{α} elements.

Symmetric matrices will appear naturally when considering unoriented graphs. They have strong and useful properties. A matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ is *Hermitian* (respectively, *unitary*) if $\overline{\mathbf{A}}^T = \mathbf{A}$ (respectively, $\overline{\mathbf{A}}^T = \mathbf{A}^{-1}$).

FACT 8.7.— A Hermitian matrix (with possibly complex entries) has only real eigenvalues (thus, they can be ordered) and it is diagonalizable by a unitary matrix. In particular, a real symmetric matrix only has real eigenvalues.

Note that a real symmetric matrix \mathbf{M} has non-real eigenvectors as well as real ones. If $\mathbf{x} \in \mathbb{C}^n \setminus \{0\}$ is such that $\mathbf{M}\mathbf{x} = \alpha\mathbf{x}$ with $\alpha \in \mathbb{R}$, then since \mathbf{M} is real, $\mathfrak{Re}(\mathbf{x})$ and $\mathfrak{Im}(\mathbf{x})$ are eigenvectors with real components. Conversely, if $\mathbf{x} \in \mathbb{R}^n$ is an eigenvector of \mathbf{M} , so is $i\mathbf{x}$. With a bit more of an argument, we can prove the following.

FACT 8.8.— A real symmetric matrix is diagonalizable by an orthogonal matrix, i.e. a real matrix S such that $S^TS = SS^T = I$. Otherwise stated, there exists an orthonormal basis of \mathbb{C}^n made up of n eigenvectors belonging to \mathbb{R}^n .

Note that if $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^n$ form a basis of \mathbb{C}^n , then they are linearly independent over \mathbb{R} , and thus they also form a basis of \mathbb{R}^n . We let $||\mathbf{x}||$ denote the 2-norm $\sqrt{\mathbf{x}^T\mathbf{x}}$ of the vector $\mathbf{x} \in \mathbb{R}^n$.

LEMMA 8.9.— Let M be a real symmetric matrix and λ be its largest eigenvalue. We have

$$\lambda = \sup_{\substack{\mathbf{x} \in \mathbb{R}^n \\ ||\mathbf{x}|| = 1}} \mathbf{x}^T \mathbf{M} \mathbf{x} = \sup_{\mathbf{x} \in \mathbb{R}^n \setminus \{0\}} \frac{\mathbf{x}^T \mathbf{M} \mathbf{x}}{||\mathbf{x}||^2}.$$

The supremum is achieved precisely for the eigenvectors corresponding to λ .

PROOF.— Let $\mathbf{v}_1 \in \mathbb{R}^n$ be an eigenvector corresponding to λ and such that $||\mathbf{v}_1|| = 1$. The existence of such a vector in \mathbb{R}^n comes from fact 8.8. As $\mathbf{v}_1^T \mathbf{M} \mathbf{v}_1 = \lambda$, we obviously have

$$\lambda \leq \sup_{\substack{\mathbf{x} \in \mathbb{R}^n \\ ||\mathbf{x}||=1}} \mathbf{x}^T \mathbf{M} \mathbf{x}.$$

Since \mathbf{M} is symmetric (fact 8.7), we let $\lambda = \lambda_1 \geq \cdots \geq \lambda_n$ denote its eigenvalues repeated with their multiplicities. From fact 8.8, there exist vectors $\mathbf{v}_2, \ldots, \mathbf{v}_n$ such that $\mathbf{M}\mathbf{v}_i = \lambda_i \mathbf{v}_i$ and $\mathbf{v}_i^T \mathbf{v}_j = \delta_{i,j}$ for all $i, j \in \{1, \ldots, n\}$ and $\mathbf{v}_1, \ldots, \mathbf{v}_n$ form a basis of \mathbb{R}^n . Now assume that $\mathbf{y} \in \mathbb{R}^n$ has a norm equal to 1. Since we have a basis, there exist real coefficients $\alpha_1, \ldots, \alpha_n$ such that

$$\mathbf{y} = \sum_{i=1}^{n} \alpha_i \mathbf{v}_i$$

and, using the fact that $\mathbf{v}_1, \dots, \mathbf{v}_n$ are orthonormal,

$$\mathbf{y}^T \mathbf{M} \mathbf{y} = \sum_{i=1}^n \alpha_i^2 \lambda_i \le \lambda \sum_{i=1}^n \alpha_i^2 = \lambda ||\mathbf{y}|| = \lambda.$$
 [8.1]

This proves that

$$\sup_{\substack{\mathbf{x} \in \mathbb{R}^n \\ ||\mathbf{x}||=1}} \mathbf{x}^T \mathbf{M} \mathbf{x} \le \lambda.$$

Recall that the eigenvalues are ordered: if $\lambda_i \neq \lambda$, then $\lambda_i < \lambda$. We have equality exactly in [8.1] when, for each i such that $\alpha_i \neq 0$, we have $\lambda_i = \lambda$. This means that \mathbf{y} belongs to the eigenspace of λ .

8.2. Adjacency matrix

Since graphs are special instances of digraphs, we give a single definition for the adjacency matrix of a digraph.

DEFINITION 8.10.— Let G=(V,E) be a directed multigraph. The adjacency matrix of G is a square matrix $\mathbf{A}(G)=(\mathbf{A}(G))_{u,v\in V}$ of dimension #V indexed by the vertices of V where, for all $u,v\in V$,

$$[\mathbf{A}(G)]_{u,v}$$
 is the number of edges from u to v .

In particular, we can speak of the eigenvalues, eigenvectors, eigenspaces, spectrum of a graph G. For a simple digraph, the adjacency matrix is hollow: all its diagonal entries are zero.

Recall that (undirected) graphs are special cases of digraphs. Thus, a multigraph G is undirected if and only if $\mathbf{A}(G)$ is symmetric. In particular, an undirected multigraph has only real eigenvalues (see fact 8.7).

It is important to note that if a result is stated for directed graphs, it can also be applied to undirected graphs. Nevertheless, the converse is not true (in particular, when using the fact that A(G) is symmetric).

REMARK 8.11.— Let G = (V, E) be a directed multigraph. We can recover the outdegree and indegree of a vertex as follows:

$$\sum_{v \in V} [\mathbf{A}(G)]_{u,v} = \deg^+(u) \text{ and } \sum_{u \in V} [\mathbf{A}(G)]_{u,v} = \deg^-(v).$$

Otherwise stated, if e denotes the $n \times 1$ column vector whose entries are all equal to 1, we have

$$\mathbf{A}(G) \mathbf{e} = \left(\mathsf{deg}^+(v_1) \, \cdots \, \mathsf{deg}^+(v_n) \right)^T$$

and

$$\mathbf{e}^T \mathbf{A}(G) = (\mathsf{deg}^-(v_1) \cdots \mathsf{deg}^-(v_n)).$$

In the undirected case, since A(G) is symmetric, if G has **no loop**, the degree of a vertex is obtained by summing up elements of the row or of the column corresponding to it.

Recall that loops have a double contribution to the degree, see [1.1]. This does not show up in the adjacency matrix. This is the reason why we add the no loop assumption. Otherwise, we would have to count twice the diagonal entries.

REMARK 8.12.— If two multigraphs G_1 and G_2 are isomorphic (see Definition 7.4), then they have the same adjacency matrix up to a permutation of the indices. There exists a permutation matrix $P \in \{0,1\}^{n \times n}$ with exactly one entry 1 on each row and each column such that

$$\mathbf{A}(G_2) = \mathbf{P}^{-1}\mathbf{A}(G_1)\mathbf{P}.$$

¹ If you are not familiar with this concept, experiment with your favorite 3-vertex graph and number the vertices in two different ways.

It is an easy exercise to prove that the two matrices have the same characteristic polynomial.

In group theory, in particular for groups of automorphisms of graphs, the order of an element x is the smallest positive integer n such that $x^n = id$.

PROPOSITION 8.13.— [MOW 71] Let G be a digraph. If all the eigenvalues of $\mathbf{A}(G)$ are different, then every automorphism f of G has order 1 or 2, i.e. $f = \operatorname{id} \operatorname{or} f^2 = \operatorname{id}$.

PROOF.– From remark 7.9, we know that every automorphism corresponds to a permutation matrix \mathbf{P} such that $\mathbf{P}^{-1}\mathbf{A}(G)\mathbf{P} = \mathbf{A}(G)$. Our aim is to show that $\mathbf{P}^2 = \mathbf{I}$. Let \mathbf{x} be an eigenvector of \mathbf{A} associated with the eigenvalue λ . It yields

$$\mathbf{A}(G)\mathbf{P}\mathbf{x} = \mathbf{P}\mathbf{A}(G)\mathbf{x} = \lambda \mathbf{P}\mathbf{x}.$$

Thus, $\mathbf{P}\mathbf{x}$ is also an eigenvector of $\mathbf{A}(G)$ associated with the eigenvalue λ . Since all the eigenvalues of $\mathbf{A}(G)$ are different, the geometric multiplicity of every eigenvalue is equal to one. Hence, $\mathbf{P}\mathbf{x}$ and \mathbf{x} are linearly dependent. But the entries of \mathbf{x} and $\mathbf{P}\mathbf{x}$ are just permuted. Thus, the two vectors have the same norm and we conclude² that $\mathbf{P}\mathbf{x} = \alpha\mathbf{x}$ where $\alpha \in \mathbb{C}$ is such that $\alpha^2 = 1$. In particular, $\mathbf{P}^2\mathbf{x} = \mathbf{x}$ for all eigenvectors \mathbf{x} of $\mathbf{A}(G)$. A matrix whose eigenvalues are all different is diagonalizable, i.e. has a basis of eigenvectors. So the equality $\mathbf{P}^2\mathbf{x} = \mathbf{x}$ stands for the elements of a basis of \mathbb{C}^n and thus for every element in \mathbb{C}^n . In particular, it holds for the unitary column vector e_j whose components are all zero except the jth component equal to 1. Hence, we conclude that $\mathbf{P}^2 = \mathbf{I}$.

The setting of the next proposition generalizes the notion of bipartite graphs to directed graphs.

PROPOSITION 8.14.— Let G = (V, E) be a directed multigraph. If there exists a partition of V into two subsets V_1 and V_2 such that $E \subseteq (V_1 \times V_2) \cup (V_2 \times V_1)$, then for every eigenvalue $\lambda \in \mathbb{C}$ of G, $-\lambda$ is also an eigenvalue of G.

² There exists $\alpha \in \mathbb{C}$ such that $\mathbf{P}\mathbf{x} = \alpha \mathbf{x}$. Assume that a, b are two non-zero entries of \mathbf{x} that are interchanged by \mathbf{P} . Then, $\alpha a = b$ and $\alpha b = a$.

PROOF.— If we order V by first considering the vertices in V_1 , second those in V_2 , then $\mathbf{A}(G)$ is a block matrix

$$\begin{pmatrix} \mathbf{0} & \mathbf{B} \\ \mathbf{C} & \mathbf{0} \end{pmatrix}$$

where the submatrix **B** (respectively, **C**) has dimensions $\#V_1 \times \#V_2$ (respectively, $\#V_2 \times \#V_1$). Let **x** be a non-zero eigenvector of $\mathbf{A}(G)$ with eigenvalue λ . We can consider **x** as a block matrix

$$\mathbf{x} = \begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix}$$

where \mathbf{y} (respectively, \mathbf{z}) is a column of height $\#V_1$ (respectively, $\#V_2$). Since $\mathbf{A}(G)\mathbf{x} = \lambda \mathbf{x}$, then $\mathbf{B}\mathbf{z} = \lambda \mathbf{y}$ and $\mathbf{C}\mathbf{y} = \lambda \mathbf{z}$. Now consider the non-zero column vector

$$\widetilde{\mathbf{x}} = \begin{pmatrix} \mathbf{y} \\ -\mathbf{z} \end{pmatrix}.$$
 [8.2]

We get
$$\mathbf{A}(G)\widetilde{\mathbf{x}} = -\lambda \widetilde{\mathbf{x}}$$
 showing that $-\lambda$ is an eigenvalue.

The next statement gives more insight about the multiplicities of opposite eigenvalues (in the unoriented case).

COROLLARY 8.15.— Let G=(V,E) be a bipartite graph. If λ is an eigenvalue of G, then $-\lambda$ is an eigenvalue of G with the same multiplicity³.

PROOF.— From the previous result, we know that the spectrum of $\mathbf{A}(G)$ is symmetric with respect to 0. Let λ be an eigenvalue of $\mathbf{A}(G)$. Since $\mathbf{A}(G)$ is diagonalizable (because it is symmetric – fact 8.8), the algebraic and geometric multiplicities of λ coincide. Let $\mathbf{x}_1, \ldots, \mathbf{x}_r$ be a basis of the eigenspace associated with λ . Applying the same transformation as in [8.2], thus using the same notation, the vectors $\widetilde{\mathbf{x}_1}, \ldots, \widetilde{\mathbf{x}_r}$ all belong to the eigenspace $E_{-\lambda}$ associated with $-\lambda$. Since we are only permuting rows, any linear relation occurring between the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_r$ also hold for the

³ Reading the proof, you will see that algebraic and geometric multiplicities coincide. Thus, there is no need to be more specific.

vectors $\widetilde{\mathbf{x}_1}, \dots, \widetilde{\mathbf{x}_r}$ and conversely, i.e.

$$\sum_{i=1}^{r} \lambda_i \, \mathbf{x}_i = 0 \Leftrightarrow \sum_{i=1}^{r} \lambda_i \, \widetilde{\mathbf{x}}_i = 0.$$

Thus, $\widetilde{\mathbf{x}_1}, \dots, \widetilde{\mathbf{x}_r}$ are linearly independent elements in $E_{-\lambda}$ and $\dim E_{\lambda} \leq \dim E_{-\lambda}$. If we apply the same argument starting with a basis of $E_{-\lambda}$, we get $\dim E_{\lambda} \geq \dim E_{-\lambda}$.

EXAMPLE 8.16.— The graph⁴ with 30 vertices depicted in Figure 8.1 has the following eigenvalues (with the corresponding algebraic multiplicities):

$$-6(1\times)$$
, $-3(5\times)$, $-1(9\times)$, $1(9\times)$, $3(5\times)$, $6(1\times)$.

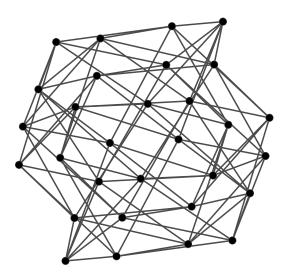


Figure 8.1. The bipartite Kneser graph H(6,2)

Observe once more that all the eigenvalues are real because we have an unoriented graph (fact 8.7). From proposition 8.13, we also deduce that this

⁴ The bipartite Kneser graph H(n,k) is the graph whose two bipartite sets of vertices represent the k-subsets and (n-k)-subsets of $\{1,\ldots,n\}$ and where two vertices are connected if and only if they are in different sets and one is a subset of the other.

graph has an automorphism of order at least 3. Note that Aut(H(6,2)) contains 1,440 elements.

The adjacency matrix of a graph is useful to count walks of a given length. We allow walks of length 0 on each vertex. This is consistent with the convention as in section 1.2.1. Even though the next result is quite elementary, we will explore it in various contexts (for instance, graphs with primitive components in section 9.4.2).

THEOREM 8.17.— Let G be a directed multigraph. For all $n \geq 0$ and $u, v \in V(G)$, $[\mathbf{A}(G)^n]_{u,v}$ is the number of walks of length n from u to v.

PROOF.—We proceed by induction on n. The cases n=0 and n=1 are clear from the definition of $\mathbf{A}(G)$. Assume that the property holds for $n\geq 1$ and prove it for n+1. By definition of the product of two matrices, we have

$$[\mathbf{A}(G)^{n+1}]_{u,v} = \sum_{w \in V(G)} [\mathbf{A}(G)^n]_{u,w} [\mathbf{A}(G)]_{w,v}.$$

It suffices to get a combinatorial interpretation of this formula. By induction hypothesis, $[\mathbf{A}(G)^n]_{u,w}$ is the number of walks of length n from u to w. To conclude with the proof, notice that the walks of length n+1 from u to v are obtained from walks of length n from u to w followed by walks of length 1 from w to v and we get different walks when w ranges over V(G).

We will spend a lot of time discussing the number of walks between two vertices. Thus, it deserves a special notation.

DEFINITION 8.18.— We let $nW_{u\to v}: \mathbb{N} \to \mathbb{N}$ denote the function that maps n > 0 to the number of walks of length n from u to v.

COROLLARY 8.19.— Let G be a directed multigraph with d vertices. There exist integer constants c_0, \ldots, c_{d-1} such that, for all $n \ge 0$,

$$\mathsf{nW}_{u \to v}(n+d) = \sum_{i=0}^{d-1} c_i \, \mathsf{nW}_{u \to v}(n+i).$$

Said otherwise, the sequences $(nW_{u\to v}(n))_{n\geq 0}$, $u,v\in V$, satisfy the same recurrence relation. Two such sequences may only differ due to their initial conditions $nW_{u\to v}(0),\ldots,nW_{u\to v}(d-1)$.

Note that this result can also be applied to the number of vertices in the different levels of the unraveling of a digraph (see section 5.5).

PROOF.— Let $p(z) \in \mathbb{Z}[z]$ be the characteristic polynomial of $\mathbf{A}(G)$. It is a monic polynomial of degree d=#V(G). From the Cayley–Hamilton theorem, we know that $p(\mathbf{A}(G))=0$. Therefore, there exist integers c_{d-1},\ldots,c_0 such that

$$\mathbf{A}(G)^d = \sum_{i=0}^{d-1} c_i \mathbf{A}(G)^i.$$

Multiplying both sides by $\mathbf{A}(G)^n$ shows that $(\mathbf{A}(G)^j)_{j\geq 0}$ satisfies a linear recurrence equation. Thus, all components of this matrix satisfy this recurrence equation as well, and we know from the previous theorem that $[\mathbf{A}(G)^n]_{u,v}$ is the number of walks $\mathsf{nW}_{u\to v}(n)$ of length n from u to v.

8.3. Playing with linear recurrences

It is probably worth recalling standard results about linear recurrence sequences (see, for instance, [GRA 94]).

THEOREM 8.20.— Let $d \ge 1$ and $r_0, \ldots, r_{d-1} \in \mathbb{R}$, $r_0 \ne 0$. Let $(U_n)_{n \ge 0}$ be a sequence satisfying, for all $n \ge 0$,

$$U_{n+d} = r_{d-1} U_{n+d-1} + \dots + r_0 U_n.$$
 [8.3]

Let $\alpha_1, \ldots, \alpha_t \in \mathbb{C}$ be the roots with multiplicities m_1, \ldots, m_t of the characteristic polynomial of the relation [8.3]

$$X^{d} - r_{d-1}X^{d-1} - \dots - r_{0}.$$
 [8.4]

There exist t polynomials $P_1, \ldots, P_t \in \mathbb{C}[z]$ of degree, respectively, less than m_1, \ldots, m_t and depending only on the initial conditions U_0, \ldots, U_{d-1} such that

$$\forall n \ge 0, \ U_n = P_1(n) \, \alpha_1^n + \dots + P_t(n) \, \alpha_t^n.$$
 [8.5]

REMARK 8.21.— In the relation [8.3], if $r_0 = \cdots = r_{\ell-1} = 0$, then the sequence $(U_n)_{n\geq 0}$ does not depend on the first ℓ initial conditions $U_0, \ldots, U_{\ell-1}$. We can consider the shifted sequence whose first term is U_ℓ and we are back to the assumption of the theorem (with a relation of smaller order). Observe that $r_0 = 0$ if and only if 0 is a root of the characteristic polynomial [8.4] of the relation.

EXAMPLE 8.22 (Binet's Formula⁵).— With the digraph G depicted in Figure 8.2, let us illustrate the above results by counting the number of closed walks of length n from u to itself.



Figure 8.2. Counting number of walks

We have

$$\mathbf{A}(G) = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$
 and $p_{\mathbf{A}}(z) = z^2 - z - 1$.

Thus, the sequence $(nW_{u\to u}(n))_{n>0}$ satisfies the equation

$$U_{n+2} = U_{n+1} + U_n, \ \forall n \ge 0$$

and $nW_{u\to u}(0)=1$, $nW_{u\to u}(1)=1$. This is exactly the ubiquitous Fibonacci sequence. The roots of $p_{\mathbf A}(z)$ are the golden ratio $(1+\sqrt{5})/2$ and its conjugate $(1-\sqrt{5})/2$. From [8.5], we derive that

$$\mathsf{nW}_{u \to u}(n) = A \left(\frac{1 + \sqrt{5}}{2}\right)^n + B \left(\frac{1 - \sqrt{5}}{2}\right)^n, \ \forall n \ge 0$$

where A and B are constants (because the two roots are simple). The initial conditions lead to the system for n=0 and n=1

$$\begin{cases} 1 = A + B \\ 1 = A\left(\frac{1+\sqrt{5}}{2}\right) + B\left(\frac{1-\sqrt{5}}{2}\right). \end{cases}$$

⁵ The formula was probably known from others, but the name of Jacques Philippe Marie Binet (1786–1856) is usually associated with the famous formula expressing the nth Fibonacci number.

We find
$$A = (5 + \sqrt{5})/10$$
, $B = (5 - \sqrt{5})/10$ and

$$\mathsf{nW}_{u \to u}(n) = \frac{5 + \sqrt{5}}{10} \left(\frac{1 + \sqrt{5}}{2} \right)^n + \frac{5 - \sqrt{5}}{10} \left(\frac{1 - \sqrt{5}}{2} \right)^n, \ \forall n \ge 0.$$

The latter relation is sometimes referred to as Binet's relation that provides a closed form for the nth Fibonacci number.

We can also make use of a bit of linear algebra whenever A(G) is diagonalizable or, more generally, is reduced to the canonical Jordan form. Indeed, in that case, it is easy to derive the form of a matrix to the power n.

Let us pursue the previous example, with

$$\mathbf{S} = \begin{pmatrix} \frac{1}{2} \left(1 + \sqrt{5} \right) & \frac{1}{2} \left(1 - \sqrt{5} \right) \\ 1 & 1 \end{pmatrix}$$

then

$$\mathbf{S}^{-1}\mathbf{A}(G)\mathbf{S} = \begin{pmatrix} \frac{1+\sqrt{5}}{2} & 0\\ 0 & \frac{1-\sqrt{5}}{2} \end{pmatrix}.$$

This is not a miracle, we have to find eigenvalues and eigenvectors of $\mathbf{A}(G)$. Hence,

$$\mathbf{A}(G)^n = \mathbf{S} \begin{pmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^n & 0\\ 0 & \left(\frac{1-\sqrt{5}}{2}\right)^n \end{pmatrix} \mathbf{S}^{-1}.$$

Knowing the two matrices S and S⁻¹, we get back Binet's relation by expressing $[\mathbf{A}(G)^n]_{u,u}$.

REMARK 8.23.— Here is an alternative to theorem 8.20 and the two methods have the same problem. It is equivalent to find the roots of the characteristic polynomial of a recurrence relation or the eigenvalues of a matrix. In general, for a $k \times k$ matrix \mathbf{B} , there exists an invertible matrix $\mathbf{S} \in \mathbb{C}^{k \times k}$ such that $\mathbf{S}^{-1}\mathbf{B}\mathbf{S}$ is a block diagonal matrix \mathbf{D} where the blocks on the diagonal are square matrices (Jordan blocks) of the form

$$\mathbf{J}_{\lambda} = \begin{pmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix}$$

where λ is an eigenvalue of **B**. It is easy to prove by induction on n that, if \mathbf{J}_{λ} is such a block of size r, then entries of \mathbf{J}_{λ}^{n} above the diagonal are of the form $P(n) \lambda^{n}$ where P is a polynomial of degree at most r-1. For instance, for r=2, for all $n \in \mathbb{N}$,

$$\begin{pmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{pmatrix}^n = \begin{pmatrix} \lambda^n & n\lambda^{n-1} & \frac{1}{2}(n-1)n\lambda^{n-2} \\ 0 & \lambda^n & n\lambda^{n-1} \\ 0 & 0 & \lambda^n \end{pmatrix}.$$

In particular, if all the Jordan blocks appearing in $S^{-1}BS$ are 1×1 matrices, then B is diagonalizable. Since $B^n = SD^nS^{-1}$, then every entry of B^n is a linear combination of some polynomials in n times eigenvalues of B to the power n. Moreover, the degree of these polynomials is less than the maximal size of the associated Jordan blocks. If B is diagonalizable, then every entry of B^n is a linear combination of the eigenvalues of B to the power n.

EXAMPLE 8.24.— We will not give much details here but consider the graph depicted in Figure 8.3.



Figure 8.3. Digraph and Jordan normal form

The corresponding Jordan normal form is given by

$$\begin{pmatrix} \frac{1+\sqrt{5}}{2} & 1 & 0 & 0\\ 0 & \frac{1+\sqrt{5}}{2} & 0 & 0\\ 0 & 0 & \frac{1-\sqrt{5}}{2} & 1\\ 0 & 0 & 0 & \frac{1-\sqrt{5}}{2} \end{pmatrix}.$$

Having Jordan blocks of size 2 implies that some sequences $(nW_{u\to v}(n))_{n\geq 0}$ will asymptotically behave like $n((1+\sqrt{5})/2)^n$. This will be elaborated in section 9.4.

Another convenient tool to consider when dealing with recurrence sequences is *formal power series* (also called *generating function*). With a

sequence $(U_n)_{n\geq 0}\in \mathbb{K}^{\mathbb{N}}$, where \mathbb{K} is a ring, is associated the series (in variable z)

$$g_U(z) = \sum_{n=0}^{+\infty} U_n \, z^n.$$

This object is usually seen purely as an algebraic object used to encode a sequence and to work with it (we generally do not look at convergence). One can apply various operations on those series, which in turn have interpretations in terms of the initial sequence. For a good account, see [WIL 06] or [GRA 94, Chapter 7]. In some cases, but not always, analytic tools provide extra information such as asymptotic formulas [FLA 09]. The set of these series is denoted by $\mathbb{K}[[z]]$. Endowed with term-wise addition and with *Cauchy product* extending the product of two polynomials, $\mathbb{K}[[z]]$ is a ring:

$$\sum_{n=0}^{+\infty} U_n z^n + \sum_{n=0}^{+\infty} V_n z^n = \sum_{n=0}^{+\infty} (U_n + V_n) z^n,$$
 [8.6]

$$\sum_{n=0}^{+\infty} U_n z^n \cdot \sum_{n=0}^{+\infty} V_n z^n = \sum_{n=0}^{+\infty} \left(\sum_{i=0}^{n} (U_i + V_{n-i}) \right) z^n.$$

A trivial but useful observation is that, by definition, two formal series $\sum_{n=0}^{+\infty} U_n z^n$ and $\sum_{n=0}^{+\infty} V_n z^n$ are equal if and only if $U_n = V_n$ for all n. A polynomial of $\mathbb{K}[z]$ is a formal power series where all but a finite number of coefficients are zero.

Before stating the next result, we say that the **reciprocal polynomial** of a polynomial $P(z) = a_n z^n + \cdots + a_0$, $a_n \neq 0$ is the polynomial $z^n P(1/z) = a_n + \cdots + a_0 z^n$. Roughly, we have to mirror the coefficients.

In the next statement, we are discussing rational functions thus we assume that we are working with recurrence equations whose coefficients and initial conditions belonging to a field. For our purposes, it is enough to work over \mathbb{C} . Note that the same sequence can satisfy several linear recurrence equations. For instance, the Fibonacci sequence $1,1,2,3,5,8,13,\ldots$ satisfies the equation $U_{n+2}=U_{n+1}+U_n$ for all $n\geq 0$ but also an equation of order four $V_{n+4}=V_{n+3}+V_{n+1}+V_n$ for all $n\geq 0$. So we must speak of the characteristic polynomial of a particular relation (not of the sequence, since

several relations are associated with one sequence⁶). In the first case, it is the polynomial $X^2 - X - 1$ and in the second case, it is $X^4 - X^3 - X - 1$.

THEOREM 8.25.— The sequence $U=(U_n)_{n\geq 0}$ satisfies a linear recurrence equation of degree d of the form [8.3], with 7 $r_0\neq 0$, if and only if its generating function $\mathbf{g}_U(z)$ is a rational function that can be written as the quotient P/Q of two polynomials where $\deg(P)\leq d-1$ and Q is the reciprocal polynomial of the characteristic polynomial [8.4] of equation [8.3] satisfied by U. In particular, Q(0)=1, $\deg(Q)=d$ and the roots of Q are the reciprocals of the roots of the characteristic polynomial of the relation [8.3]. Moreover, the polynomial P only depends on the initial conditions of the recurrence.

PROOF.- With algebraic manipulations, we have

$$\begin{split} \mathbf{g}_{U}(z) &= \sum_{n \geq 0} U_{n+d} \, z^{n+d} + \sum_{i=0}^{d-1} U_{i} \, z^{i} \\ &= \sum_{i=0}^{d-1} r_{i} z^{d-i} \sum_{n \geq 0} U_{n+i} \, z^{n+i} + \sum_{i=0}^{d-1} U_{i} \, z^{i} \\ &= \sum_{i=0}^{d-1} r_{i} z^{d-i} \left(\mathbf{g}_{U}(z) - \sum_{k=0}^{i-1} U_{k} \, z^{k} \right) + \sum_{i=0}^{d-1} U_{i} \, z^{i}. \end{split}$$

Hence, we deduce that

$$\underbrace{\left(1 - \sum_{i=0}^{d-1} r_i z^{d-i}\right)}_{=:Q(z)} \mathbf{g}_U(z) = \underbrace{\sum_{i=0}^{d-1} \left(U_i z^i - r_i z^{d-i} \sum_{k=0}^{i-1} U_k z^k\right)}_{=:P(z)}$$
[8.7]

where the right-hand side is a polynomial P(z) of degree at most d-1. Note that Q(z) is indeed the reciprocal polynomial of [8.4].

⁶ One could introduce the minimal polynomial of a linear recurrent sequence. It is associated with a recurrence relation of minimal order and we can show that this polynomial is unique and thus well defined.

⁷ As observed in remark 8.21, this simple extra condition means that there is no degeneracy, an element really depends on the d previous ones. In particular, 0 is not a root of the characteristic polynomial.

For the converse, proceed by long division of P by Q but starting with terms of lowest degree first. The easiest thing to do is to proceed with an example. Take the rational function $(1+2z)/(1-2z-5z^2)$

Indeed, the series expansion yields

$$1 + 4z + 13z^{2} + 46z^{3} + 157z^{4} + 544z^{5}$$

+ 1,873z⁶ + 6,466z⁷ + 22,297z⁸ + $\mathcal{O}(z^{9})$.

It seems that the coefficients of the power series satisfies the equation $U_{n+2} = 2U_{n+1} + 5U_n$. It is not difficult to prove this. The long division means that

$$1 + 2z = (1 - 2z - 5z^{2}) \sum_{n=0}^{+\infty} U_{n} z^{n}.$$

If we proceed to the Cauchy product on the right-hand side and equal the coefficients of the terms with same degree, we get

$$1 = U_0, \ 2 = U_1 - 2U_0, \ 0 = U_2 - 2U_1 - 5U_0$$

and, for all n > 0,

$$0 = U_{n+2} - 2U_{n+1} - 5U_n.$$

What we have done on an example is general. Since $\deg(P) \leq d-1$, the coefficients of P uniquely determine U_0, \ldots, U_{d-1} . Since $r_0 \neq 0$, the polynomial Q is the reciprocal polynomial of [8.4] and has degree d. Hence U_{n+d} satisfies [8.3] for all $n \geq 0$.

Since g_U is a rational function whenever U satisfies a linear recurrence equation, we will make use of another classical result.

PROPOSITION 8.26 (Partial Fractions Decomposition).— Let $Q \in \mathbb{C}[z]$ be a polynomial with roots z_1, \ldots, z_k of multiplicity d_1, \ldots, d_k i.e. there exists $c \in \mathbb{C} \setminus \{0\}$ such that

$$Q(z) = c \prod_{i=1}^{k} (z - z_i)^{d_i}.$$

Let $P/Q \in \mathbb{C}(z)$ be a rational function with $\deg P < \deg Q$, then P/Q can be decomposed in a unique way as

$$\sum_{i=1}^{k} \sum_{j=1}^{d_i} \frac{a_{i,j}}{(z-z_i)^j}$$

where the $a_{i,j}$'s are constants.

REMARK 8.27.— In the setting of theorem 8.25, 0 is not a root of the denominator. Let ρ be a non-zero complex number. For all integers $j \geq 1$, we only have to recall the power series expansion of a fraction of the form $\frac{a}{(z-\rho)^j}$ as

$$(-1)^{j} \frac{a}{\rho^{j}} \frac{1}{\left(1 - \frac{z}{\rho}\right)^{j}} = (-1)^{j} \frac{a}{\rho^{j}} \sum_{n=0}^{+\infty} {j+n-1 \choose j-1} \left(\frac{1}{\rho}\right)^{n} z^{n}.$$

Putting together theorem 8.25, proposition 8.26 and the above remark provides a general method for solving recurrences, i.e. expressing the general term of the sequence.

EXAMPLE 8.28.— Using formal power series, we can reobtain Binet's relation in an alternative way (useful in the following chapter). The last line [8.7] of the first part of the proof of theorem 8.25 applied to that example gives (with d=2, $r_0=r_1=1$, $U_0=U_1=1$)

$$\sum_{n=0}^{+\infty} U_n \, z^n = \frac{1}{1 - z - z^2}.$$

The trick is to decompose the rational function into partial fractions. Let $\varphi=(1+\sqrt{5})/2$ and $\psi=(1-\sqrt{5})/2$. The roots of the denominator are the reciprocals of the roots of the characteristic polynomial, thus

$$\frac{1}{1 - z - z^2} = \frac{a}{z - 1/\varphi} + \frac{b}{z - 1/\psi}.$$

Determining a and b yields $a = -b = -\sqrt{5}/5$. Now, we have

$$\frac{a}{z-1/\varphi} = \frac{-a\,\varphi}{1-\varphi\,z} = -a\varphi\sum_{n=0}^{+\infty}\varphi^n\,z^n$$

and $-a\varphi=(5+\sqrt{5})/10$. We get back the first term expressing the nth Fibonacci number. Proceed in the same way to get the second term.

8.4. Interpretation of the coefficients

After this digression on linear recurrence sequences, we are back to our graph business. The first few coefficients of the characteristic polynomial of the adjacency matrix have a nice combinatorial interpretation as stated in the next result, which follows from the multilinearity of the determinant.

LEMMA 8.29.– Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. Let

$$p_{\mathbf{A}}(z) = \sum_{i=0}^{n} c_i (-z)^{n-i}$$
 [8.8]

be its characteristic polynomial. We have $c_0 = 1$ and for i > 0, the coefficient c_i is the sum of the determinants of all the principal $i \times i$ submatrices of \mathbf{A} , i.e. obtained by removing n-i rows and columns such that the sets of row indices and column indices that have been removed are the same. In particular, $c_1 = tr(\mathbf{A})$ is the sum of the elements on the diagonal (the trace of \mathbf{A}) and $c_n = \det(\mathbf{A})$.

A *triangle* (or 3-cycle) in a graph is a subgraph equal to K_3 .

PROPOSITION 8.30.— Let G be a graph and p be its characteristic polynomial given as in [8.8]. Then

- 1) c_1 is the number of loops, in particular, $c_1 = 0$ whenever G is simple;
- 2) if G is simple, $-c_2$ is the number of edges in G;
- 3) if G is simple, c_3 is twice the number of triangles in G.

PROOF.— If we consider the principal 2×2 submatrices of $\mathbf{A}(G)$ associated with the vertices u and v, they are of two kinds

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$
, or $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

if there is no edge $\{u, v\}$, or if this edge belongs to the graph. The determinant of the second is equal to -1. If we consider the principal 3×3 submatrices of $\mathbf{A}(G)$ associated with the vertices u, v and w, they are of three kinds (not including the zero matrix)

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \text{ or } \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \text{ or } \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

Only the last one has a non-zero determinant equal to 2 and corresponding to the case where $\{u, v\}, \{v, w\}, \{u, w\}$ all belong to the graph.

8.5. A theorem of Hoffman

We were looking for a good pretext to introduce an algebra of polynomials associated with a multigraph. If \mathbf{A} is a square matrix, a *polynomial* in \mathbf{A} is an expression of the form $\sum_{i=0}^d c_i \mathbf{A}^i$.

DEFINITION 8.31.— Let G = (V, E) be a multigraph. We let A_G denote the algebra of polynomials in $\mathbf{A}(G)$ over \mathbb{C} .

Since we have a vector space, we can make linear combinations of polynomials or multiply together polynomials of the adjacency matrix of G. In particular, powers of $\mathbf{A}(G)$ belongs to \mathcal{A}_G . In this section, we only consider unoriented graphs.

DEFINITION 8.32.— Let G be a connected multigraph. The diameter of G is given by

$$\mathsf{diam}(G) = \max_{u,v \in V} \mathsf{d}(u,v)$$

where the distance d was discussed in remark 1.31 and d(u, v) is realized by a shortest path between u and v.

As a result of Cayley–Hamilton theorem, \mathcal{A}_G is a finite dimensional vector space over \mathbb{C} , thus we can speak of its dimension. We have already discussed the fact that $\mathbf{A}(G)$ is diagonalizable. Let $m_{\mathbf{A}}(X)$ be the minimal polynomial of $\mathbf{A}(G)$, i.e. the non-zero monic polynomial of smallest degree

such that $m_{\mathbf{A}}(\mathbf{A}(G)) = \mathbf{0}$. In particular, if $\deg m_{\mathbf{A}} = d$, we have a non-trivial linear combination of $\mathbf{I}, \mathbf{A}(G), \dots, \mathbf{A}(G)^d$ being equal to zero. Otherwise stated, $\dim \mathcal{A}_G \leq \deg m_{\mathbf{A}}$.

PROPOSITION 8.33.— Let G = (V, E) be a connected multigraph. We have $\dim \mathcal{A}_G > \operatorname{diam}(G)$.

PROOF.— Let $(v_0, v_1, \ldots, v_\ell)$ be a path realizing the diameter ℓ of G. This means that, for all $j \leq \ell$, we have a path from v_0 to v_j but no shorter path. Translating this, we have $[\mathbf{A}(G)^j]_{v_0,v_j} > 0$ and $[\mathbf{A}(G)^k]_{v_0,v_j} = 0$ if k < j. Thus, the matrices $\mathbf{I}, \mathbf{A}(G), \ldots, \mathbf{A}(G)^\ell$ are linearly independent and $\dim \mathcal{A}_G \geq \ell + 1$.

FACT 8.34.— The roots of the minimal polynomial of a matrix are exactly its eigenvalues. A matrix is diagonalizable if and only if all the roots of its minimal polynomial are simple. In that case, the degree of this polynomial is equal to the number of eigenvalues. Actually, the multiplicity of a root λ of the minimal polynomial of \mathbf{A} gives the size of the largest Jordan block \mathbf{J}_{λ} associated with λ .

As a result of the previous proposition, a connected multigraph G has at least ${\sf diam}(G)+1$ distinct eigenvalues.

Let **J** be a square matrix where all entries are equal to one, i.e. $\mathbf{J} = \mathbf{e} \, \mathbf{e}^T$.

THEOREM 8.35 (Hoffman).— A multigraph with no loop G is connected and regular if and only if J belongs to the algebra A_G .

For further information, see the original paper [HOF 63] where more is proved.

PROOF.— Assume that $J \in A_G$. Thus, J is a polynomial in A(G) and we deduce that J.A(G) = A(G).J. Because of remark 8.11, for all u, v, we have

$$\deg(v) = [\mathbf{J}.\mathbf{A}(G)]_{u,v} = [\mathbf{A}(G).\mathbf{J}]_{u,v} = \deg(u).$$

Note that this cannot hold for graphs with loops because loops have a double contribution to the degree (or, to keep loops, we would have to tweak the definition of the adjacency matrix by doubling the values on the diagonal). Thus, G is regular: all vertices have the same degree. Proceed by contradiction and assume that G is not connected. There exist two vertices u, v such that $[\mathbf{A}(G)^n]_{u,v} = 0$ for all $n \geq 0$. Thus, for any matrix in \mathcal{A}_G

being a linear combination of powers of A(G), the same relation holds and J cannot belong to that algebra.

Now assume that G is connected and k-regular for some k. It is easy to see that k is an eigenvalue of $\mathbf{A}(G)$. Indeed, the vector \mathbf{e} from remark 8.11 is an eigenvector:

$$\mathbf{A}(G) \mathbf{e} = (\deg(v_1) \cdots \deg(v_n))^T = k \mathbf{e}.$$

We will revisit this with more details in proposition 9.8. From fact 8.8, $\mathbf{A}(G)$ is diagonalizable. Thus, using fact 8.34, the roots of the minimal polynomial of the adjacency matrix are simple. In particular, it holds for the root k and this polynomial is of the form

$$m_{\mathbf{A}}(z) = (z - k) q(z)$$

where q is a polynomial such that $q(k) \neq 0$. Evaluating the above relation in $\mathbf{A} = \mathbf{A}(G)$ yields

$$\mathbf{A}.q(\mathbf{A}) = k \, q(\mathbf{A}).$$

Said otherwise, every column of the matrix $q(\mathbf{A})$ is an eigenvector of \mathbf{A} with eigenvalue k. Note that $q(\mathbf{A}) \neq \mathbf{0}$ because $\deg q < \deg m_{\mathbf{A}}$.

To conclude with the proof, we need a bit more insight about k. The fact that G is connected implies that k is a simple eigenvalue. (Let us assume this result granted; for a proof, see again proposition 9.8 but we postpone the proof because it makes use of the theorem of Perron–Frobenius.) Thus, every column of $q(\mathbf{A})$ is a multiple of the vector \mathbf{e} . Since \mathbf{A} is symmetric, this also holds for $q(\mathbf{A})$. Consequently, every column of $q(\mathbf{A})$ must be equal to the same (non-zero) multiple of \mathbf{e} and $q(\mathbf{A}) = \alpha \mathbf{J}$, whence $\mathbf{J} \in \mathcal{A}_G$.

We can pursue the above reasoning a bit further. If the distinct eigenvalues of ${\bf A}$ are k and $\lambda_1,\ldots,\lambda_s$, using fact 8.34, they are all simple roots of $m_{\bf A}$ and $q(z)=\prod_{j=1}^s(z-\lambda_j).$ Since $m_{\bf A}$ is a monic polynomial, q(z) is also a monic polynomial. The eigenvalues of $q({\bf A})$ are q(k) and $q(\lambda_j)=0$ for all j. Since $\alpha {\bf J}=q({\bf A})$, the only non-zero eigenvalue of $\alpha {\bf J}$ is q(k). On the other hand, if G has n vertices, i.e. if ${\bf A}$ is a $n\times n$ matrix, then αn is an eigenvalue of $\alpha {\bf J}$ (with the eigenvector ${\bf e}$). Hence, $q(k)=\alpha n$ and we derive the following expression for ${\bf J}$

$$\mathbf{J} = \frac{n}{q(k)} \, q(\mathbf{A}).$$

8.6. Counting directed spanning trees

In section 5.4, we were counting the number $\tau(G)$ of spanning trees of a connected multigraph but the contraction/deletion formula was quite unsatisfactory from a practical point of view. In this section, we boldly move to the oriented case (and get as a special bonus a result in the unoriented case). Let G be a directed multigraph with no loops. Our aim is to count the number of arborescences in G as they were introduced in section 1.7. This is again a nice pretext to introduce another matrix related to G. But also recall that the number of arborescences is useful for determining the number of Eulerian circuits in an Eulerian digraph. Let us recall the definition.

DEFINITION 8.36.— An arborescence rooted at w in a directed multigraph G is a digraph where, for all vertices $v \in V(G)$, there is exactly one path from w to v.

A first example of arborescences was seen in Figure 1.26. Here, we consider a running example for this section.

EXAMPLE 8.37.— Consider the digraph depicted in Figure 8.4. In Figure 8.5, we have represented three arborescences (there is no restriction on the root). Others can be found. You can simply note that already two choices can be considered for the edge from 1 to 2.

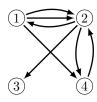


Figure 8.4. How many arborescences in this digraph?

DEFINITION 8.38.— We let $\mathbf{D}(G)$ denote the indegree matrix associated with the directed multigraph G = (V, E) and defined as follows, for all $u, v \in V$,

$$[\mathbf{D}(G)]_{v,v} = \mathsf{deg}^-(v)$$

and, if $u \neq v$,

$$[\mathbf{D}(G)]_{u,v} = -(\#(\omega^+(u) \cap \omega^-(v))) = -[\mathbf{A}(G)]_{u,v}.$$

Otherwise stated, $[\mathbf{D}(G)]_{u,v}$ is the opposite of the number of edges joining u to v. Note that each column of $\mathbf{D}(G)$ sums to 0.

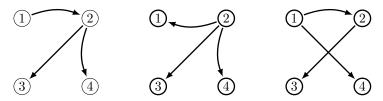


Figure 8.5. Some arborescences (two rooted at 1 and one rooted at 2)

If G has no loops and if we let $\mathbf{D}^-(G)$ denote the diagonal matrix whose entries are the indegrees of the vertices, then a simple formulation of the indegree matrix is given by

$$\mathbf{D}(G) = \mathbf{D}^{-}(G) - \mathbf{A}(G).$$

REMARK 8.39.— For other applications, we can similarly introduce the outdegree matrix. For simple graphs and digraphs, this matrix is usually referred to as the Laplacian matrix⁸.

With the digraph depicted in Figure 8.4, we have

$$\mathbf{D}(G) = \begin{pmatrix} 1 & -2 & 0 & -1 \\ -1 & 3 & -1 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 2 \end{pmatrix}.$$

REMARK 8.40.— Here is a trivial necessary condition for having an arborescence. Except for the column associated with the root (which is zero), every column of the indegree matrix associated with an arborescence has exactly 1 in diagonal position and another coefficient -1.

⁸ The name comes from the discrete Laplacian operator that is a classical differential operator.

With the first digraph depicted in Figure 8.5, we have

$$\mathbf{D} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We can find several terminologies. We have mentioned in remark 8.39 that we can also speak of the Laplacian matrix and what we call the Bott–Mayberry theorem, which has several other names: Kirchhoff's theorem, Matrix-Tree theorem (for instance, see [CHA 78]).

THEOREM 8.41 (Bott and Mayberry).— Let G be a directed multigraph with no loops. The number $t_v(G)$ of arborescences rooted at v is equal to the (v,v)-minor of $\mathbf{D}(G)$: the determinant of the indegree matrix associated with G where we remove the row and column corresponding to v.

This result will easily follow from the next statement [BOT 54].

THEOREM 8.42.— Let G be a digraph with no loops such that the indegree of each vertex is at most 1. The (v,v)-minor of the indegree matrix $\mathbf{D}(G)$ is equal to 1 (respectively, 0) if G is an arborescence rooted at v (respectively, otherwise).

To apply this result, we first select a potential root v. Then, we make a selection each time a vertex has several ingoing edges. We let $G^{(v)}$ denote the multigraph induced by $E \setminus \omega^-(v)$, i.e. we suppress all edges entering v. Now that the potential root v is selected the idea is that we will check whether or not there is an arborescence for each choice of edges. For all $u \neq v$, if $[\mathbf{D}(G^{(v)})]_{u,u} = r_u \geq 2$, i.e. u has r_u ingoing edges, then the column corresponding to u can be uniquely written as a sum of column vectors

$$C_{u,1},\ldots,C_{u,r_n}$$

where, for all $j \in \{1, \dots, r_u\}$, the component $[C_{u,j}]_u$ is equal to 1 and exactly one other component is equal to -1. Replacing the column corresponding to u with one of the $C_{u,j}$'s means that we select a single edge entering u. For each such choice, we have one candidate matrix/digraph to which we apply theorem 8.42 to sort out which ones are arborescences. The total number of choices is

$$n_v = \prod_{u \neq v} [\mathbf{D}(G^{(v)})]_{u,u}.$$

For instance, on the example, we have the decomposition of the second column as

$$\begin{pmatrix} -2\\3\\0\\-1 \end{pmatrix} = \underbrace{\begin{pmatrix} -1\\1\\0\\0 \end{pmatrix}}_{\mathbf{X}} + \underbrace{\begin{pmatrix} -1\\1\\0\\0 \end{pmatrix}}_{\mathbf{Y}} + \underbrace{\begin{pmatrix} 0\\1\\0\\-1 \end{pmatrix}}_{\mathbf{Z}}$$

which means that we have three choices for an edge entering the vertex 2: two possible edges from 1 to 2 and one from 4 to 2.

Let us consider $G^{(3)}$. Since $r_1=1$, $r_2=3$ and $r_4=2$, there are $n_3=6$ candidates for arborescences corresponding to six matrices. For the first (respectively, last) three, we have chosen the edge from 1 (respectively, 2) to 4. For the third and sixth one, we have chosen the edge from 4 to 2. In the other four matrices, we have chosen one of the two edges from 1 to 2.

$$\begin{pmatrix} 1 & -1 & 0 & -1 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \underbrace{0}_{\mathbf{x}} & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & -1 & 0 & -1 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \underbrace{0}_{\mathbf{y}} & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & -1 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \underbrace{-1}_{\mathbf{z}} & 0 & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & \underbrace{0}_{\mathbf{x}} & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & \underbrace{0}_{\mathbf{y}} & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & \underbrace{-1}_{\mathbf{z}} & 0 & 1 \end{pmatrix}.$$

The six (3,3)-minors all being equal to zero, if theorem 8.42 holds, then there is no arborescence rooted at 3.

We let $\mathbf{D}_1,\ldots,\mathbf{D}_{n_v}$ denote the matrices resulting from the above construction (i.e. choosing v as root and each matrix corresponds to one choice of ingoing edges). From the properties of the determinant (multilinear function of the columns), it is obvious that the (v,v)-minor of $\mathbf{D}(G)$ is the sum of the (v,v)-minors of the matrices $\mathbf{D}_1,\ldots,\mathbf{D}_{n_v}$. Thus, theorem 8.41 is an immediate corollary of theorem 8.42.

For arborescences rooted at 2, you can check that the following two (2,2)-minors are equal to 1

$$\begin{pmatrix} 1 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 0 & -1 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

PROOF OF THEOREM 8.42.— Assume first that G contains an arborescence A rooted at v. Thus, G=A or G has an extra edge e ingoing to v as depicted in Figure 8.6 because by assumption the indegree of v could be equal to 1. If we enumerate the vertices of G by breadth-first traversal, starting with the root v, then every edge (except e if it exists) is of the form (x,y) where x is enumerated before y. The resulting matrix $\mathbf{D}(G)$ is upper triangular, up to a coefficient -1 appearing in the first column (corresponding to the edge e). Hence, the (v,v)-minor is equal to 1 (we compute the determinant of $\mathbf{D}(G)$ without its first row and column, so it is not a problem if a -1 occurs in the first column).

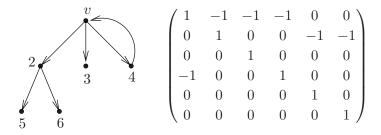


Figure 8.6. An arborescence with an extra edge ingoing to the root

Now assume that G has no arborescence rooted at v. If there exists $u \neq v$ such that $\deg^-(u) = 0$, then the corresponding column in $\mathbf{D}(G)$ is zero and the (v,v)-minor vanishes. We can thus assume that, for all $u \neq v$, $\deg^-(u) = 1$. Hence starting from every vertex, we can follow the ingoing edges backwards. If for all u, we can backtrack to v, then G has an arborescence rooted at v. So there exists at least one vertex that cannot be reached from v. Since every vertex has indegree one, we conclude that there must exist a cycle not containing v. In the indegree matrix $\mathbf{D}(G)$, the sum of the columns corresponding to the vertices in this cycle is zero and thus the (v,v)-minor is zero.

REMARK 8.43.— Theorem 8.41 shows that $t_v(G)$ can be computed in polynomial time (because the determinant⁹ is). In the exercises section, we will consider a generalization of this result that permits us to enumerate all rooted arborescences by attaching variables to the edges.

COROLLARY 8.44.— Let G be an undirected multigraph with no loops. If we consider the directed version G' where every edge $\{u,v\}$ of G is replaced with two edges (u,v) and (v,u) in G', then each (w,w)-minor of the corresponding indegree matrix $\mathbf{D}(G')$ is equal to the number $\tau(G)$ of trees spanning G.

With the graph depicted in Figure 5.10, the indegree matrix where edges are seen as going in both ways is given by

$$\begin{pmatrix}
3 & -1 & -1 & -1 \\
-1 & 2 & 0 & -1 \\
-1 & 0 & 2 & -1 \\
-1 & -1 & -1 & 3
\end{pmatrix}$$

and we can check that each minor corresponding to a diagonal element is equal to $\tau(G)=8$. This is somehow quite remarkable that all these minors are equal.

PROOF.— Let v be a vertex. With every tree T spanning G, we associate a unique arborescence in G' rooted at v and using edges in T. The choice of v induces an orientation of the edges of T. Conversely, every arborescence in G' rooted at v corresponds to a spanning tree of G. Said otherwise, $\tau(G) = t_v(G')$ for all vertices v.

8.7. Comments

There are several good sources for further study of the many relationships existing between linear algebra and graph theory. I particularly enjoy the short book [BRU 11] by R. A. Brualdi, which could be a nice way to study the subject deeper (and it provides many pointers to the bibliography). The book [BAP 14] also covers classical material and includes extra topics not covered here (e.g. Laplacian matrix). We will also mention the classical books [BIG 93, CVE 95]. Finally, [GOD 01] is also of interest as well as the survey paper [GOD 95] that shows how linear algebra can be applied in combinatorics.

⁹ The LUP decomposition of a $n \times n$ matrix can be obtained in $\mathcal{O}(n^3)$ operations. In this decomposition, we obtain a lower and a upper triangular matrices whose determinant are easily obtained.

As an example, the following interlacing results are presented in [BRU 11, Chapter 1]. For two sequences of real numbers $\lambda_1 \geq \cdots \geq \lambda_n$ and $\mu_1 \geq \cdots \geq \mu_m$ with m < n, the second sequence is said to *interlace* the first one if $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i=1,\ldots,m$. Another reference is in [HAE 95].

THEOREM 8.45.— Let \mathbf{A} be a real symmetric $n \times n$ matrix with $\lambda_1 \ge \cdots \ge \lambda_n$ as eigenvalues (repeated with their multiplicities). Let \mathbf{A}' be a principal $m \times m$ submatrix of \mathbf{A} , i.e. obtained by removing certain rows and columns such that the sets of row indices and column indices that have been removed are the same. Let $\mu_1 \ge \cdots \ge \mu_m$ be the eigenvalues of \mathbf{A}' (repeated with their multiplicities). Then

$$\lambda_i \ge \mu_i \ge \lambda_{n-m+i}$$
 for all $i \in \{1, \dots, m\}$.

COROLLARY 8.46.— Let G be a multigraph with n vertices and u be a vertex of G. Let $\lambda_1 \geq \cdots \geq \lambda_n$ be its eigenvalues (repeated with their multiplicities). Let $\mu_1 \geq \cdots \geq \mu_{n-1}$ be the eigenvalues of G-u. Then, we have

$$\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n$$
.

8.8. Exercises

- 1) This exercise follows the same lines as the proof of lemma 8.9. Let $\mathbf{M} \in \mathbb{R}^{n \times n}$ be a symmetric matrix and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be its eigenvalues repeated with their multiplicities. Let $\mathbf{v_1} \in \mathbb{R}^n \setminus \{0\}$ be an eigenvector associated with λ_1 . Prove the following:
 - a) We have

$$\lambda_2 = \sup_{\substack{\mathbf{x} \in \mathbb{R}^n \\ ||\mathbf{x}|| = 1, \mathbf{x} \perp \mathbf{v}_1}} \mathbf{x}^T \mathbf{M} \mathbf{x}.$$

The supremum is achieved precisely for the eigenvectors corresponding to λ_2 . If $\lambda_1 = \lambda_2$, the supremum is achieved precisely for the eigenvectors corresponding to λ_1 and orthogonal to \mathbf{v}_1 .

b) We have

$$\lambda_n = \inf_{\substack{\mathbf{x} \in \mathbb{R}^n \\ ||\mathbf{x}|| = 1}} \mathbf{x}^T \mathbf{M} \mathbf{x}.$$

The infimum is achieved precisely for the eigenvectors corresponding to λ_n .

- 2) Prove that the eigenvalues of the complete bipartite graph $K_{m,n}$ are $\pm \sqrt{mn}$ and 0.
 - 3) Count the number of closed walks of length ℓ in the complete graph K_n .
- 4) Count the number of closed walks of length ℓ in the complete tripartite graph $K_{2,2,2}$.
 - 5) Let C_n be a cycle of length n. What is the spectrum of C_n ?
- 6) Let $a,b \geq 1$ be integers. Consider the complete bipartite graph $K_{a,b}$. Count the number of automorphisms of $K_{a,b}$. If $\lambda_1,\ldots,\lambda_{a+b}$ are the eigenvalues of the graph (repeated with their multiplicity), prove that there are exactly $\lambda_1^n+\cdots+\lambda_{a+b}^n$ closed walks of length n. Prove that 0 is an eigenvalue of $K_{a,b}$ if a+b>2. What is its algebraic multiplicity?
- 7) Let n > 0. Consider the complete tripartite graph $K_{n,n,n}$. What is the algebraic multiplicity of the eigenvalue 0. If $\lambda_1, \ldots, \lambda_{3n}$ are the eigenvalues of $K_{n,n,n}$ (repeated with their multiplicity), compute for $j = 1, 2, 3, \sum_{i=1}^{3n} \lambda_i^j$.
- 8) Let $\bf A$ be the adjacency matrix of the Petersen graph (Figure 1.8). Prove that $\bf M = A^2 + A 2I$ has all its entries equal to 1. Diagonalize $\bf M$ and deduce that the eigenvalues of the Petersen graph belong to $\{-2,1,3\}$. Determine the algebraic multiplicities of the eigenvalues of $\bf A$. Count the number of closed walks of length 100 in the Petersen graph.
- 9) Let G be a graph with $\{1,\ldots,n\}$ as set of vertices and let σ be a permutation belonging to the symmetric group S_n . Prove that σ is an automorphism of G if and only if every eigenspace of the adjacency matrix $\mathbf{A}(G)$ is invariant under the matrix \mathbf{P}_{σ} associated with σ .
- 10) If G is a simple graph with adjacency matrix \mathbf{A} , show that $tr(\mathbf{A}^2)$ equals twice the number of edges and $tr(\mathbf{A}^3)$ is equal to six times the number of triangles. Explain why the latter observation leads to an efficient algorithm for detecting a triangle.
- 11) What can be said, as in proposition 8.30 about c_2 or c_3 if G is a non-simple graph, i.e. loops are allowed? When G is simple, give a combinatorial interpretation of c_4 .
- 12) With a digraph where the edges have k different labels (or colors), we may associate k adjacency matrices (one for each label). For instance, with the graph depicted in Figure 1.15, we have two such matrices M_B and M_R for

blue and red edges, respectively:

$$M_B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad M_R = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

We will assume that each row of these matrices contains exactly one entry equal to 1, the other entries are 0. A labeled digraph is *synchronizing*, i.e. there exist a vertex p and a finite sequence of colors s such that starting from any vertex and following the sequence s leads to p. Prove that this property is equivalent to the fact that there exists a product of matrices in $\{M_B, M_R\}^*$ where one column corresponding to p is the vector e made of 1 and all other columns are zero. Have a look at the *triple rendezvous problem* where one looks for the shortest sequence s such that there exist three vertices that, when following the sequence s from these three vertices leads to a common vertex [GON 16].

- 13) Study the spectrum, and in particular the largest eigenvalue, of trees [LOV 73].
- 14) Study the spectrum of the Cartesian product of a directed acyclic graph with a directed multigraph G.
- 15) The Laplacian matrix is quite similar to the indegree matrix (see remark 8.39). It is defined as follows. Let G be a simple graph, $[\mathbf{L}(G)]_{v,v} = \deg(v)$ and for $u \neq v$, $[\mathbf{L}(G)]_{u,v} = -[\mathbf{A}(G)]_{u,v}$. Study the first properties of this matrix: all eigenvalues of $\mathbf{L}(G)$ are non-negative, zero is an eigenvalue and its multiplicity is the number of connected components. See the survey [MER 94]. Variants exist for directed multigraphs.
- 16) Prove the following extended Bott–Mayberry theorem (theorem 8.41). Let us define a generalized indegree matrix. Let G be a directed multigraph with no loops. With each edge (u,v) is associated a variable $x_{(u,v)}$. If we have multiple edges, we consider several different variables $x_{(u,v),1},\ldots,x_{(u,v),n}$. Define the matrix $\mathbf{D}'(G)$ as follows. If $u\neq v$, $[\mathbf{D}'(G)]_{u,v}$ is the opposite of the sum of all the variables $x_{(u,v),i}$ corresponding to edges from u to v and $[\mathbf{D}'(G)]_{u,u}$ is the sum of the variable $x_{(v,u),i}$ for all $v\neq u$ corresponding to the edges entering v. With the graph depicted in Figure 8.4, the matrix $\mathbf{D}'(G)$

is given by

$$\begin{pmatrix} x_{(2,1)} & -x_{(1,2),1} - x_{(1,2),2} & 0 & -x_{(1,4)} \\ -x_{(2,1)} & x_{(1,2),1} + x_{(1,2),2} + x_{(4,2)} & -x_{(2,3)} & -x_{(2,4)} \\ 0 & 0 & x_{(2,3)} & 0 \\ 0 & -x_{(4,2)} & 0 & x_{(1,4)} + x_{(2,4)} \end{pmatrix}.$$

Now, prove that the (v,v)-minor of the matrix $\mathbf{D}'(G)$ is a homogeneous polynomial (sometimes referred to as Kirchoff polynomial) where each term corresponds to an arborescence rooted at v. For example, with v=1, we obtain

$$\begin{split} x_{(1,2),1}x_{(1,4)}x_{(2,3)} + x_{(1,2),1}x_{(2,3)}x_{(2,4)} + x_{(1,4)}x_{(2,3)}x_{(4,2)} \\ + x_{(1,4)}x_{(2,3)}x_{(1,2),2} + x_{(2,3)}x_{(2,4)}x_{(1,2),2}. \end{split}$$

Finally, note that setting all the variables to 1 returns the original result of Bott and Mayberry.

Perron-Frobenius Theory

Let $\bf A$ and $\bf B$ be two matrices with the same dimensions. Notation such as $\bf A \geq 0$, $\bf A > 0$ or $\bf A \leq \bf B$ has to be understood component-wise. In this chapter, we are dealing with square matrices $\bf A \geq 0$, i.e. with non-negative entries. There is a rich theory about their spectra, eigenspaces and powers that turns out to be of particular interest when considering adjacency matrices of graphs. This theory also has many applications ranging from probability theory and Markov chains to dynamical systems (see, for instance, [BRI 02]). Perron's theorem is at the core of Google's PageRank algorithm discussed in the following chapter. For standard textbooks on matrix theory including discussions about Perron–Frobenius theory see, for instance, [HOR 13] or [SEN 06, GAN 59]. The reader will not find a proof of Perron's theorem in this book.

9.1. Primitive graphs and Perron's theorem

We will start with a quite specific property (more restrictive than strong connectedness) that has an important asymptotic consequence expressed by relation [9.3].

Let $t \geq 1$ be an integer. A matrix $\mathbf{A} \in \mathbb{R}^{t \times t}$ with non-negative entries is *primitive* if there exists an integer N such that \mathbf{A}^N is positive, i.e. all the

¹ See Chapter 10.

entries in ${\bf A}^N$ are positive. Primitive matrices have strong properties known as Perron–Frobenius² theory.

DEFINITION 9.1.— A directed multigraph is **primitive** if its adjacency matrix is primitive. This means that G is not only strongly connected but there exists a length N such that between any two vertices (respectively, for any vertex), there exists a walk (respectively, a closed walk) of length N connecting them. The definition also applies to the undirected case.

Having in mind the forthcoming relation [9.3], note that in the following statement we normalize eigenvectors in a specific way.

THEOREM 9.2 (Perron's theorem).— Let $\mathbf{A} \in \mathbb{R}_{\geq 0}^{t \times t}$ be a primitive matrix. The following properties hold:

- 1) There exists a unique real number $\lambda > 0$ such that λ is an eigenvalue of \mathbf{A} and all the other (possibly complex) eigenvalues of \mathbf{A} have modulus less than λ . We say that λ is the **Perron eigenvalue** of \mathbf{A} .
- 2) The Perron eigenvalue λ is simple: it is a simple root of the characteristic polynomial of **A**. Thus, the dimension of the corresponding eigenspace E_{λ} is also one.
- 3) There exists an eigenvector $\mathbf{v}_{\lambda} \in \mathbb{R}^{t \times 1}$ with eigenvalue λ whose components are all positive. We normalize this vector so that the sum of its components is one.
- 4) Similarly, there exists a left eigenvector $\mathbf{w}_{\lambda} \in \mathbb{R}^{t \times 1}$ such that $\mathbf{w}_{\lambda}^{T} \mathbf{A} = \lambda \mathbf{w}_{\lambda}^{T}$ and whose components are all positive. We normalize this vector so that $\langle \mathbf{v}_{\lambda}, \mathbf{w}_{\lambda} \rangle = \mathbf{w}_{\lambda}^{T} \mathbf{v}_{\lambda} = 1$.
- 5) Any (right) eigenvector of **A** whose components are all positive real numbers is a multiple of \mathbf{v}_{λ} . Similarly, the same holds for left eigenvectors.

In particular, the spectral radius of a primitive matrix is one of its eigenvalues (see remark 8.2).

Recall definition 8.18. We let $\mathsf{nW}_{u \to v} : \mathbb{N} \to \mathbb{N}$ denote the function that maps $n \geq 0$ to the number of walks of length n from u to v. Motivated by theorem 8.17 and looking for estimates about the asymptotic behavior of

² Oskar Perron (1880–1975) is a well-known German mathematician. He worked on differential equations and continued fractions. The present result was given in [PER 07].

 $\mathsf{nW}_{u \to v}(n)$ in a primitive digraph, let us proceed with some linear algebra. Let **A** be a primitive matrix with $\lambda > 0$ as the Perron eigenvalue. The matrix

$$\mathbf{P} = \mathbf{v}_{\lambda} \mathbf{w}_{\lambda}^{T}$$

is a projection onto the eigenspace E_{λ} . Indeed, from the choice of the normalized right and left eigenvectors \mathbf{v}_{λ} and \mathbf{w}_{λ} (see theorem 9.2 parts (3) and (4) for the normalization conditions), we derive immediately that $\mathbf{P}^2 = \mathbf{P}$. Next, for any vector $\mathbf{x} \in \mathbb{C}^{t \times 1}$, the vector $\mathbf{P}\mathbf{x}$ belongs to the eigenspace E_{λ} . In particular, $\mathbf{P}\mathbf{v}_{\lambda} = \mathbf{v}_{\lambda}$ and the range of \mathbf{P} is E_{λ} . Otherwise stated, \mathbf{P} is the (spectral) projector on $E_{\lambda} = \ker(\mathbf{A} - \lambda \mathbf{I})$ along the range of $\mathbf{A} - \lambda \mathbf{I}$ denoted by $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$. Indeed, for every vector $\mathbf{x} \in \mathbb{C}^{t \times 1}$, $\mathbf{A}\mathbf{x} - \lambda \mathbf{x}$ belongs to $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$ and $\mathbf{P}(\mathbf{A}\mathbf{x} - \lambda \mathbf{x}) = 0$. Set $\mathbf{Q} := \mathbf{I} - \mathbf{P}$. In fact, \mathbf{Q} is the projector on $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$ along $\ker(\mathbf{A} - \lambda \mathbf{I})$.

We have

$$\mathbb{C}^{t \times 1} = E_{\lambda} \oplus \operatorname{rg}(\mathbf{A} - \lambda \mathbf{I}). \tag{9.1}$$

We can therefore construct a basis of $\mathbb{C}^{t \times 1}$ from the single vector \mathbf{v}_{λ} , which is a basis of E_{λ} and a basis of $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$ made up of t-1 elements $\mathbf{z}_2, \ldots, \mathbf{z}_t$. Let \mathbf{S} be the matrix whose columns are $\mathbf{v}_{\lambda}, \mathbf{z}_2, \ldots, \mathbf{z}_t$. Since the two subspaces E_{λ} and $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$ are obviously closed under \mathbf{A} , because \mathbf{A} and $\mathbf{A} - \lambda \mathbf{I}$ commute³, using [9.1], we get

$$\mathbf{S}^{-1}\mathbf{A}\mathbf{S} = \begin{pmatrix} \lambda & 0 \\ 0 & \mathbf{B} \end{pmatrix}$$

for some ${\bf B}$ in $\mathbb{C}^{(t-1)\times(t-1)}$. Since ${\bf A}$ and ${\bf S}^{-1}{\bf A}{\bf S}$ have the same characteristic polynomial, we deduce that the characteristic polynomial of ${\bf A}$ is $(z-\lambda)$ times the characteristic polynomial of ${\bf B}$. Hence, the eigenvalues of ${\bf B}$ are those of ${\bf A}$ except for λ . From the primitivity of ${\bf A}$, this means that the modulus of any eigenvalue of ${\bf B}$ is less than λ . Since ${\bf I}={\bf P}+{\bf Q}$, we have ${\bf A}={\bf A}{\bf P}+{\bf A}{\bf Q}$. By the choice of ${\bf S}$ and since ${\bf P}$, ${\bf Q}$ are projectors, we get

$$\mathbf{S}^{-1}\mathbf{APS} = \begin{pmatrix} \lambda & 0 \\ 0 & 0 \end{pmatrix}, \ \mathbf{S}^{-1}\mathbf{AQS} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{B} \end{pmatrix}.$$

³ If \mathbf{x} belongs to $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$, then there exists \mathbf{y} such that $\mathbf{x} = (\mathbf{A} - \lambda \mathbf{I})\mathbf{y}$. Thus, $\mathbf{A}\mathbf{x} = \mathbf{A}(\mathbf{A} - \lambda \mathbf{I})\mathbf{y} = (\mathbf{A} - \lambda \mathbf{I})\mathbf{A}\mathbf{y}$ belongs to $\operatorname{rg}(\mathbf{A} - \lambda \mathbf{I})$.

So APAQ = 0 = AQAP, and thus

$$\mathbf{A}^{n} = (\mathbf{A}\mathbf{P})^{n} + (\mathbf{A}\mathbf{Q})^{n} = \mathbf{S} \begin{pmatrix} \lambda^{n} & 0 \\ 0 & 0 \end{pmatrix} \mathbf{S}^{-1} + \mathbf{S} \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{B}^{n} \end{pmatrix} \mathbf{S}^{-1}.$$
 [9.2]

It is well known (see remark 8.23) that every entry of \mathbf{B}^n is expressed as a linear combination of polynomials⁴ times eigenvalues of \mathbf{B} to the power n, i.e. each entry is of the form $\sum_{i=1}^{t-1} P_i(n)\alpha_i^n$ with $|\alpha_i| < \lambda$ for all i. Hence, \mathbf{B}^n/λ^n tends to 0 as n tends to infinity.

Note that the first term of the sum on the right-hand side in [9.2] is the product of λ^n by the first column of **S** (which is equal to \mathbf{v}_{λ}) times the first row of \mathbf{S}^{-1} . This row is equal to \mathbf{w}_{λ}^T because, from

$$\mathbf{S}^{-1}\mathbf{A} = \begin{pmatrix} \lambda & 0 \\ 0 & 0 \end{pmatrix} \mathbf{S}^{-1},$$

we deduce that the first row of \mathbf{S}^{-1} is a left eigenvector of \mathbf{A} with eigenvalue λ . It is thus a multiple of \mathbf{w}_{λ}^{T} but since $\mathbf{S}^{-1}\mathbf{S} = \mathbf{I}$, it is exactly \mathbf{w}_{λ}^{T} . We have just shown that for a primitive matrix \mathbf{A} with Perron eigenvalue λ ,

$$\lim_{n \to +\infty} \frac{\mathbf{A}^n}{\lambda^n} = \mathbf{v}_{\lambda} \mathbf{w}_{\lambda}^T.$$
 [9.3]

Note that since \mathbf{v}_{λ} is a $t \times 1$ column vector and \mathbf{w}_{λ}^{T} is a $1 \times t$ row vector, both with positive entries only, then $\mathbf{v}_{\lambda}\mathbf{w}_{\lambda}^{T}$ is a $t \times t$ matrix whose entries are positive. An equivalent formulation of [9.3] is to write

$$\mathbf{A}^n = \lambda^n \, \mathbf{v}_{\lambda} \mathbf{w}_{\lambda}^T + o(\lambda^n).$$

A term r is in $o(\lambda^n)$ if r/λ^n tends to 0 when n tends to infinity. As a first application of this formula, we derive the asymptotic growth rate of the number of walks of length n in a primitive digraph when n tends to $+\infty$. Consider the digraph depicted in Figure 9.1. The adjacency matrix is given by \mathbf{A} and it is primitive as shown when computing its third power,

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{A}^3 = \begin{pmatrix} 4 & 2 & 3 \\ 1 & 1 & 1 \\ 2 & 1 & 2 \end{pmatrix}.$$

⁴ These polynomials have a degree related to the size of the blocks of the Jordan decomposition of **B**. If **B** is diagonalizable, then the polynomials are reduced to constants.

We find the characteristic polynomial

$$p_{\mathbf{A}}(z) = -z^3 + z^2 + z + 1.$$

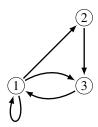


Figure 9.1. A primitive digraph

From this we compute left and right eigenvectors (here numerically approximated) associated with the Perron eigenvalue λ

$$\mathbf{v}_{\lambda} = \begin{pmatrix} 0.543689 \\ 0.160713 \\ 0.295598 \end{pmatrix}, \quad \mathbf{w}_{\lambda}^{T} = \begin{pmatrix} 0.419643 \ 0.228155 \ 0.352201 \end{pmatrix}.$$

The left eigenvector is normalized so that the sum of its entries sum up to one. We are thus fine with theorem 9.2 (part 3). The real λ is approximately 1.839286. The other two eigenvalues are $-0.419643 \pm 0.606291i$ whose modulus is close to 0.737. Since $\mathbf{w}_{\lambda}^T \mathbf{v}_{\lambda} = 0.368933$, in view of theorem 9.2 (part 4), we replace \mathbf{w}_{λ} with $\mathbf{w}_{\lambda}/(\mathbf{w}_{\lambda}^T \mathbf{v}_{\lambda})$ before computing the matrix

$$\mathbf{v}_{\lambda}\mathbf{w}_{\lambda}^{T} = \begin{pmatrix} 0.61842 & 0.336228 & 0.519032 \\ 0.182804 & 0.0993883 & 0.153425 \\ 0.336228 & 0.182804 & 0.282192 \end{pmatrix}.$$

As an application, we have information about the asymptotic behavior (i.e. when n tends to infinity) of the number of walks of length n within the digraph. For instance, because of theorem 8.17 and [9.3], we deduce (up to the numerical approximations and truncations⁵) that

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{2 \to 2}(n)}{0.0994 \ 1.84^n} = 1.$$

⁵ You have to be careful with these approximations, the difference with the exact value may grow exponentially fast.

Again, this means that $nW_{2\rightarrow 2}(n)$ asymptotically behaves up to a multiplicative constant as λ^n . For all vertices u,v, we write

$$\mathsf{nW}_{u\to v}(n) \sim_C \lambda^n$$

meaning that

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{u \to v}(n)}{\lambda^n}$$

is a positive constant.

REMARK 9.3.— A matrix $\mathbf{A} \geq 0$ is primitive if and only if there exists N such that $\mathbf{A}^i > 0$ for all $i \geq N$.

PROOF.—If $\mathbf{A}^N>0$ for some N, then every column of \mathbf{A} is non-zero because \mathbf{A} only contains non-negative entries. Indeed, if the ith column of \mathbf{A} is zero, then so is the ith column of \mathbf{A}^n for all $n\geq 1$. Now, $\mathbf{A}^N.\mathbf{A}>0$ and we conclude with an induction argument.

9.2. Irreducible graphs

For a matrix with non-negative entries or, equivalently, for connected graphs (respectively, strongly connected digraphs), there is a weaker property than primitivity and the corresponding result is called the Perron–Frobenius⁶ theorem.

Recall that, in a digraph G = (V, E), a strongly connected component (see section 1.2.1) is a maximal subset $W \subseteq V$ such that, for all vertices $v, w \in W$, there exists a walk from v to w.

DEFINITION 9.4.— A matrix $\mathbf{A} \in \mathbb{R}^{t \times t}_{\geq 0}$ is irreducible if, for all indices $i, j \in \{1, \dots, t\}$, there exists an integer $N_{i,j}$ such that $[\mathbf{A}^{N_{i,j}}]_{i,j}$ is positive. We say that a directed multigraph is **irreducible** if its adjacency matrix is irreducible.

Note that a directed multigraph G is strongly connected if and only if $\mathbf{A}(G)$ is irreducible. The definition readily applies to the undirected connected multigraphs.

⁶ Ferdinand Georg Frobenius (1849–1917) is another famous German mathematician best known for his work in group theory or elliptic functions. His generalization of Perron's theorem first appeared in [FRO 12].

Contrarily to theorem 9.2, we may have several eigenvalues of maximal modulus.

THEOREM 9.5 (Perron–Frobenius theorem).— Let $\mathbf{A} \in \mathbb{R}^{t \times t}_{\geq 0}$ be an irreducible matrix. The following properties hold:

- 1) There exists a unique real number $\lambda > 0$ such that λ is an eigenvalue of **A** and all the other (possibly complex) eigenvalues of **A** have modulus less or equal to λ . We say that λ is the **Perron–Frobenius eigenvalue** of **A**.
 - 2) The Perron–Frobenius eigenvalue λ is simple.
- 3) There exists a (right) eigenvector with eigenvalue λ whose components are all positive.
- 4) Similarly, there exists a left eigenvector with eigenvalue λ whose components are all positive.
- 5) Any eigenvector of **A** whose components are all positive real numbers is associated with λ .
- 6) There exists a positive integer h, called the period⁷ of \mathbf{A} , such that \mathbf{A} has exactly h eigenvalues with modulus λ . These eigenvalues are simple roots of the characteristic polynomial of \mathbf{A} . They are exactly equal to $\lambda e^{2in\pi/h}$ for $n = 0, \ldots, h-1$.
 - 7) The Perron–Frobenius eigenvalue satisfies the following inequalities

$$\min_{i} \sum_{j=1}^{t} \mathbf{A}_{i,j} \leq \lambda \leq \max_{i} \sum_{j=1}^{t} \mathbf{A}_{i,j} \text{ and}$$

$$\min_{j} \sum_{i=1}^{t} \mathbf{A}_{i,j} \leq \lambda \leq \max_{j} \sum_{i=1}^{t} \mathbf{A}_{i,j}.$$
[9.4]

In particular, the spectral radius of an irreducible matrix is one of its eigenvalues. See remark 8.2.

Figure 9.2 shows the differences between the spectra of a primitive matrix on the left where all eigenvalues distinct from λ belong to the interior of the disk of radius λ and an irreducible matrix on the right where we have five

⁷ The term *period* will be made clear in section 9.4.4.

eigenvalues of modulus equal to λ distributed along the fifth roots of the unity. Recall that the characteristic polynomial p of the adjacency matrix has real coefficients, thus if it has a root x in $\mathbb{C} \setminus \mathbb{R}$, then its conjugate \overline{x} is also a root of p.

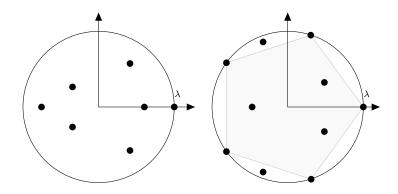


Figure 9.2. Typical spectra of primitive and irreducible matrices (h = 5)

REMARK 9.6.— Even though the Perron—Frobenius theorem is quite powerful, the existence of other eigenvalues of maximal modulus implies that a behavior such as in [9.3] does not hold. Simply consider a cycle of length 3 with **A** as adjacency matrix. We have

$$\mathbf{A}^{3n} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \mathbf{A}^{3n+1} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \ \mathbf{A}^{3n+2} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

For instance, the sequence $(nW_{1\rightarrow 2}(n))_{n\geq 0}$ is $0,1,0,0,1,0,\ldots$ We have three eigenvalues of modulus 1: $\lambda=1,\ e^{2i\pi/3},\ e^{4i\pi/3}$. Thus, because of this cyclic structure $\lim_{n\rightarrow +\infty} nW_{1\rightarrow 2}(n)/\lambda^n$ does not exist. From remark 8.23, powers of different eigenvalues with the same modulus may cancel each other.

9.3. Applications

In this short section, we give a few graph theoretic results where parts of the proof involve the use of the Perron–Frobenius theorem. To get a grasp about the meaning of the first result, recall that the spectral radius of a matrix is generally not an eigenvalue of the matrix (remark 8.2). The subtlety of this first result is that G is not necessarily connected and that the entries of the eigenvector are non-negative (versus positive).

THEOREM 9.7.— Let G be a directed multigraph. The spectral radius of G is an eigenvalue of G and it is associated with an eigenvector with non-negative entries.

PROOF.— If G is strongly connected, the result immediately follows from the Perron–Frobenius theorem. Otherwise, let G_1,\ldots,G_k be the strongly connected components of G with $\lambda_1,\ldots,\lambda_k$ the corresponding Perron–Frobenius eigenvalues. Let $\lambda=\max_i\lambda_i$. If j is such that $\lambda_j=\max_i\lambda_i$, then $\mathbf{A}(G_j)\mathbf{x}=\lambda_j\mathbf{x}$ for some positive \mathbf{x} . Completing, in a convenient way, \mathbf{x} with zeroes to get a column vector of size #V(G) gives an eigenvector of $\mathbf{A}(G)$ with eigenvalue λ because $\mathbf{A}(G)$ can be written as a block-diagonal matrix whose blocks are $\mathbf{A}(G_1),\ldots,\mathbf{A}(G_k)$.

Let $k \geq 1$ be an integer. Recall that a directed multigraph is k-regular if, for all vertices v, $\deg^+(v) = k$. In the undirected case, it is called k-regular if, for all vertices v, $\deg(v) = k$. In both cases, recalling remark 8.11, this means that each row of the adjacency matrix sums to k. Remember that we used this statement in the proof of Hoffman theorem.

PROPOSITION 9.8.— Let G be a k-regular directed multigraph. We have

- 1) k is an eigenvalue of G;
- 2) for each eigenvalue $\alpha \in \mathbb{C}$ of G, we have $|\alpha| < k$;
- 3) if G is strongly connected, then k is a simple eigenvalue.

PROOF.—The vector $(1 \cdots 1)^T$ is clearly an eigenvector of eigenvalue k. Let us prove the second point of the statement.

Let y be a non-zero eigenvector associated with an eigenvalue α of $\mathbf{A}(G)$. Let j be such that y_j is a component of maximal modulus. We have⁸

$$|\alpha| |y_j| = |[\mathbf{A}(G)y]_j| \le \sum_{i=1}^n [\mathbf{A}(G)]_{j,i} |y_i| \le |y_j| \sum_{i=1}^n [\mathbf{A}(G)]_{j,i} = k |y_j|$$
 [9.5]

thus $|\alpha| \leq k$.

⁸ We will also use the same argument in the proof of the next result.

The third point is a direct consequence of the Perron–Frobenius theorem. The matrix $\mathbf{A}(G)$ is irreducible and from the previous point, we know that k must be the Perron–Frobenius eigenvalue of $\mathbf{A}(G)$. Therefore, it is a simple eigenvalue.

EXERCISE 9.3.1.— Adapt the previous result to the undirected case.

If we remove at least one edge (and possibly some vertices), then we have some spectral information about the obtained graph.

PROPOSITION 9.9.— Let G be a connected multigraph and H be a proper subgraph of G. Then, the spectral radius of H, i.e. the maximal modulus among the eigenvalues of H, is less than the Perron–Frobenius eigenvalue of G.

PROOF.—We can assume that G and H have the same set of n vertices. Isolated vertices provide only zero eigenvalues. Only some edges (at least one) have been deleted from G. Thus, $\mathbf{A}(H) \leq \mathbf{A}(G)$. Let $\beta \in \mathbb{C}$ be an eigenvalue of H associated with a non-zero eigenvector $\mathbf{y} = (y_i)_{1 \leq i \leq n} \in \mathbb{C}^n$. We write \mathbf{y}_+ for the non-negative vector $(|y_i|)_{1 \leq i \leq n}$. For every component $i \in \{1, \ldots, n\}$, by taking moduli, we have a computation similar to [9.5]

$$|\beta| |y_i| = |[\mathbf{A}(H)\mathbf{y}]_i| = \left| \sum_{j=1}^n [\mathbf{A}(H)]_{i,j} y_j \right|$$

$$\leq \sum_{j=1}^n [\mathbf{A}(H)]_{i,j} |y_j| = [\mathbf{A}(H)\mathbf{y}_+]_i.$$

Since every component is non-negative and $A(H) \leq A(G)$,

$$|\beta| \mathbf{y}_{+} \le \mathbf{A}(H) \mathbf{y}_{+} \le \mathbf{A}(G) \mathbf{y}_{+}. \tag{9.6}$$

We now discuss two cases depending on the fact that \mathbf{y}_+ can have some zero components.

If all the components of \mathbf{y}_+ are positive, then the second inequality in [9.6] is strict. Let λ be the Perron–Frobenius eigenvalue of $\mathbf{A}(G)$ and \mathbf{w}_{λ}^T be a corresponding left eigenvector whose components are all positive. Thus, multiplying [9.6] by \mathbf{w}_{λ}^T yields

$$|\beta| \mathbf{w}_{\lambda}^T \mathbf{y}_+ < \mathbf{w}_{\lambda}^T \mathbf{A}(G) \mathbf{y}_+ = \lambda \mathbf{w}_{\lambda}^T \mathbf{y}_+ \text{ and } |\beta| < \lambda.$$

If one component of y_+ is zero, then multiplying [9.6] by y_+^T and dividing by $||y_+||^2$ yields

$$|\beta| \leq \frac{\mathbf{y}_+^T \mathbf{A}(G) \, \mathbf{y}_+}{||\mathbf{y}_+||^2} \leq \sup_{\mathbf{x} \in \mathbb{R}^n \backslash \{0\}} \frac{\mathbf{x}^T \mathbf{A}(G) \, \mathbf{x}}{||\mathbf{x}||^2} = \lambda.$$

The last equality comes from lemma 8.9. But the supremum is achieved only for the eigenvectors \mathbf{x} associated with λ . Since \mathbf{y}_+ has a zero component, from the Perron–Frobenius theorem, \mathbf{y}_+ is not an eigenvector associated with λ . This means that

$$\frac{\mathbf{y}_+^T\mathbf{A}(G)\,\mathbf{y}_+}{||\mathbf{y}_+||^2} < \sup_{\mathbf{x} \in \mathbb{R}^n \backslash \{0\}} \frac{\mathbf{x}^T\mathbf{A}(G)\,\mathbf{x}}{||\mathbf{x}||^2} \text{ and } |\beta| < \lambda.$$

COROLLARY 9.10.— Let G be a connected simple graph and $\Delta = \max_{v \in V(G)} \deg(v)$. The Perron–Frobenius eigenvalue λ of G satisfies

$$\sqrt{\Delta} \le \lambda \le \Delta$$
.

PROOF.—By definition of Δ , the complete bipartite graph $K_{1,\Delta}$ is a subgraph of G and G is a subgraph of the complete graph K_{Δ} . It is an exercise to prove that the Perron–Frobenius eigenvalue of $K_{1,\Delta}$ is $\sqrt{\Delta}$. Since K_{Δ} is Δ -regular, its Perron–Frobenius eigenvalue is Δ . We conclude using the previous proposition.

We can prove the converse (with the extra assumption of connectedness) of corollary 8.15 about bipartite graphs. The fact that the graph is connected allows us to use the Perron–Frobenius theorem. The proof of the following lemma is left as an exercise.

LEMMA 9.11.— A graph G=(V,E) is bipartite if and only if V can be partitioned into two subsets V_1 and V_2 such that

- 1) every walk between two vertices both belonging to V_1 has even length;
- 2) every walk between two vertices both belonging to V_2 has even length;
- 3) every walk between a vertex in V_1 and a vertex in V_2 has odd length.

⁹ We can show that the eigenvalues are $-\sqrt{\Delta} \le 0 \le \cdots \le 0 \le \sqrt{\Delta}$ (repeated with their multiplicities, i.e. 0 is repeated $\Delta-1$ times). See exercise in section 8.8.

EXERCISE 9.3.2.— Prove the previous lemma. Show that the third condition can be removed and the result remains valid.

THEOREM 9.12.— A simple connected graph G = (V, E) is bipartite if and only if the spectrum of G is symmetric with respect to 0.

We only have to prove that symmetry of the spectrum implies a bipartition. The other direction was given by corollary 8.15.

PROOF.— By assumption G is connected, so its adjacency matrix \mathbf{A} is irreducible. Let λ be its Perron–Frobenius eigenvalue and \mathbf{x} be an associated non-zero eigenvector. By assumption, $-\lambda$ is also an eigenvalue of \mathbf{A} . Let \mathbf{y} be an associated non-zero eigenvector. From linear algebra (fact 8.5), we know that non-zero eigenvectors associated with distinct eigenvalues are linearly independent.

Let G' be the multigraph having \mathbf{A}^2 as adjacency matrix 10 . Note that G and G' share the same set of vertices. By definition of G', there is an edge $\{u,v\}$ in G' if and only if there exists a walk of length 2 between u and v in G. Multiple edges correspond to distinct walks between u and v. In particular, two vertices are connected by a sequence of edges in G' if and only if there exists a walk of even length joining them in G.

The eigenvalues of G' are exactly the square of the eigenvalues of G (fact 8.4). Therefore, λ^2 is a real eigenvalue of G' of maximal modulus. Since $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ and $\mathbf{A}\mathbf{y} = -\lambda\mathbf{y}$, we conclude that \mathbf{x} and \mathbf{y} are eigenvectors of \mathbf{A}^2 for the eigenvalue λ^2 . Thus, the corresponding eigenspace has dimension at least 2. From the Perron–Frobenius theorem, we conclude that G' is not connected.

Pick a vertex u. We define two subsets V_1 and V_2 of V such that v belongs to V_1 (respectively, V_2) if and only if there exists a walk of odd (respectively, even) length between u and v in the original graph G. Since G is connected, every vertex in V belongs to at least one of these two subsets, i.e. $V = V_1 \cup V_2$.

We now show that all vertices in V_2 are connected in G'. Let v, w be two vertices in V_2 . By definition of this set, there exists a walk in G of even length \mathfrak{p} (respectively, \mathfrak{q}) between v and u (respectively, u and w). The union of these two walks has even length and join v and w in G. This means that v and w are connected in G'.

¹⁰ An illustration is given in Figure 9.3.

The argument is similar to show that all vertices in V_1 are connected within G'. Indeed, a walk obtained as the union of two walks of odd length is a walk of even length. Since G' is not connected, we must have $V_1 \cap V_2 = \emptyset$. We are almost done: we have a partition of V. We still have to prove that it is a convenient one.

We conclude using the previous lemma. Let us check the three conditions. Assume that there is a walk of odd length in G between two vertices v, w in V_1 . By definition of V_1 , there exists a walk of odd length between u and v in G. The union of these two walks has even length and connects u and w. We should conclude that w belongs to V_2 . This is a contradiction. The argument is similar for two vertices in V_2 . Finally, assume that there is a walk of even length in G between two vertices $v \in V_1$ and $v \in V_2$. By definition of v_2 , there exists a walk of even length between v and v. The union of these two walks has even length and connects between v and v. We should conclude that v belongs to v.

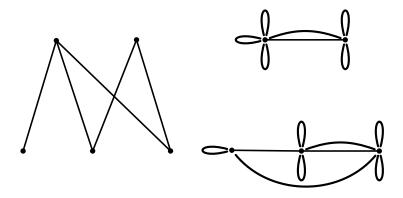


Figure 9.3. A graph G and the corresponding graph G' in the proof of theorem 9.12

9.4. Asymptotic properties

We have seen in section 9.1 of this chapter that the asymptotic behavior of A^n when $n \to +\infty$ is well explained by [9.3] whenever A is primitive. There is no need to try to solve linear recurrences. We have an exponential behavior

of $\mathsf{nW}_{u \to v}(n)$ for all u, v. In this section, we first study the asymptotic behavior of the sequence $\mathsf{nW}_{u \to v}(n)$ counting walks of length n for digraphs (or directed multigraphs) whose strongly connected components are all primitive. Then, we will study the sequence $\mathsf{nW}_{u \to v}(n)$ when the digraph is irreducible. We conclude this section with a final example mixing primitive and irreducible components.

9.4.1. Canonical form

Let G be a directed multigraph. First detect the strongly connected components C_1, \ldots, C_k of G (see section 1.2.1). Then, consider the directed acyclic graph \mathcal{A} (see end of Chapter 4) where the set of vertices is $\{C_1, \ldots, C_k\}$ and there is a unique edge from C_i to C_j if and only if there exists an edge in G from a vertex in C_i to a vertex in C_j . This graph can also be seen as the quotient of G (in section 5.3) by the relation \leftrightarrow from section 1.2.1. Now proceed to a topological sort of \mathcal{A} (again see Chapter 4) and get an ordering of the SCCs of G. Using this ordering, we can now order the vertices of G by first enumerating the vertices of the first SCC, then those of the second SCC and so on. This enumeration of the vertices leads to a special form for the adjacency matrix of G.

The matrix $\mathbf{A}(G)$ is a block triangular matrix whose diagonal blocks are square matrices of dimension equal to the size of the SCCs. Because of the topological sort of the SCCs, the elements below the block diagonal are zero. The elements above the block diagonal reflect the connections between the SCCs. We continue example 5.8.

EXAMPLE 9.13.— Consider the digraph depicted in Figure 1.13. It has four SCCs and the vertices have been ordered accordingly. The corresponding adjacency matrix is depicted below.

The SCC $\{5\}$ is trivial. From it, there are edges leading to the SCC $\{6,7\}$ and $\{8,9\}$. In the same way, the edges going out of the SCC $\{1,2,3,4\}$ enter only the SCC $\{5\}$.

REMARK 9.14.— The spectrum of a block triangular matrix is the union of the spectra of its diagonal blocks.

In the following section, we will first tackle the case where all the SCCs are primitive (or trivial, i.e. corresponding to a 1×1 zero diagonal block such as the vertex $\{5\}$ in the previous example). Then, in section 9.4.3, we will analyze the case of irreducible SCCs.

9.4.2. Graphs with primitive components

When a digraph is primitive, we can make use of the relation [9.3]. In this section, we explain how to get asymptotic information on $\mathsf{nW}_{u\to v}(n)$ for a directed multigraph whose SCCs are primitive or trivial (i.e. reduced to a single vertex). Consider the following running example. We will proceed with three steps.

Example 9.15.— The digraph depicted in Figure 9.4 seemingly has three identical primitive SCCs $\{1,2\}$, $\{4,5\}$ and $\{6,7\}$. Their Perron value is the golden ratio $\tau = (1+\sqrt{5})/2$. The digraph also has a trivial component $\{3\}$.

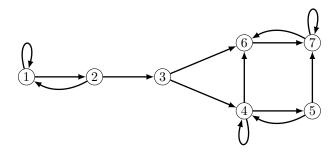


Figure 9.4. A digraph and its four SCCs

Step 0. Thanks to relation [9.3], we directly have the following asymptotics (as usual, up to a positive multiplicative constant)

$$\mathsf{nW}_{u \to v}(n) \sim_C \tau^n, \textit{ for } u, v \in \{1, 2\}; \textit{ or } u, v \in \{4, 5\}; \textit{ or } u, v \in \{6, 7\}$$

where the notation $f \sim_C g$ means that $\lim_{n\to+\infty} f(n)/g(n)$ tends to a positive constant (not necessarily equal to one).

Let us describe what we will discover in the following.

- In Step 0, we had a single primitive SCC: direct application of Perron's theorem.
- In Step 1, we will consider two primitive SCCs with the same Perron value.
- In Step 2, we will consider more primitive SCCs with the same Perron value.
- In Step 3, concluding the primitive case, we will consider several primitive SCCs with different Perron values.

Step 1]. What can be said in a more tricky situation such as $nW_{1\to 5}(n)$ or $nW_{1\to 7}(n)$? Let us start with walks of length n going through two primitive SCCs with the same Perron value. Observe that any walk of length n from the SCC $\{1,2\}$ to the SCC $\{4,5\}$ is divided into three parts: a walk of length i staying in the first component, a path from vertex i to vertex i of (bounded) length i connecting the two components and a walk of length i a staying in the second component. Hence, we get

$$\mathsf{nW}_{1\to 5}(n) = \sum_{i=0}^{n} \left(\mathsf{nW}_{1\to 2}(i).\mathsf{nW}_{4\to 5}(n-i-2) \right) \tag{9.7}$$

where we take the natural convention that $nW_{u\to v}(j)$ is set to zero if j<0. Note that [9.7] could also be written as

$$\sum_{\substack{i_1,i_2 \geq 0\\i_1+i_2=n-2}} \mathsf{nW}_{1 \to 2}(i_1).\mathsf{nW}_{4 \to 5}(i_2).$$

Such an expression involving two summatory indices i_1, i_2 will be easier to handle when we are dealing with more SCCs. Here, for the sake of simplicity, we have a single path from the SCC $\{1,2\}$ to the SCC $\{4,5\}$. The general situation will be explained later on. The point is that there are a finite number of paths connecting two SCCs.

How could we work out the sum [9.7] to derive some asymptotic result? Because of corollary 8.19 and theorem 8.25, the formal series

$$s_1(z) = \sum_{j=0}^{+\infty} \mathsf{nW}_{1 \to 2}(j) \, z^j \text{ and } s_2(z) = \sum_{j=0}^{+\infty} \mathsf{nW}_{4 \to 5}(j) \, z^j$$

are two rational functions of the form P_1/Q_1 and P_2/Q_2 . Recall that the roots of the characteristic polynomial of the recurrence relation are the reciprocals of the poles of the corresponding rational function.

LEMMA 9.16.— Let G be a primitive directed multigraph with Perron eigenvalue λ . For all vertices u, v of G, the formal series

$$\sum_{j=0}^{+\infty} \mathsf{nW}_{u \to v}(j) \, z^j$$

is a rational function of the form

$$\frac{P(z)}{Q(z)} = \frac{a}{(1 - \lambda z)} + R(z)$$

where a is non-zero constant and R(z) is a rational function whose poles have modulus larger than $1/\lambda$.

PROOF.— Since G is primitive, the polynomial Q has $1/\lambda$ as unique root of minimal modulus. When decomposing P/Q into partial fractions (see proposition 8.26), we get a single term of the form $\frac{a}{(1-\lambda z)}$ for some constant a. This term can be expanded as

$$a\sum_{j=0}^{+\infty} \lambda^n z^n.$$

In the decomposition of P/Q into partial fractions, this is the only term with this growth rate λ^n in its expansion. Again, by primitivity and [9.3], we know that $\mathsf{nW}_{u\to v}(n)\sim_C\lambda^n$. Hence, a must be non-zero.

The *Cauchy product* of the two series $s_1(z)$ and $s_2(z)$ (i.e. a discrete convolution product as defined in [8.6]) is given by

$$\sum_{n=0}^{+\infty} \left(\sum_{i=0}^{n} \mathsf{nW}_{1\to 2}(i).\mathsf{nW}_{4\to 5}(n-i) \right) z^n = \frac{P_1 P_2}{Q_1 Q_2}. \tag{9.8}$$

When decomposing this expression into partial fractions, since we have two primitive SCCs, we may apply lemma 9.16 to both $P_1/Q_1=a_1/(1-\tau z)+R_1(z)$ and $P_2/Q_2=a_2/(1-\tau z)+R_2(z)$ and distribute. Hence, P_1P_2/Q_1Q_2 is of the form

$$\frac{a_1 a_2}{(1 - \tau z)^2} + \frac{a_2 R_1(z)}{(1 - \tau z)} + \frac{a_1 R_2(z)}{(1 - \tau z)} + R_1(z) R_2(z)$$

where a_1a_2 is non-zero and $1/\tau$ is a simple pole (i.e. a pole of multiplicity one) of the central two terms. Decomposing this fraction into partial fractions, we get one term $a_1a_2/(1-\tau z)^2$, one term of the form $b/(1-\tau z)$ and terms of the form $c/(1-\alpha z)$ with $|\alpha|<\tau$. Moreover, $R_1(z)R_2(z)$ is a rational function whose poles have modulus larger than $1/\tau$. Thus, the main term for the asymptotic behavior comes from the following expansion

$$\frac{1}{(1-\tau z)^2} = \sum_{n=0}^{+\infty} (n+1)\,\tau^n\,z^n.$$
 [9.9]

Considering the coefficient of z^n in the two expansions [9.8] and [9.9], we derive that, for $n \to +\infty$,

$$\sum_{i=0}^{n} \mathsf{nW}_{1\to 2}(i).\mathsf{nW}_{4\to 5}(n-i) = a_1 a_2(n+1) \, \tau^n + o(n \, \tau^n) \sim_C n \, \tau^n. \ [9.10]$$

Recall that we are working up to a multiplicative constant, so $n\tau^n$ or $(n+1)\tau^n$ or even $(cn+d)\tau^{n+k}$ where $c,d,k\in\mathbb{Z}$ are constants (c>0) have the same asymptotic behavior: their respective limits divided by $n\tau^n$ exist (i.e. are finite) and are all positive.

The reader may object that the expression [9.10] is not exactly the one considered in [9.7]. We simply have to consider the Cauchy product $s_1(z).z^2s_2(z)$. With this finite shift of index, we obtain the same behavior because $(n-2)\,\tau^{n-2}\sim_C n\,\tau^n$. Indeed,

$$\lim_{n \to +\infty} \frac{(n-2)\tau^{n-2}}{n\tau^n} = \frac{1}{\tau^2}.$$

Numerical experiments show that

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{1 \to 5}(n)}{n \, \tau^n} = \frac{3 - \sqrt{5}}{10} \simeq 0.0764.$$

REMARK 9.17.— The reader may wonder why we cautiously argue that the constant a_1a_2 is non-zero (or equivalently, it is important in lemma 9.16 to state that the constant a is non-zero). Consider, for instance, the rational function

$$\frac{-2z^2-z+1}{2z^3+z^2-3z+1}$$

whose poles are 1/2, $2/(1+\sqrt{5})=1/\tau$ and $2/(1-\sqrt{5})=1/\tau'$ where $\tau'=(1-\sqrt{5})/2$ is the conjugate of the golden ratio. The general form of the decomposition into partial fractions is of the form

$$\frac{-2z^2-z+1}{2z^3+z^2-3z+1} = \frac{a}{1-2z} + \frac{b}{1-\tau z} + \frac{c}{1-\tau' z}$$

but determining a, b, c from

$$-2z^{2} - z + 1 = a(1 - \tau z)(1 - \tau' z) + b(1 - 2z)(1 - \tau' z) + c(1 - 2z)(1 - \tau z)$$

yields $a=0,\,b=(5+3\sqrt{5})/10,\,c=(5-3\sqrt{5})/10.$ Indeed, 1/2 is also a root of the numerator.

Let us modify slightly the previous example to consider two SCCs with the same Perron value but where several paths are connecting the two SCCs (instead of a single path).

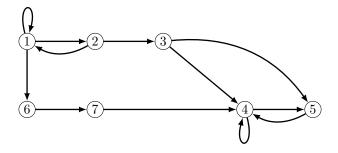


Figure 9.5. A modified example

With the digraph depicted in Figure 9.5, we have the same primitive SCCs $\{1,2\}$ and $\{4,5\}$. If we proceed as for [9.7], we have three paths connecting the two SCCs: one of length three $1\to 6\to 7\to 4$, and two of length two $2\to 3\to 4$ and $2\to 3\to 5$. We get

$$\begin{split} \mathsf{nW}_{1\to 5}(n) &= \sum_{i=0}^n \biggl(\mathsf{nW}_{1\to 1}(i).\mathsf{nW}_{4\to 5}(n-i-3) \\ &+ \mathsf{nW}_{1\to 2}(i).\mathsf{nW}_{4\to 5}(n-i-2) \\ &+ \mathsf{nW}_{1\to 2}(i).\mathsf{nW}_{5\to 5}(n-i-2) \biggr). \end{split}$$

So we essentially have to treat three expressions (up to a finite shift) similar to [9.10] and the sum of these three expressions will give the same behavior $\sim_C n\tau^n$. The main argument is that there is only a *finite number of paths connecting the two components*, all being of bounded length. Indeed, if an SCC is not primitive, then it is trivial. With trivial components, there is no cycle nor loop. Hence, we always have a finite sum of terms with the same asymptotic behavior.

As a conclusion, we have thus shown the following result.

PROPOSITION 9.18.— The number of walks of length n connecting two vertices and passing exactly through two primitive SCCs with the same Perron value α (and passing only by those SCCs excepting trivial ones) is in $\sim_C n \alpha^n$.

Step 2]. Let us move to several (two or more) primitive SCCs with the same Perron value. For the digraph in Figure 9.4, we will evaluate the quantity $nW_{1\rightarrow 6}(n)$. Note that there are two kinds of walks from 1 to 6, those passing through the SCC $\{4,5\}$ and those that do not. We will only consider those passing through that extra component (the other type of walks has been treated in the previous step – we already know that the number of walks of length n between the two SCCs and passing through the vertex 3 has a behavior in $\sim_C n \tau^n$). Let us denote the number of such walks of length n by $nW_{1\rightarrow \{4,5\}\rightarrow 6}(n)$. Using either the edge (4,6) or (5,7), we get that

 $\mathsf{nW}_{1 \to \{4,5\} \to 6}(n)$ is equal to

$$\begin{split} & \sum_{\substack{i_1,i_2,i_3 \geq 0\\ i_1+i_2+i_3=n-3}} \mathrm{nW}_{1\to 2}(i_1).\mathrm{nW}_{4\to 4}(i_2).\mathrm{nW}_{6\to 6}(i_3) \\ &+ \sum_{\substack{i_1,i_2,i_3 \geq 0\\ i_1+i_2+i_3=n-3}} \mathrm{nW}_{1\to 2}(i_1).\mathrm{nW}_{4\to 5}(i_2).\mathrm{nW}_{7\to 6}(i_3). \end{split}$$

Let us consider the second term (the first one is similar). We have already introduced the two series $s_1(z)$ and $s_2(z)$. The formal series

$$s_3(z) = \sum_{j=0}^{+\infty} \mathsf{nW}_{7\to 6}(j) \, z^j$$

is also a rational function P_3/Q_3 and we can again apply lemma 9.16. We simply consider the Cauchy product of the three series

$$s_1(z).s_2(z).s_3(z)$$

and the term with the main asymptotic contribution is derived from the expansion of

$$\frac{1}{(1-\tau z)^3} = \sum_{n=0}^{+\infty} \frac{(n+1)(n+2)}{2} \tau^n z^n.$$

Indeed, this is the same argument repeated for three SCCs: a term $a_i/(1-\tau z)$ with a non-zero constant a_i appears exactly once in the decomposition into partial fractions of P_i/Q_i , i=1,2,3 and thus a single term $a_1a_2a_3/(1-\tau z)^3$ appears in the final decomposition. We also have to consider a finite shift by multiplying by z^3 but it does not modify the growth rate that is in $\sim_C n^2 \tau^n$. Then, we have to take into account a finite union of possible connections between SCCs, each providing a term with the same growth rate.

Numerical experiments show that

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{1 \to 6}(n)}{n^2 \, \tau^n} = \frac{5 - 2\sqrt{5}}{25} \simeq 0.0211.$$

The same argument may be applied and repeated with $k \geq 2$ primitive components with the same Perron value. We just have to know the following expansion.

LEMMA 9.19.— Let $k \ge 2$ be an integer and $\alpha > 1$ be a real number. We have

$$\frac{1}{(1-\alpha z)^k} = \sum_{n=0}^{+\infty} \frac{(n+1)\cdots(n+k-1)}{(k-1)!} \alpha^n z^n.$$

We have thus proved the following result.

PROPOSITION 9.20.— The number of walks of length n connecting two vertices and passing exactly through $k \geq 1$ primitive SCCs with the same Perron value α (and passing only by those SCCs excepting trivial ones) is in $\sim_C n^{k-1}\alpha^n$.

COROLLARY 9.21.— Let G be a directed multigraph whose SCCs are all primitive with the same Perron value α . Let k be the maximal number of such primitive components that may be visited in a single walk. Then, the dimension of the largest Jordan block associated with α occurring in the Jordan decomposition of $\mathbf{A}(G)$ is k.

PROOF.— This observation follows directly from proposition 9.20 and remark 8.23. This is the only way to achieve the expected asymptotic behavior.

For instance, the Jordan decomposition of the adjacency matrix of the digraph depicted in Figure 9.4 has a block

$$\begin{pmatrix} \tau & 1 & 0 \\ 0 & \tau & 1 \\ 0 & 0 & \tau \end{pmatrix} .$$

Step 3]. The last situation to take into account (this is the general case when all the SCCs are primitive or trivial) is when we have *primitive SCCs* with different Perron values. Consider the digraph depicted in Figure 9.6 with three primitive SCCs. The components $\{1,2\}$ and $\{5,6\}$ again have the golden ratio as Perron value and $\{3,4\}$ has Perron value 2.

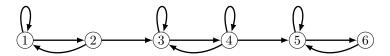


Figure 9.6. Primitive SCCs with different Perron values

For instance, we have

$$\mathsf{nW}_{1\to 6}(n) = \sum_{\substack{i_1, i_2, i_3 \geq 0 \\ i_1 + i_2 + i_3 = n - 2}} \mathsf{nW}_{1\to 2}(i_1).\mathsf{nW}_{3\to 4}(i_2).\mathsf{nW}_{5\to 6}(i_3).$$

We can proceed as before and consider the Cauchy product of three series. Two of these series are rational functions having $1/\tau$ as pole of minimal modulus 11 and the third series is a rational function with 1/2 as pole of minimal modulus. The decomposition into partial fractions of the product of these three rational functions has a term a/(1-2z) for some constant a. Since $n\tau^n/2^n$ tends to zero, this is the only term to take into account for the asymptotic behavior. We still have to argue that a is non-zero. Considering the particular walks of length n starting with the path $1 \to 2 \to 3$, followed by a walk of length n-4 between 3 and 4, and ending with the path $4 \to 5 \to 6$, we have, for large enough n.

$$\mathsf{nW}_{1\to 6}(n) \ge \mathsf{nW}_{3\to 4}(n-4).$$

Otherwise stated, this inequality is obtained by only considering a subset of the set of walks of length n: those for which only the portion of the walk contained in the SCC of maximal Perron value is allowed to vary. From the previous steps, we know that $\mathsf{nW}_{3\to 4}(n) \sim_C 2^n$. We conclude that the constant a is non-zero and $\mathsf{nW}_{1\to 6}(n) \sim_C 2^n$. We can improve the previous proposition.

THEOREM 9.22.— Let G be a directed multigraph whose SCCs are either primitive or trivial. The number of walks of length n connecting two vertices and visiting some fixed non-trivial SCCs C_1, \ldots, C_k is in $\sim_C n^{t-1}\alpha^n$ where α is the largest real number among the Perron values of C_1, \ldots, C_k and $t \in \{1, \ldots, k\}$ is the number of SCCs among C_1, \ldots, C_k having α as Perron value.

PROOF.—We just have to formalize a bit what we have discussed so far. Let C_{i_1}, \ldots, C_{i_t} be the t primitive SCCs in $\{C_1, \ldots, C_k\}$ with maximal Perron value α . Among the walks of length n connecting u and v and passing through C_1, \ldots, C_k , consider a shortest path \mathfrak{p}_1 (possibly empty) from u to a vertex

¹¹ We always neglect the fact that 0 can be a pole (in this example, 0 is an eigenvalue of the SCC $\{3,4\}$). Indeed, such a pole simply corresponds to a finite shift of the considered linearly recurrent sequence. Thus, it does not affect its asymptotic behavior (up to a multiplicative constant). So by pole of minimal modulus, we always refer to the set of non-zero poles.

in C_{i_1} denoted by $v_{i_1,0}$, then for $j=2,\ldots,t$, a shortest path \mathfrak{p}_j connecting a vertex $v_{i_{j-1},1}$ in $C_{i_{j-1}}$ and a vertex $v_{i_j,0}$ in C_{i_j} , and finally a shortest path \mathfrak{p}_{t+1} from a vertex $v_{i_t,1}$ in C_{i_t} to v. Among those walks of length n, if we only consider those for which only the portion of the walk contained in C_{i_1},\ldots,C_{i_t} is allowed to vary and using the fixed paths $\mathfrak{p}_1,\ldots,\mathfrak{p}_{t+1}$ as connectors, we derive that

$$\begin{aligned} & \mathsf{nW}_{u \to C_1 \to \cdots \to C_k \to v}(n) \\ & \geq \sum_{j_1 + \cdots + j_t = n - \ell} \mathsf{nW}_{v_{i_1,0} \to v_{i_1,1}}(j_1) \cdots \mathsf{nW}_{v_{i_t,0} \to v_{i_t,1}}(j_t) \end{aligned}$$

where ℓ is the total length of the paths \mathfrak{p}_j . From proposition 9.20, we know that the right-hand side is in $\sim_C (n-\ell)^{t-1}\alpha^{n-\ell}$. But ℓ is bounded (by the number of vertices in G), thus this behavior is the same as $\sim_C n^{t-1}\alpha^n$. Applying lemma 9.16, the formal series

$$\sum_{n=0}^{+\infty} \mathsf{nW}_{u \to C_1 \to \dots \to C_k \to v}(n) \, z^n$$

is a rational function with $1/\alpha$ as a pole of multiplicity t. Moreover, its decomposition into partial fractions has a single term of the form $a/(1-\alpha z)^t$. Since $1/\alpha$ is the pole of smallest modulus, it provides the main contribution to the asymptotic expansion. We conclude using lemma 9.19 and from the above discussion, the constant a is non-zero.

REMARK 9.23.— As in corollary 9.21, we can derive information about the largest block associated with the largest Perron value occurring in the Jordan decomposition of the adjacency matrix of a directed multigraph with primitive or trivial SCCs.

9.4.3. Structure of connected graphs

Theorem 9.22 gives the growth rate of the number of walks of length n in a directed multigraph when all the components are primitive (or trivial). The aim of this section is to see what could happen when some of the SCCs are not primitive (but they are necessarily irreducible). For that purpose, it is enough to discuss the case of a single SCC.

Consider the strongly connected directed multigraph depicted in Figure 9.7. It is mostly built from two cycles of length 3 and a cycle of length 6. It is easy to see that the digraph is not primitive. For instance, consider closed walks starting and ending in vertex 3. The only such walks have length 3m because they are made of 3-cycles and 6-cycles. Otherwise stated,

 $[(\mathbf{A}(G))^n]_{3,3}$ is zero for infinitely many n. Thus, the adjacency matrix is not primitive. The shortest path connecting 1 to 2 has length 7. There are six such paths (because of the 2 multiedges) and from the cyclic structure of the digraph, we see that $\mathsf{nW}_{1\to 2}(n)>0$ if and only if n=3m+1 with $m\geq 2$. Similarly, $\mathsf{nW}_{1\to 3}(n)>0$ if and only if n=3m+2 with $m\geq 1$ and $\mathsf{nW}_{1\to 4}(n)>0$ if and only if n=3m with $m\geq 2$. As observed in remark 9.6, we cannot look for a limit behavior as in the previous section. Nevertheless, the first few values m>0 of the sequence $(m)_{1\to 2}(3j+1)_{j>0}$ are

0, 6, 12, 42, 120, 366, 1092, 3282, 9840, 29526

and we can prove that

$$\lim_{j \to +\infty} \frac{\mathsf{nW}_{1 \to 2}(3j+1)}{3^j} = \frac{1}{2}.$$
 [9.11]

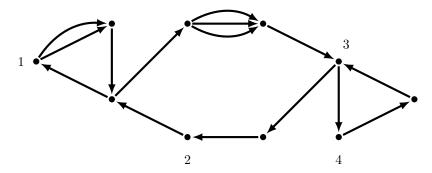


Figure 9.7. An irreducible multigraph

We can write $nW_{1\rightarrow 2}(3j+1) \sim_C 3^j$. This introductory example lets us foresee what to expect:

- 1) we will define a notion of *period* relevant with the structure of the digraph. For the digraph in Figure 9.7, the period is 3;
- 2) this period p will have the following property. For any two vertices u and v, there exists a unique integer $r_{u,v}$ such that every walk connecting u to v has length congruent to $r_{u,v}$ modulo p. In the example, we have seen that the walks

¹² These values have been computed by taking powers of the adjacency matrix.

between 1 and 2 (respectively, 3, 4) have length congruent to 1 (respectively, 2, 0) modulo 3;

3) finally, we will try to get some asymptotic information about the number of such walks as in the previous limit [9.11].

The gcd of an infinite set of positive integers

$$X = \{x_1 < x_2 < \cdots \}$$

is defined as the largest integer that divides every element in X. If X contains two coprime elements, then the gcd of X is equal to one. This gcd is also less than or equal to x_1 .

DEFINITION 9.24.— The **period** of a vertex v is the gcd of the lengths of the closed walks passing through it. It is denoted by per(v). It is undefined if no cycle passes through v. (Note that for a strongly connected non-trivial digraph, the period of each vertex is well defined.)

We use the notation given in section 1.2.1.

LEMMA 9.25.— Let G be a directed multigraph. Let u, v be two vertices such that $u \leftrightarrow v$. Then, per(u) = per(v). In particular, all the vertices belonging to an SCC have the same period.

PROOF.— Assume that a closed walk $\mathfrak w$ of length s passes through v. By assumption, there exists a walk $\mathfrak p$ (respectively, $\mathfrak q$) of length m (respectively, n) from u to v (respectively, from v to u). Thus, there exists a closed walk $\mathfrak p\mathfrak q$ passing through u of length m+s+n. Taking $\mathfrak w$ twice, there also exists a closed walk passing through u of length m+2s+n. By definition of the period of u, $\operatorname{per}(u)$ divides m+s+n and m+2s+n. Thus, $\operatorname{per}(u)$ divides the difference s for every s that is the length of a closed walk passing through v. By definition, $\operatorname{per}(v)$ is the gcd of all such s. Hence, $\operatorname{per}(v) \geq \operatorname{per}(u)$. We conclude the proof by symmetry on u and v.

The previous lemma allows us to define the **period** of a strongly connected multigraph G denoted by per(G). It is equal to the period of any vertex of G. Note that per(G) is less than or equal to the number of vertices of G.

COROLLARY 9.26.— Let G be a strongly connected multigraph. If G has two closed walks with coprime lengths, then per(G) = 1. In particular, if G has a loop on a vertex, then per(G) = 1.

PROOF.— Let u (respectively, v) be a vertex belonging to a closed walk of length p (respectively, q) with p,q coprime integers. Since $u \leftrightarrow v$, by the previous lemma, the period of G divides p and q. Thus, per(G) = 1.

The admissible lengths of walks between two vertices is related to the notion of period.

THEOREM 9.27.— Let G be a strongly connected directed multigraph of period p = per(G). Let v, w be two vertices in G:

- 1) there exists a unique integer $r_{v,w} \in \{0, \dots, p-1\}$ such that if there exists a walk of length ℓ from v to w, then $\ell \equiv r_{v,w} \pmod{p}$;
- 2) moreover, for all large enough n, there is a walk of length $np + r_{v,w}$ between v and w.

In particular, if the period p = 1, then G is primitive.

The second part of the proof relies on the next two results. The first one has an arithmetic flavor. For a generalization of this theorem, see exercise 9.4.1. The first arithmetic question below is recurrent and related to the so-called Frobenius problem (see the final remark 9.40).

LEMMA 9.28.— Let $X \subseteq \mathbb{N}_{\geq 1}$ be an infinite set of positive integers that is closed under addition, i.e. for all $m, n \in X$, m+n belongs to X. Then, X contains all but a finite number of the positive multiples of the gcd of X, i.e. all sufficiently large multiples of the gcd belong to X.

EXAMPLE 9.29.— Assume that X is a subset of \mathbb{N} closed under addition and containing 2 and 7, then the first few elements of X are

$$2, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, \dots$$

Since 6 and 7 belong to the set, then all integers $n \ge 6$ belong to X by adding convenient multiples of 2. Note that the gcd of the elements in X is 1.

PROOF.—Without loss of generality, we may assume that the gcd of X is equal to 1: simply divide every element by this gcd. There exists a finite subset $F = \{x_1, \ldots, x_k\}$ of X such that $\gcd F = 1$. If this was not the case, then we would conclude that $\gcd X > 1$. Note that the number of elements in F could be larger than 2, e.g. with $F = \{6, 10, 15\}$ any two elements are not coprime.

We apply Bezout's theorem: there exist $\lambda_1, \ldots, \lambda_k \in \mathbb{Z}$ such that

$$\sum_{i=1}^{k} \lambda_i \, x_i = \gcd F = 1.$$

We may sort the positive and the negative coefficients. Up to reordering, assume that $\lambda_1, \ldots, \lambda_\ell$ are positive and $\lambda_{\ell+1}, \ldots, \lambda_k$ are negative. We set

$$m:=\sum_{i=1}^\ell \lambda_i\,x_i \quad ext{ and } \quad n:=-\sum_{i=\ell+1}^k \lambda_i\,x_i.$$

Thus, m-n=1. Since X is closed under addition, m and n belong to X. Let q be an integer larger than or equal to n(n-1). Considering the Euclidean division of q by n yields

$$q = a n + b$$

with $0 \le b < n$ and $a \ge n-1$. In particular, a-b is non-negative. Since 1 = m-n, we have

$$q = a n + b(m - n) = (a - b) n + b m$$

showing that each $q \geq n(n-1)$ belongs to X because X is closed under addition.

We have a first interpretation of the period.

COROLLARY 9.30.— Let G be a strongly connected directed multigraph of period p. For all vertices v and all large enough n, there exists a closed walk of length np passing through v.

PROOF.— Consider two closed walks passing through the vertex v. Since the period of G is p, these walks have length a multiple of p, say kp and ℓp . The union of the two walks is again a closed walk passing through v. Its length is $(k+\ell)p$. Otherwise stated, the set of lengths of the closed walks passing through v is a subset X of $\mathbb N$ closed under addition and such that $\gcd X = p$. The conclusion follows from lemma 9.28.

PROOF OF THEOREM 9.27.— Assume that we have two walks from v to w of respective lengths m and n. It is enough to prove that $n \equiv m \pmod p$. Since the digraph is strongly connected, there exists a walk of length ℓ from w to v.

Hence, we have two closed walks passing through v, one of length $m+\ell$ and one of length $n+\ell$. By definition of the period, p divides $m+\ell$ and $n+\ell$ thus it divides the difference. Otherwise stated, $m-n\equiv 0\pmod p$.

The second part of the statement follows from corollary 9.30. Since G is strongly connected, there exists a walk of length ℓ from v to w. From the first part, we know that ℓ is of the form $mp+r_{v,w}$ for some integer m. From the previous corollary, there exists N_v such that there is a closed walk of length np passing through v for all $n \geq N_v$. Let $N_{v,w} = m + N_v$. For all $k \geq N_{v,w}$, we have $kp+r_{v,w} = np+(mp+r_{v,w})$ for some $n \geq N_v$. We know that there is a closed walk of length np on v and a walk of length $\ell = mp+r_{v,w}$ from v to w. Thus for all $k \geq N_{v,w}$, there is a walk of length $kp+r_{v,w}$ from v to w.

The particular case is obvious. If p=1, then $r_{v,w}=0$ for all pairs (v,w). Thus for all v,w, there exists $N_{v,w}$ such that there is a walk of length n from v to w for all $n \geq N_{v,w}$. Take $N = \max_{v,w} N_{v,w}$. There is a walk of length N from v to w for all vertices v,w showing that the digraph is primitive.

As a consequence of theorem 9.27, we can define an equivalence relation partitioning the set of vertices of a strongly directed multigraph G of period p = per(G).

DEFINITION 9.31.— Two vertices v and w are equivalent if and only if $r_{v,w}=0$, i.e. every walk between v and w has a length that is a multiple of p. Moreover, strong connectedness implies that fixing a vertex v_0 , for all $i \in \{0, \ldots, p-1\}$, there must exist some vertex v_i such that there is a walk from v_0 to v_i of length congruent to i modulo p. This means that we have exactly p (non-empty) equivalence classes $\mathfrak{C}_0, \ldots, \mathfrak{C}_{p-1}$ partitioning the set of vertices V(G). We have, for all $j \in \{0, \ldots, p-1\}$,

$$\mathfrak{C}_{j} = \{ w \in V(G) \mid r_{v_0, w} = j \}.$$

Note that if two vertices belong to the same class \mathfrak{C}_j then, by definition of the relation, all walks between these two vertices have a length that is a multiple of p. For convenience, we set $\mathfrak{C}_p = \mathfrak{C}_0$. Therefore, the set of edges satisfies

$$E(G) \subseteq \bigcup_{i=0}^{p-1} (\mathfrak{C}_i \times \mathfrak{C}_{i+1}).$$

Moreover, since the digraph is strongly connected, we have that, for all $i \in \{0, \dots, p-1\}$, $E(G) \cap (\mathfrak{C}_i \times \mathfrak{C}_{i+1})$ is non-empty and between any two

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vertices in the same class, there exists a walk of length a multiple of p. Since, for every vertex, the in-degree and the out-degree are positive, the structure of the digraph partitioned into the equivalence classes is depicted in Figure 9.8.

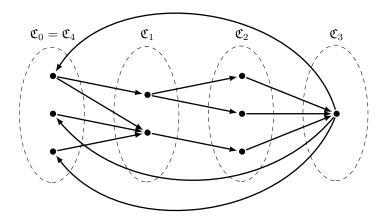


Figure 9.8. A schematic view of the equivalence classes (p = 4)

DEFINITION 9.32 (G_p) .— Similarly to the proof of theorem 9.12, we will consider the multigraph G_p having \mathbf{A}^p as adjacency matrix (in that proof, the graph G' should here be denoted G_2). The two directed multigraphs G and G_p share the same set of vertices¹³. There is an edge (u,v) in G_p if and only if there exists a walk of length p between u and v in G. Multiple edges reflect multiple walks.

The directed multigraph G_p can be deduced from G: every closed walk in G (and we know, by definition of the period, that each such walk has a length which is a multiple of p) gives a closed walk in G_p whose length is divided by p (thus, the corresponding period is also divided by p). Since every walk in G between two vertices of the same equivalence class \mathfrak{C}_j has length a multiple of p (and at least one such walk exists), in G_p , all vertices of \mathfrak{C}_j are connected.

¹³ G_p is related to the strict pth power of G introduced in definition 5.2 but this is not the same construction. In general, G is not a subgraph of G_p .

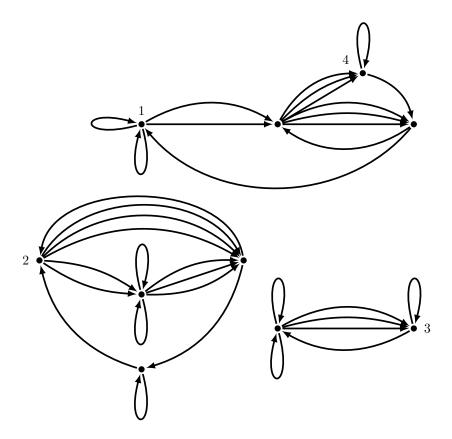


Figure 9.9. The digraph G_3 associated with the digraph G in Figure 9.7

If we compute G_4 for the digraph depicted in Figure 9.8, its adjacency matrix is given below. It reflects the four classes.

Hence, the equivalence classes $\mathfrak{C}_0,\dots,\mathfrak{C}_{p-1}$ are the strongly connected components of the directed multigraph G_p . Since the length of every closed walk in G_p has been divided by p comparing with closed walks in the original digraph G, the period of such an SCC is 1. So, by theorem 9.27, $\mathfrak{C}_0,\dots,\mathfrak{C}_{p-1}$ are primitive components of G_p . More about the Perron value of these components will be said in remark 9.35. Moreover, these components are totally disconnected: let $v\in\mathfrak{C}_i$ and $w\in\mathfrak{C}_j$ be two vertices belonging to different classes $(i\neq j)$. There is no walk in G_p between these two vertices. Otherwise, there should exist a walk in G of length that is a multiple of p between v and w, i.e. v and w should belong to the same equivalence class which is a contradiction. Continuing the running example given by the multigraph in Figure 9.7, we get the directed multigraph G_3 depicted in Figure 9.9. Note that the vertices 1 and 4 of the initial digraph belong to the same component. To build the digraph G_3 , simply consider every possible walk of length 3 in the initial digraph.

REMARK 9.33.— If the reader wonders what happens when we consider G_n where n is not a multiple per(G), we have given some of these digraphs in Figure 9.10 computed from the digraph G in Figure 9.7. To increase readability, we have written weights representing the number of edges between two vertices instead of multiple edges. Note that G_6 can be deduced from G_3 by taking walks of length 2.

9.4.4. Period and the Perron–Frobenius theorem

We have defined the period of a strongly connected digraph but there is also a special integer associated with every irreducible matrix. In this section, we prove that these two quantities are equal.

Let G be a strongly connected multigraph having \mathbf{A} as adjacency matrix. Let λ be the Perron–Frobenius eigenvalue of the irreducible matrix \mathbf{A} . Assume that \mathbf{A} has $period\ h$, in terms of the statement of theorem 9.5 part 6): the eigenvalues of maximal modulus are exactly $\lambda\ e^{2ik\pi/h}$ for $k=0,\ldots,h-1$. In particular (fact 8.4), h is the $\underline{\text{smallest}}$ integer n such that \mathbf{A}^n has a unique (real) eigenvalue of maximal modulus, i.e. any other eigenvalue α of \mathbf{A}^h is such that $|\alpha| < \lambda^h$. This is one notion of period.

¹⁴ From corollary 9.30, in G there are closed walks of length np in every vertex v and for all large enough n. Thus in G_p , there are closed walks in every vertex v for all large enough lengths.

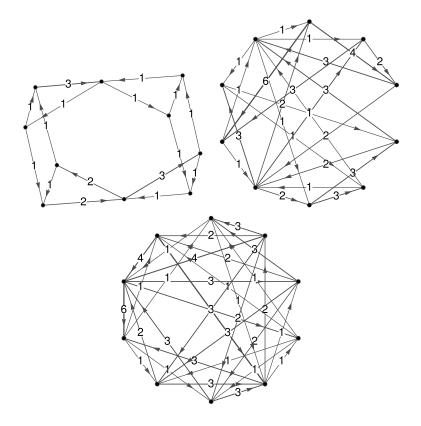


Figure 9.10. The digraphs G_2 , G_4 and G_5 associated with the digraph G in Figure 9.7

Thanks to definition 9.24, we have also introduced the period of G, denoted by per(G). We are now ready to prove that the two notions of period introduced so far are the same, that is h = per(G).

With the discussion of the previous section, we know that $\mathbf{A}^{\mathsf{per}(\mathsf{G})}$ is a block-diagonal matrix with primitive matrices¹⁵

$$\mathbf{R}_0, \dots, \mathbf{R}_{\mathsf{per}(\mathsf{G})-1} \tag{9.12}$$

¹⁵ Think, for instance, about the digraph in Figure 9.9.

on the diagonal, we can apply the theorem of Perron: each block \mathbf{R}_j has its own Perron eigenvalue λ_j and each eigenvalue α of \mathbf{R}_j distinct from λ_j is such that $|\alpha| < \lambda_j$. Then, any eigenvalue α of $\mathbf{A}^{\mathsf{per}(G)}$ distinct from $\max_j \lambda_j$ is such that $|\alpha| < \max_j \lambda_j$, i.e. $\mathbf{A}^{\mathsf{per}(G)}$ has a unique real eigenvalue of maximal modulus. Consequently, due to the minimality of h discussed above, we have $\mathsf{per}(G) \geq h$.

If the reader has in mind the general form of an irreducible multigraph of period $p = \operatorname{per}(G)$ decomposed into equivalence classes (e.g. a model is given in Figure 9.7) and if we order the vertices of G starting with those belonging to \mathfrak{C}_0 , then $\mathfrak{C}_1,\mathfrak{C}_2,\ldots$ up to \mathfrak{C}_{p-1} , then the adjacency matrix has a particular form

$$\mathbf{A} = \begin{pmatrix} 0 & \mathbf{B}_0 & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{B}_1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{B}_{p-2} \\ \mathbf{B}_{p-1} & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

The block \mathbf{B}_j has $\#\mathfrak{C}_j$ rows and $\#\mathfrak{C}_{j+1}$ columns (with the usual convention that $\mathfrak{C}_p = \mathfrak{C}_0$). It stores the edges connecting two consecutive equivalence classes and we know that there are no other edges. As an example, consider the digraph decomposed into four classes depicted in Figure 9.8. The matrices $\mathbf{B}_0, \ldots, \mathbf{B}_3$ are represented below.

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & \boxed{1} & \boxed{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{0} & 1 & \boxed{0} & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{0} & \boxed{1} & \boxed{0} & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{0} & \boxed{1} & \boxed{1} & \boxed{0} & \boxed{0} & 0 \\ 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} & \boxed{1} & \boxed{0} & \boxed{0} \\ 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{0} & \boxed{1} & \boxed{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{0} & \boxed{1} & \boxed{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} & \boxed{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} & \boxed{0} \\ \boxed{1} & \boxed{1} & \boxed{1} & \boxed{0} & 0 & 0 & 0 & \boxed{0} & \boxed{0} & \boxed{0} \end{pmatrix}$$

REMARK 9.34.— The structure of the block matrix above reflects the cyclic structure of the digraph. Indeed, look at the cycle depicted in Figure 9.11 and the corresponding adjacency matrix.

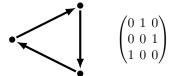


Figure 9.11. Adjacency matrix of a cycle

Let \mathbf{x} be a (right) eigenvector of \mathbf{A} for one eigenvalue α . This column vector is split accordingly into p subvectors $\mathbf{x}_0, \dots, \mathbf{x}_{p-1}$ corresponding to the p equivalence classes ¹⁶. Since $\mathbf{A}\mathbf{x} = \alpha \mathbf{x}$, we get for $j = 1, \dots, p-1$

$$\mathbf{B}_{j-1}\mathbf{x}_j = \alpha \, \mathbf{x}_{j-1}$$
 and $\mathbf{B}_{p-1}\mathbf{x}_0 = \alpha \, \mathbf{x}_{p-1}$.

Now consider the vector \mathbf{x}' whose subvectors are

$$\mathbf{x}_0, e^{2i\pi/p} \mathbf{x}_1, \dots, e^{2i(p-1)\pi/p} \mathbf{x}_{p-1}.$$

So to define \mathbf{x}' , we replace \mathbf{x}_j with $\mathbf{x}_j' = e^{2ij\pi/p}\mathbf{x}_j$. We get $\mathbf{A}\mathbf{x}' = e^{2i\pi/p}\alpha \mathbf{x}'$ because, for $j=1,\ldots,p-1$,

$$\mathbf{B}_{j-1}\mathbf{x}_{j}' = \mathbf{B}_{j-1}e^{2ij\pi/p}\mathbf{x}_{j} = e^{2i\pi/p}\alpha \underbrace{e^{2i(j-1)\pi/p}\mathbf{x}_{j-1}}_{\mathbf{x}_{j}'}$$

and $\mathbf{B}_{p-1}\mathbf{x}_0'=e^{2i\pi/p}\alpha\,e^{2i(p-1)\pi/p}\mathbf{x}_{p-1}=e^{2i\pi/p}\alpha\,\mathbf{x}_{p-1}'$. We have just proved that for any eigenvalue $\alpha\in\mathbb{C}$ of an irreducible matrix \mathbf{A} such that G has period p, the complex numbers $\alpha\,e^{2in\pi/p}$ for $n=0,\ldots,p-1$ are all eigenvalues of \mathbf{A} . The set of eigenvalues of \mathbf{A} is invariant under the transformation $z\mapsto z\,e^{2i\pi/p}$, where we recall that $p=\operatorname{per}(G)$. In particular, the numbers $\lambda\,e^{2ik\pi/p}$ for $k=0,\ldots,p-1$ are eigenvalues of \mathbf{A} of maximal modulus λ . This means that

$$\{\lambda\,e^{2ik\pi/p}\mid 0\leq k\leq p-1\}\subseteq \{\lambda\,e^{2ik\pi/h}\mid 0\leq k\leq h-1\}$$

where h is given by the Perron–Frobenius theorem. Consequently, p divides h and $h \ge p$. We conclude that h = p.

¹⁶ We follow the lines of [SEN 06].

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REMARK 9.35.— Each block \mathbf{R}_i introduced in [9.12] has a real dominating eigenvalue, which is simple, $i=0,\ldots,p-1$ and $p=\mathsf{per}(G)$. But the multiplicity of λ^p as an eigenvalue of \mathbf{A}^p is p (fact 8.4). Hence, we deduce that all the primitive blocks $\mathbf{R}_0,\ldots,\mathbf{R}_{p-1}$ must have λ^p as Perron eigenvalue.

We can restate this observation as follows.

PROPOSITION 9.36.— Let G be a strongly connected multigraph. Let $n \ge 1$ be an integer such that G_n is the union of totally disconnected primitive components. All these components have the same Perron value α and the Perron–Frobenius value of the initial digraph G is $\sqrt[n]{\alpha}$.

In this proposition, n could be a multiple of per(G).

9.4.5. Concluding examples

We put together the material that we have seen so far and consider digraphs with several primitive or irreducible SCCs. We will see that we need to carry out a careful analysis. In the third example, we will show that existence of a limit is not always guaranteed. We mix primitive and irreducible components as follows:

- in the first example, the dominating Perron-Frobenius eigenvalue is associated with a primitive component only;
- in the second example, the dominating Perron–Frobenius eigenvalue is the same for a primitive and an irreducible component;
- in the third example, the dominating Perron-Frobenius eigenvalue is associated with an irreducible component of period larger than 1 only;
- the digraph in Figure 9.12 has $\{1,2\}$ and $\{3,4\}$ as a primitive SCC with the golden ratio $\tau=(1+\sqrt{5})/2$ as Perron value. The SCC $\{5,6,7,8\}$ is irreducible of period 2. The eigenvalues of maximal modulus for this component are $\sqrt{\tau}$ and $-\sqrt{\tau}$. (This is a good exercise to check 17).

¹⁷ Either you compute the eigenvalues of a 5×5 matrix or, you consider the digraph G_2 associated with that component.

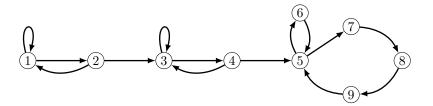


Figure 9.12. Two primitive SCCs and an irreducible one (different dominating eigenvalues)

If we proceed as in [9.7] and section 9.4.2, we have

$$\mathsf{nW}_{1\to 8}(n) = \sum_{\substack{i_1,i_2,i_3 \geq 0\\ i_1+i_2+i_3=n-2}} \mathsf{nW}_{1\to 2}(i_1).\mathsf{nW}_{3\to 4}(i_2).\mathsf{nW}_{5\to 8}(i_3).$$

As before, we have to consider the Cauchy product of three formal series that are rational. In the decomposition into partial fractions, the main term that appears is of the form $a/(1-\tau z)^2$ with a non-zero constant a. Indeed, the third SCC provides the decomposition with terms proportional to $1/(1-\sqrt{\tau}z)$ and $1/(1+\sqrt{\tau}z)$ and possibly other terms all having poles of modulus larger than $1/\tau$.

Consequently, we have a behavior similar to the one described in proposition 9.18, $nW_{1\rightarrow 8}(n)\sim_C n\, \tau^n$. We can, for instance, obtain (a long but not difficult exercise) that

$$\lim_{n\to +\infty} \frac{\mathsf{nW}_{1\to 8}(n)}{n\,\tau^n} = \frac{\tau-1}{10}.$$

– Let us proceed to a second example. The digraph depicted in Figure 9.13 has $\{1,2\}$ and $\{3,4\}$ as primitive SCC with 2 as Perron value, compared with the digraph in Figure 9.12, we have extra loops on the vertices 2 and 4. The SCC $\{5,6\}$ is irreducible of period 2. The eigenvalues of maximal modulus for this component are 2 and -2. Thus, the situation is more interesting than in the previous example because primitive and irreducible components have the same dominating eigenvalue.

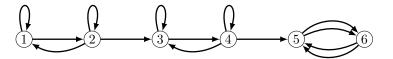


Figure 9.13. Two primitive SCCs and an irreducible one (same dominating eigenvalue)

If we are interested in the behavior of $nW_{1\rightarrow 6}(n)$, as before, we will consider the Cauchy product of three series. The three series have 1/2 as a pole, in particular,

$$\sum_{n=0}^{+\infty} \mathsf{nW}_{5\to 6}(n)\, z^n = \frac{z}{1-2z} + \frac{z}{1+2z} = \sum_{n=0}^{+\infty} (2^n + (-2)^n)\, z^{n+1}.$$

The decomposition into partial fractions of the Cauchy product of the three series is of the form (as usual, we do not consider the occurrence of zero as a pole¹⁸)

$$\frac{a_3}{(1-2z)^3} + \frac{a_2}{(1-2z)^2} + \frac{a_1}{(1-2z)} + \frac{a_0}{(1+2z)}.$$

Let us prove that $a_3 \neq 0$. If we consider walks of even length, we can make use of the digraph G_2 given in definition 9.32. It has four primitive components $\{1,2\}, \{3,4\}, \{5\}$ and $\{6\}$ with Perron value 4, see Figure 9.14.

We are back to the case discussed in section 9.4.2 with walks visiting three primitive SCCs. By theorem 9.22, in G_2 , the number of walks of length m from 1 to 6 behaves like m^24^m . Walks of length 2n in G correspond to walks of length n in G_2 , thus we can deduce that in the original digraph $n \mathbb{W}_{1 \to 6}(2n) \sim_C n^24^n = \frac{1}{4}(2n)^22^{2n}$. Hence, a_3 must be non-zero and consequently,

$$nW_{1\to 6}(n) \sim_C n^2 2^n$$
.

We can prove that

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{1 \to 5}(n)}{n^2 \, 2^n} = \frac{1}{64} \text{ and } \lim_{n \to +\infty} \frac{\mathsf{nW}_{1 \to 6}(n)}{n^2 \, 2^n} = \frac{1}{64}.$$

^{18 0} is an eigenvalue with multiplicity 2 of the adjacency matrix. This eigenvalue will not affect the general asymptotic behavior that we are looking for.

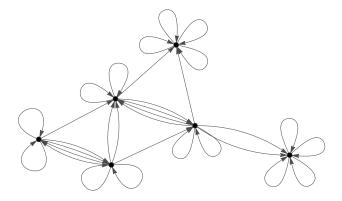


Figure 9.14. The digraph G_2 associated with the digraph depicted in Figure 9.13

– The third example is more tricky (even though at first glance, it looks similar to the previous one). The digraph in Figure 9.15 has $\{1,2\}$ and $\{3,4\}$ as primitive SCC with 2 as Perron value. The SCC $\{5,6\}$ is irreducible of period 2. The eigenvalues of maximal modulus for this component are 3 and -3.

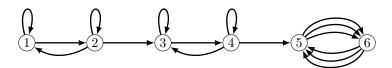


Figure 9.15. Two primitive SCCs and an irreducible one

We are again interested in $nW_{1\rightarrow 6}(n)$. With our usual arguments, we get

$$\sum_{n=0}^{+\infty} \mathsf{nW}_{1\to 6}(n)\, z^n = \frac{a_2}{(1-2z)^2} + \frac{a_1}{(1-2z)} + \frac{b_1}{(1-3z)} + \frac{b_2}{(1+3z)}.$$

Here, we will show that the coefficients b_1 and b_2 are non-zero and distinct. The sequence $(U_n)_{n\geq 0}=(\mathsf{nW}_{1\to 6}(n))_{n\geq 5}$ satisfies the relation

$$U_{n+4} = 4U_{n+3} + 5U_{n+2} - 36U_{n+1} + 36U_n, \quad \forall n \ge 0$$

with initial conditions 3, 12, 63, 204. We have

$$\sum_{n=0}^{+\infty} U_n z^n = \frac{3}{-36z^4 + 36z^3 - 5z^2 - 4z + 1}$$

which can be decomposed as

$$\frac{-12/5}{(1-2z)^2} + \frac{-216/25}{(1-2z)} + \frac{27/2}{(1-3z)} + \frac{27/50}{(1+3z)}.$$

Recall that

$$\frac{27}{2} \frac{1}{1 - 3z} = \frac{27}{2} \sum_{n=0}^{+\infty} 3^n z^n,$$

$$\frac{27}{50} \frac{1}{1+3z} = \frac{27}{50} \sum_{n=0}^{+\infty} (-3)^n z^n.$$

Hence, we get

$$\lim_{n \to +\infty} \frac{U_{2n}}{3^{2n}} = \frac{27}{2} + \frac{27}{50} \text{ and } \lim_{n \to +\infty} \frac{U_{2n+1}}{3^{2n+1}} = \frac{27}{2} - \frac{27}{50}$$

and consequently, we obtain two subsequences converging to different limits

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{1 \to 6}(2n+5)}{3^{2n+5}} = \frac{1}{3^5} \lim_{n \to +\infty} \frac{U_{2n}}{3^{2n}} = \frac{13}{225} \simeq 0.05778$$

$$\lim_{n \to +\infty} \frac{\mathsf{nW}_{1 \to 6}(2n+6)}{3^{2n+6}} = \frac{1}{3^5} \lim_{n \to +\infty} \frac{U_{2n+1}}{3^{2n+1}} = \frac{4}{75} \simeq 0.05333.$$

This fluctuation is explained by the fact that the dominating term in the asymptotic expansion is derived from a non-primitive component only. So, we have to deal with the two eigenvalues 3 and -3.

We conclude with a few exercises where several irreducible components are involved. More exercises will be given in section 9.6.

EXERCISE 9.4.1.— Consider walks starting from a vertex u, ending in a vertex v and visiting exactly k irreducible SCCs of respective periods p_1, \ldots, p_k . Assume that at least such a walk exists. Let $P = \gcd\{p_1, \ldots, p_k\}$. Prove that there exists $r_{u,v} \in \{0, \ldots, P-1\}$ such that every walk of the prescribed form from u to v has length congruent to $r_{u,v}$ modulo P and there exists N such that, for all $n \geq N$, there is such a walk of length $nP + r_{u,v}$. (Hint: generalization of theorem 9.27 where k = 1, application of lemma 9.28 to the smallest set of integers that is closed under addition and containing p_1, \ldots, p_k .)

EXERCISE 9.4.2.— Study the sequence

$$(\mathsf{nW}_{1\to 2}(n))_{n\geq 0} = 0, 0, 0, 2, 0, 2, 4, 2, 4, 10, \dots$$

for the digraph depicted in Figure 9.16.

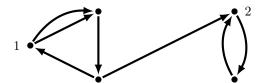


Figure 9.16. A multigraph with two irreducible SCCs (coprime periods)

Prove that $(\mathsf{nW}_{1\to 2}(n))_{n\geq 5}$ satisfies the recurrence relation $U_{n+5} = U_{n+3} + 2U_{n+2} - 2U_n$ and, with the initial conditions 2,4,2,4,10, we have

$$\sum_{n=0}^{+\infty} U_n z^n = \frac{-4z^3 + 4z + 2}{2z^5 - 2z^3 - z^2 + 1}.$$

Moreover, show that

$$\lim \frac{\mathsf{nW}_{1\to 2}(3n)}{2^n} = \lim \frac{\mathsf{nW}_{1\to 2}(3n+1)}{2^{n-1}} = \lim \frac{\mathsf{nW}_{1\to 2}(3n+2)}{2^n} = \frac{4}{3}.$$

EXERCISE 9.4.3.— *Study the sequence*

$$(\mathsf{nW}_{1\to 2}(n))_{n\geq 4} = 4, 0, 4, 0, 20, 0, 20, 0, 84, 0, 84, 0, 340, 0, 340, 0, \dots$$

for the digraph depicted in Figure 9.17.

Prove that $nW_{1\rightarrow 2}(n) = 0$ *if* n *is odd and*

$$\lim \frac{\mathsf{nW}_{1\to 2}(4n)}{4^n} = \lim \frac{\mathsf{nW}_{1\to 2}(4n+2)}{4^n} = \frac{4}{3}.$$

Figure 9.17. A multigraph with two irreducible SCCs (periods 2 and 4)

9.5. The case of polynomial growth

In this section, we consider the special case where the maximal Perron–Frobenius eigenvalue of the different SCCs is 1. Let G be a finite directed multigraph. Let u,v be two vertices in G such that there are infinitely many walks from u to v, i.e. $\mathsf{nW}_{u \to v}(n) > 0$ for infinitely many n. To give the reader an image, keep in mind the digraph depicted in Figure 9.20. With this digraph, if we compute the first values of $(\mathsf{nW}_{u \to v}(n))_{n \ge 0}$, say by taking powers of the adjacency matrix, we get the graphic in Figure 9.18 and the reader can already figure out what we mean by polynomial growth.

If there are infinitely many walks from u to v, there exists a path $\mathfrak p$ from u to v passing through a vertex w such that w belongs to a cycle $\mathfrak c$. Consequently 19, there are walks of length $|\mathfrak p|+k|\mathfrak c|$ from u to v for all $k\geq 0$.

From the previous section (application of theorem 9.27, introduction of the period p of a strongly connected graph G and then considering the graph G_p in definition 9.32 that leads to primitive components), we know that there exist $\lambda \geq 1$, an integer d, a positive constant c and an infinite increasing sequence $(n_i)_{i>0}$ of integers such that

$$\mathsf{nW}_{u \to v}(n_i) \sim c \, n_i^d \, \lambda^{n_i}, \quad i \to +\infty.$$

¹⁹ This argument is similar to one used in the pumping lemma for regular languages, see [ALL 03, RIG 14].

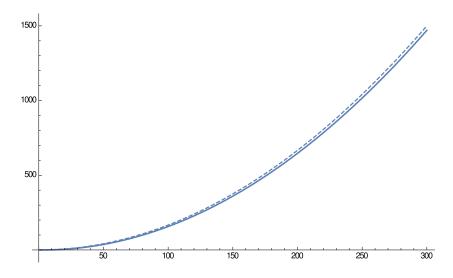


Figure 9.18. Comparing $nW_{u\to v}(n)$ with $x\mapsto \frac{x^2}{60}$ (dashed)

Indeed, the sequence $(n_i)_{i\geq 0}$ depends on the structure of the digraph and the periods of the encountered SCCs. For instance, if a digraph contains only cycles of even length, then we could imagine that $\mathsf{nW}_{u\to v}(2n) = 0$, for all n, and $\mathsf{nW}_{u\to v}(2n+1)$ will have a polynomial growth (or conversely).

The title of this section suggests that we will be interested in digraphs where the only admissible behavior is of the form

$$\mathsf{nW}_{u\to v}(n_i) \sim c\,n_i^d, \qquad i\to +\infty.$$

This is what we call a polynomial growth. We will see that these digraphs have a very special form.

Assume that there exists a path $\mathfrak p$ from u to v passing through a vertex w such that w belongs to two different closed walks $\mathfrak c$ and $\mathfrak c'$ (i.e. $\mathfrak c$ and $\mathfrak c'$ can share some edges but they have at least a distinct edge). In Figure 9.19, we have depicted several cases where two different closed walks occur. For instance, we have the walks $(\mathfrak r,\mathfrak t)$ and $(\mathfrak s,\mathfrak t)$, the walks $(\mathfrak a,\mathfrak b,\mathfrak c)$ and $(\mathfrak d,\mathfrak e,\mathfrak f)$, the walks $(\mathfrak h,\mathfrak g,\mathfrak i,\mathfrak k,\mathfrak j)$ and $(\mathfrak h,\mathfrak g,\mathfrak m,\mathfrak j)$.

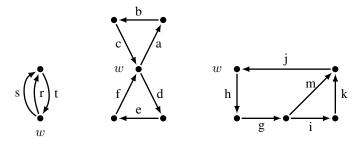


Figure 9.19. Examples of different closed walks

In that case, let us give a lower bound for the number of closed walks passing through w. The number of closed walks of length $m|\mathfrak{c}|+n|\mathfrak{c}'|$ is at least

$$\binom{m+n}{m} = \frac{(m+n)!}{m! \, n!}$$

because we have at least all the sequences made of m walks $\mathfrak c$ and n walks $\mathfrak c'$ in any order and any two such sequences provide different closed walks because $\mathfrak c \neq \mathfrak c'$. In the special case m=n, the number of closed walks of length $n(|\mathfrak c|+|\mathfrak c'|)$ on w is at least $(2n)!/(n!)^2$. From Stirling's approximation formula²⁰, the number of closed walks of length $n(|\mathfrak c|+|\mathfrak c'|)$ is, for large enough n, greater than

$$\frac{4^n}{\sqrt{\pi n}}$$

We conclude that, if we encounter two different closed walks passing through the same vertex, then $\mathsf{nW}_{u\to v}(n)$ must have an exponential growth (at least for infinitely many lengths). The next statement summarizes what we have done so far.

LEMMA 9.37.— If there exist C and d such that, for all n,

$$\mathsf{nW}_{u \to v}(n) \le Cn^d$$
,

then every vertex belonging to a path from u to v belongs to at most one closed walk.

$$\frac{1}{20 n!} \sim \sqrt{2\pi n} (n/e)^n.$$

PROOF.— Proceed by contradiction. If this is not the case, there is a vertex belonging to two closed walks and we must have an exponential growth for infinitely many values.

The general structure of the digraphs we are dealing with is thus prescribed by the above result. We have depicted in Figure 9.20 an example of a digraph such that every vertex belongs to at most one closed walk. More precisely, a digraph with that property is a union of digraphs made up of consecutive closed walks – in automata theory [SZI 92], we find the terminology *tiered graph* (meaning that it is made up of successive layers). We will never revisit a vertex belonging to a closed walk visited before. A more general situation is depicted in Figure 9.21. But we may decompose this digraph into six elementary subcases similar to the one considered in Figure 9.20 (see Figure 9.22). The six cases come from the two choices: either edge 1 or 2 and the three choices between the edges 3,4,5.

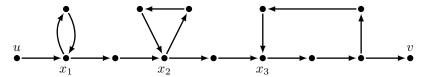


Figure 9.20. A digraph with polynomial growth

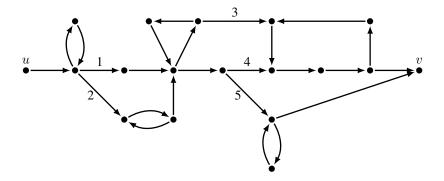


Figure 9.21. A more complex digraph with polynomial growth

To conclude this section, we would like to say a bit more about the degree of the polynomials that we encounter. It is linked to the number of closed walks that may be visited.

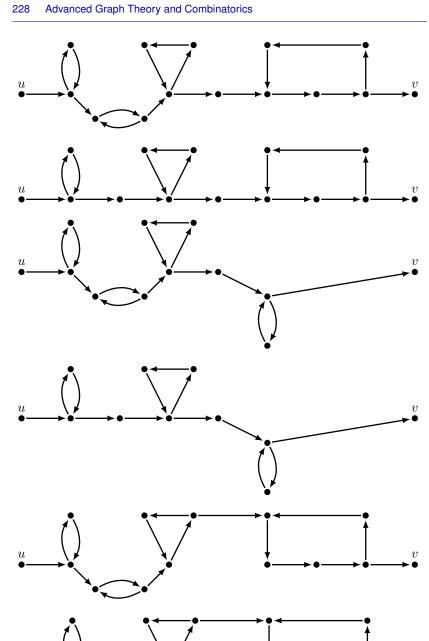


Figure 9.22. Decomposition of a complex digraph

Assume that we may encounter up to t consecutive cycles of respective (positive) length c_1, \ldots, c_t and we use ℓ extra edges to connect them together, so we have walks from u to v of length

$$\ell + n_1 c_1 + \cdots + n_t c_t$$

with $n_1,\ldots,n_t\in\mathbb{N}$. To give an idea, we would like to count paths in a digraph resembling the one depicted in Figure 9.20 (where $\ell=8,\,c_1=2,\,c_2=3,\,c_3=5$ because we have a path of length 1 from u to x_1 , of length 2 from x_1 to x_2 and from x_2 to x_3 and finally of length 3 from x_3 to v). As a result of lemma 9.28, there exist walks of length $\ell+m\gcd\{c_1,\ldots,c_t\}$ for all large enough m. Without loss of generality, we will not take ℓ into account in the following lines (it is only a shift by a constant) and we will also assume that $\gcd\{c_1,\ldots,c_t\}=1$. Said otherwise, there are walks from u to v for every large enough length. But the question is to determine how many walks of a given length n are there?

As a gentle introduction, it is an easy result in enumerative combinatorics to see that

$$\#\{(n_1,\ldots,n_t)\in\mathbb{N}^t\mid n_1+\cdots+n_t=n\}=\binom{n+t-1}{t-1}$$

which is a polynomial in n^{t-1} (see [BRU 92]). A way to prove this result is sometimes referred to as *stars and bars* method [FEL 50]. We count the number of *partitions* of n as a sum of t non-negative integers. What we want is a bit more: we want estimates on

$$f(n) := \#\{(n_1, \dots, n_t) \in \mathbb{N}^t \mid n_1 c_1 + \dots + n_t c_t = n\}.$$
 [9.13]

The generating function satisfies

$$\sum_{n=0}^{+\infty} f(n) z^n = \prod_{j=1}^{t} \frac{1}{1 - z^{c_j}}.$$

Indeed, this simply follows from the Cauchy product of the series

$$\left(\sum_{n_1=0}^{+\infty} z^{c_1 n_1}\right) \cdots \left(\sum_{n_t=0}^{+\infty} z^{c_t n_t}\right).$$

The coefficient of z^n in this product is indeed equal to f(n).

Example 9.38. With $c_1 = 2$, $c_2 = 3$, $c_3 = 5$, the series expansion of

$$\frac{1}{1-z^2} \, \frac{1}{1-z^3} \, \frac{1}{1-z^5}$$

yields

$$1 + z^{2} + z^{3} + z^{4} + 2z^{5} + 2z^{6} + 2z^{7} + 3z^{8} + 3z^{9} + 4z^{10} + 4z^{11} + 5z^{12} + 5z^{13} + 6z^{14} + 7z^{15} + \mathcal{O}(z^{16}).$$

For instance, 8 = 2 + 2 + 2 + 2 + 2, 8 = 2 + 3 + 3 or 8 = 3 + 5. There are three ways to partition 8 using the integers 2, 3, 5. In the digraph depicted in Figure 9.20, there are 3 walks of length 16 from u to v (we add the eight horizontal edges to the total length).

The next proposition says that if we encounter t different cycles for the walks of length n, then we have a behavior in n^{t-1} for $nW_{u\to v}(n)$. Remember that it also gives insight on the largest Jordan block associated with eigenvalue 1.

PROPOSITION 9.39.— With the above setting and notation [9.13], if $gcd\{c_1,\ldots,c_t\}=1$, then

$$f(n) = \left(\prod_{j=1}^{t} \frac{1}{c_j}\right) \frac{n^{t-1}}{(t-1)!} + \mathcal{O}(n^{t-2}).$$

This result is proved in [NAT 00, p. 456] and this is exactly what we were looking for.

For decision issues, given a digraph, decide if the growth rate of $nW_{u\to v}(n)$ is polynomial or exponential (see, for instance, [GAW 08]). See also [SHU 08] and [JUN 09, Chapter 3].

REMARK 9.40.— A related interesting combinatorial problem is the so-called Frobenius problem. Let c_1, \ldots, c_t be positive integers such that $\gcd\{c_1, \ldots, c_t\} = 1$. Any large enough integer can be written as a linear combination of the c_i 's with non-negative coefficients. The question is to determine the largest N that cannot be written in this way (see, for instance, [RAM 05]).

9.6. Exercises

1) Consider the digraph depicted in Figure 9.23.

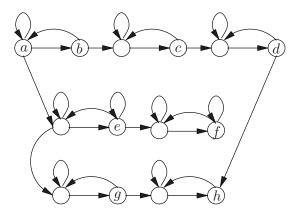


Figure 9.23. A digraph with primitive SCCs

Could you provide the asymptotic behavior of $nWa \rightarrow x(n)$ for $x = b, \ldots, h$?

2) Consider the directed multigraph depicted in Figure 9.24.



Figure 9.24. A directed multigraph

Compute the graphs G_j (definition 9.32) for j=2,3,4,5,6. What do you observe? What is the period of this strongly connected graph? For any two vertices u,v determine the sequence $(\mathsf{nW}_{u\to v}(n))_{n\geq 0}$. Could you add a single edge to make the digraph primitive?

- 3) Have you already worked out the exercises 9.4.1, 9.4.2 and 9.4.3?
- 4) Build a directed multigraph whose spectrum contains $\sqrt{3}$ and $-\sqrt{3}$.

- 5) Let n, p, q be integers such that $n \ge 2$ and $p \le q$. Build a directed multigraph with spectral radius equal to $n^{p/q}$.
- 6) Build a directed multigraph with spectral radius equal to $\sqrt[3]{30}$ and $\max \deg^+(v) \leq 5$.
- 7) Generalize the previous exercise. Build a directed multigraph with spectral radius equal to $n^{1/\ell}$ where the prime decomposition of n is $p_1^{\alpha_1}\cdots p_k^{\alpha_k}$, $\ell \geq \alpha_1+\cdots+\alpha_k$ and $\max \deg^+(v) \leq \max_{i \in \{1,\dots,k\}} p_i$.
- 8) Build the strict third power of the digraph depicted in Figure 9.7 and compare it with Figure 9.9.
 - 9) Build digraphs where $nW_{u\to v}(n)$ behaves like n^k for k=1,2,3,4.
- 10) Have a look at Shur's paper [SHU 08] for applications in formal language theory.
 - 11) Work out a proof of proposition 9.39.
- 12) Devise an algorithm determining the number of cycles a vertex belongs to. From this algorithm, test whether or not the number of walks in a directed multigraph behaves with a polynomial growth.

Google's Page Rank

We will now start one of my favorite topics when lecturing or giving talks to a general audience¹. Indeed, we will see that Perron's theorem is behind the famous search engine and how powerful this result is. In this chapter, we will describe the basic ideas behind the PageRank algorithm. This is only an introduction to the subject. Entire books are devoted to this important topic [LAN 06]. The PageRank of a page is only one of the ingredients (but an important one) used by Google to provide its ranking of Webpages. This requires a more complex formula to include, for instance, information about the user (language, searcher's last queries, geographic location, which links are usually clicked on, operating system or browser, etc.) to obtain a personalization of the search. Even though many improvements have been made over two decades, the idea behind PageRank link analysis is fundamental.

Search engines (SEs) play a major role in what pages users effectively see. They have a tremendous power in their hands. People click more on the pages they see at the top. No one goes on the third page of results provided by Google. There is an ongoing debate about how results should be displayed by SE. *Organic search* is the result given by the SE based on relevance only (versus *non-organic search* including pay-per-click advertisement). If the user clicks on some particular item, the SE makes more money. The SE has to find a good balance between maximizing revenue and keeping relevant results [LEC 16, VAR 07, WRI 12].

¹ Thus, I really have to give crystal clear explanations! I have given these talks almost a hundred times.

REMARK 10.1.— Before going further, let me mention that Google is not the only model. Parallel and independent works exist. At the same period as the Google conceptors were developing their algorithms, J. Kleinberg was devising an algorithm called HITS [KLE 99]. As pointed out in [LAN 12], similar ideas already existed long before PageRank became popular: see [KEE 93] where the author J. Keener worked in the analysis of evolutionary systems and biological dynamics. Other earlier works [KEN 55, SAA 87] dating back to 1955 can also be found.

We can rank Webpages but we could also rank soccer teams, academic journals, chess players, etc. (see example 10.15 at the end of this chapter). As soon as we are dealing with a digraph, we can rank its vertices. Indeed, recall that the World Wide Web can be seen as a (huge) digraph where the vertices are the Webpages and the edges are the links between pages (example 1.6). The edges are directed: we can have a link from a page A referencing a page B and there is no reason that B should refer to A. We will use the words link and reference interchangeably.

A positive real number called **PageRank** is associated with every Webpage. We will use the words *PageRank* and *Score* equally. This quantity should measure the relevance (or authority) of a page based on two "natural" criteria as originally described by Larry Page and Sergey Brin [BRI 98] almost 20 years ago:

- pages referenced by pages having a high PageRank should also get a high
 PageRank roughly speaking, if an "expert" in a particular field of interest
 tells us that this person is good or excellent in this field, we are more inclined
 to believe it because an expert says so²;
- the importance of a link has to be relativized with respect to how many links the page it comes from is distributing roughly speaking, if someone claims to have a thousand friends, are all these people true friends or only vague acquaintances? If someone else claims to have a couple of friends, these relationships are probably much stronger.

REMARK 10.2.— We can already note that this ranking does not depend on the content or the data found on the pages but only on the links between them. It is not a problem. As soon as every page receives its score, when a user makes a query by typing some keywords, Google selects the subset of pages relevant to

² I usually take the following example: if you need surgery, would you choose a world famous surgeon, i.e. an expert, or a first-year student in an obscure medical faculty? We are confident in authoritative figures.

these keywords (this is another problem about information retrieval and Webcrawling software³). Then, simply compare the scores of the pages belonging to this subset. As an example, if we have a dataset with chess games between various players, we compute the PageRank of every player, and then we can sort out two rankings for the male or female players.

Let $V=\{1,\ldots,n\}$ be the set of Webpages on the World Wide Web. You can easily assume that n is larger than 10^{10} . From the above criteria, if π_j denotes the PageRank of j, then we set

$$\pi_j = \sum_{i \in \mathsf{pred}(j)} \frac{\pi_i}{\mathsf{deg}^+(i)}.$$
 [10.1]

Indeed, in this formula π_j depends only on the scores of the pages referencing j and the presence of the denominator $\deg^+(i)$ divides the importance of π_i with respect to the total number of references sent by page i to other pages. Since i belongs to $\operatorname{pred}(j)$, we never divide by 0.

Hence [10.1] provides a recursive definition of the π_j 's: the score of a page depends on the score of the pages linking to it. We have a system of linear equations determining π_1, \ldots, π_n . Can we hope to solve this system? Does it have at least one solution? Probably, it would be better to look for a unique solution because if we have more than one solution, it would mean that we will have several incomparable rankings. Finally, if everything goes well from a theoretical point of view, it is also desirable to compute the solution efficiently. Indeed, we have billions of Webpages, thus the system has billions of unknowns.

Hopefully, we can answer these questions positively. But first, we add an extra requirement.

³ Googlebots scan new and updated pages indexing every word. The programs are following links from page to page, they literally crawl through the Web. The indexing of pages includes keywords but also metadata such as number of occurrences, font size and type, capitalization (i.e. lower/upper case), position on the page of the keyword, etc. Then, an inverted index is created to point from keywords to relevant pages.

REMARK 10.3.— There is no restriction to assume (and it will soon become clear why, see remark 10.6) that the scores satisfying [10.1] are also normalized, i.e.

$$\sum_{i=1}^{n} \pi_i = 1. ag{10.2}$$

Since the π_i 's are positive and sum to 1, we could interpret them as some probability (see section 10.4).

EXAMPLE 10.4.— Recall that by convention, vectors are column vectors. Thus row vectors will be denoted with transpose. We again take example 1.6, relations [10.1] give the matrix equation

where $\Pi^T = (\pi_1 \ \pi_2 \ \pi_3 \ \pi_4 \ \pi_5)$ and **H** stands for "hyperlinks". Equivalently, we can rewrite it as a homogeneous system of five linear equations with five unknowns

$$\Pi^{T}\left(\mathbf{H} - \mathbf{I}\right) = \mathbf{0}.$$

Since the system is homogeneous, it always has the solution $\mathbf{0}$. Unfortunately, on this example, the matrix $\mathbf{H} - \mathbf{I}$ is invertible. Thus, we obtain the unique solution $\Pi^T = \mathbf{0}$, i.e. $\pi_1 = \cdots = \pi_5 = 0$. It is unfortunate because you have to recall that we want to rank Webpages and with such a solution we are unable to do the job properly.

With this example, we have just discovered that we are looking for a (left) eigenvector Π^T of the matrix \mathbf{H} associated with the eigenvalue 1. If you are used to right eigenvectors, do not worry: the same theory applies for left eigenvectors (you can simply transpose everything). Note that the matrix \mathbf{H} is quite close to the adjacency matrix of the digraph and can easily be derived from it. The formal definition is given in the following (definition 10.7).

With the results from the previous chapter, you can already imagine what we are looking for: if the matrix **H** was primitive, Perron's theorem would

provide an eigenvector (and hopefully associated with the eigenvalue 1 but we will have to check) with positive entries. Moreover, any multiple of an eigenvector is again an eigenvector, thus we could find a normalized solution. It is not by chance that Brin and Page thought about Perron's theorem. Sergei Brin's father, Michael Brin, is a well-known mathematician⁴ working on dynamical systems and ergodic theory. In this branch of mathematics, Perron–Frobenius theory is widely used. For an account, see [BRI 02, section 4.12].

Before filling the gap, let us consider an example as bad as the previous one.

EXAMPLE 10.5.— Again we consider a minimal Web with five Webpages and links between these pages as depicted in Figure 10.1.

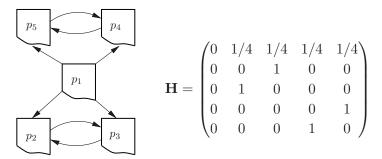


Figure 10.1. Some links and Webpages

The vectors

$$\Pi^T = \begin{pmatrix} 0 \ 0 \ 0 \ 1/2 \ 1/2 \end{pmatrix}$$

and

$$\Pi'^T = \begin{pmatrix} 0 & 1/2 & 1/2 & 0 & 0 \end{pmatrix}$$

⁴ He is a retired professor of mathematics at the University of Maryland. The *Michael Brin Prize in Dynamical Systems* was created in 2008 and is awarded to young mathematicians having obtained outstanding results in the field of dynamical systems.

are both eigenvectors of \mathbf{H} with eigenvalue 1. So, even for such a simple situation, we get two different and incomparable rankings. It is not surprising looking at the structure of the digraph. Indeed, the existence of these two solutions reflects the symmetry in the digraph: we have exactly the same relations between the first three pages and the pages p_1, p_4, p_5 .

REMARK 10.6.— One of our initial questions was the uniqueness of the ranking. Since the set of solutions of a homogeneous system of linear equations is a vector space, any linear combination (and in particular any multiple) of solutions is again a solution. If this vector space has dimension 1, then the solution Π^T will be defined up to multiplication by a constant. Nevertheless, this is not a problem for ranking: if $\pi_i < \pi_j$, then $k \pi_i < k \pi_j$ for all k > 0. Even though the two solutions Π^T and $k \Pi^T$ are distinct (for $k \neq 1$), they will provide the same ranking. Naturally, for k < 0, we get the reversed ranking (but it does not really matter). This remark also ensures us that whenever there exists a solution, we can derive a normalized one in the sense of remark 10.3.

10.1. Defining the Google matrix

We will introduce three matrices \mathbf{H} , \mathbf{S} and finally \mathbf{G} . All these matrices depend on the adjacency matrix $\mathbf{A}(G)$ and thus on the initial digraph G. Since the context is clear (G is given), we will not write explicitly the dependency on G.

DEFINITION 10.7.— Let $G = (\{1, ..., n\}, E)$ be a digraph with adjacency matrix $\mathbf{A}(G)$. The hyperlink matrix \mathbf{H} is defined by

$$H_{ij} = \begin{cases} \mathbf{A}(G)_{ij}/\mathsf{deg}^+(i), & \textit{if}\,\mathsf{deg}^+(i) > 0; \\ 0, & \textit{if}\,\mathsf{deg}^+(i) = 0. \end{cases}$$

Note that the sum of the elements on every non-zero row is equal to one.

Let us introduce a useful variant of this matrix,

$$S_{ij} = \begin{cases} \mathbf{A}(G)_{ij}/\deg^{+}(i), & \text{if } \deg^{+}(i) > 0; \\ 1/n, & \text{if } \deg^{+}(i) = 0. \end{cases}$$

Compared with H, note that S is stochastic⁵: each row sums to one.

⁵ We could even say *row-stochastic* to be more precise.

With the digraph of the Web, take its adjacency matrix and its hyperlink matrix **H**. Replacing **H** with **S** amounts to adding to sinks (that are dead-end Webpages) external links to every pages of the Web. It makes sense: assume that you are browsing the Web and at some stage, you end up on a page with no link. Take, for instance, a link to a picture. You click on the link and the picture shows up in your browser. What will you do? What will an "average" surfer do? One will use either the "back" button or proceed to a new search or enter a url given by some friend, etc. The point is that after visiting a page with no link, on the next step (i.e. the next visited page) the surfer could virtually be on any page of the Web. Thus, this is reasonable to get rid of sinks proceeding in that way⁶.

Having no sink does not mean that the digraph is strongly connected (to apply Perron–Frobenius theorem, recall that we need an irreducible matrix). There is one last trick to consider.

DEFINITION 10.8.— Let $G = (\{1, ..., n\}, E)$ be a digraph with adjacency matrix $\mathbf{A}(G)$. The Google matrix \mathbf{G} is defined by

$$\mathbf{G} = \alpha \,\mathbf{S} + (1 - \alpha) \,\mathbf{J}/n \tag{10.3}$$

where \mathbf{S} has been given in definition 10.7 and \mathbf{J} is a $n \times n$ matrix whose entries are all equal to 1 and α is a fixed real number in (0,1) (we have seen this matrix in section 8.5). Imagine a segment in the space $\mathbb{R}^{n \times n}$ of matrices whose endpoints are \mathbf{S} and \mathbf{J} . The closer α is to 1 the closer to the matrix derived from the links on the internet (up to getting rid of the sinks) \mathbf{G} is. The closer α is to 0, the closer to the matrix associated with the complete graph K_n (we have lost any information on the existing links) \mathbf{G} is.

EXAMPLE 10.9.— Continuing example 10.4, the corresponding matrix G for various values of $\alpha = 0.1, 0.3, 0.5$ and 0.7 are given below.

$$\begin{pmatrix} 0.18 & 0.23 & 0.23 & 0.18 & 0.18 \\ 0.2 & 0.2 & 0.2 & 0.2 & 0.2 \\ 0.18 & 0.18 & 0.18 & 0.23 & 0.23 \\ 0.23 & 0.18 & 0.23 & 0.18 & 0.18 \\ 0.18 & 0.213 & 0.213 & 0.213 & 0.18 \end{pmatrix}$$

⁶ There were several other attempts to deal with sinks; one can for instance suggest to model the "back button" by replacing ingoing edges with symmetric edges. See, for instance, [LAN 06, section 8.4].

$$\begin{pmatrix} 0.14 & 0.29 & 0.29 & 0.14 & 0.14 \\ 0.2 & 0.2 & 0.2 & 0.2 & 0.2 \\ 0.14 & 0.14 & 0.14 & 0.29 & 0.29 \\ 0.29 & 0.14 & 0.29 & 0.14 & 0.14 \\ 0.14 & 0.239 & 0.239 & 0.239 & 0.14 \end{pmatrix}$$

$$\left(\begin{array}{cccccc} 0.1 & 0.35 & 0.35 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.2 & 0.2 & 0.2 \\ 0.1 & 0.1 & 0.1 & 0.35 & 0.35 \\ 0.35 & 0.1 & 0.35 & 0.1 & 0.1 \\ 0.1 & 0.265 & 0.265 & 0.265 & 0.1 \end{array} \right)$$

$$\begin{pmatrix} 0.06 & 0.41 & 0.41 & 0.06 & 0.06 \\ 0.2 & 0.2 & 0.2 & 0.2 & 0.2 \\ 0.06 & 0.06 & 0.06 & 0.41 & 0.41 \\ 0.41 & 0.06 & 0.41 & 0.06 & 0.06 \\ 0.06 & 0.291 & 0.291 & 0.291 & 0.06 \end{pmatrix}$$

REMARK 10.10.— Another possibility to define \mathbf{G} is to adapt \mathbf{J} to the user, because not all pages are likely to be visited by a specific user. In [10.3], we replace \mathbf{J}/n with \mathbf{ev}^T where \mathbf{e} is a vector with all components equal to 1 and \mathbf{v}^T is a probability vector that is supposed to reflect the preferences of the user. Note that $\mathbf{J} = \mathbf{ee}^T$.

We will not give many details here but the value of α has to be carefully chosen. First note that any positive $\alpha \neq 1$ does a good job: every entry in \mathbf{G} is positive and thus \mathbf{G} is trivially primitive. At first guess, we could take $\alpha = 0.999$ because \mathbf{G} will be "close" to \mathbf{S} (i.e. close to the real links occurring in the Web) but for computational reasons, the closer α is to 1, the more prohibitive are the computations to get the needed precision on the scores. Also, the results will be more dependent on the small modifications that occur on the Web (many minor pages appear and disappear every day). It seems that a good (heuristic) compromise is a value $\alpha = 0.85$.

EXAMPLE 10.11.— Continuing example 10.4, the corresponding matrix **G** is given by

$$0.85 \begin{pmatrix} 0 & 1/2 & 1/2 & 0 & 0 \\ 1/5 & 1/5 & 1/5 & 1/5 & 1/5 \\ 0 & 0 & 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 0 & 1/3 & 1/3 & 1/3 & 0 \end{pmatrix} + 0.15 \frac{\mathbf{J}}{5}$$

$$= \begin{pmatrix} 3/100 & 91/200 & 91/200 & 3/100 & 3/100 \\ 1/5 & 1/5 & 1/5 & 1/5 & 1/5 & 1/5 \\ 3/100 & 3/100 & 3/100 & 91/200 & 91/200 \\ 91/200 & 3/100 & 91/200 & 3/100 & 3/100 \\ 3/100 & 47/150 & 47/150 & 47/150 & 3/100 \end{pmatrix}.$$

More details can be found in [LAN 06]. In particular, the authors proposed the results in Table 10.1. We can imagine that, to be able to distinguish billions of pages, we need a precision of 10 decimal digits. Also see the concluding section 10.5.

α	Number of iterations
0.5	34
0.75	81
0.8	104
0.85	142
0.9	219
0.95	449
0.99	2,292
0.999	23,015

Table 10.1. Needed iterations depending on the chosen α

10.2. Harvesting the primitivity of the Google matrix

Instead of considering the initial equations [10.1], we will tweak it a bit and finally consider the matrix equation

$$\Pi^T \mathbf{G} = \Pi^T \tag{10.4}$$

where the unknown is the vector Π . We will be able to easily conclude.

Since $\mathbf S$ and $\mathbf J/n$ are both stochastic matrices, then $\mathbf G$ is also stochastic (because the coefficients in the definition of $\mathbf G$ are such that $\alpha+(1-\alpha)=1$). As a corollary of proposition 9.8, every $n\times n$ stochastic matrix $\mathbf T$ with rational coefficients has 1 as eigenvalue and every eigenvalue $\alpha\in\mathbb C$ is such that $|\alpha|\leq 1$. For the proof, observe that $q\mathbf T$ is the adjacency matrix of a q-regular graph where q is the lowest common multiple (lcm) of the denominators of the entries of $\mathbf T$ (this is why we need rational entries).

Thus, G is primitive and has 1 as largest eigenvalue. By Perron's theorem, 1 must be the Perron eigenvalue of G. To summarize our observations:

THEOREM 10.12.— The Google matrix **G** is primitive and 1 is its Perron eigenvalue.

By Perron's theorem (theorem 9.2), there exists a left eigenvector Π^T associated with 1 whose components are all positive. Up to multiplication by a constant, we can assume that the sum of the components of this eigenvector is equal to 1. Since the Perron eigenvalue is simple, we have uniqueness of the scores: there is a unique vector Π satisfying both [10.2] and [10.4].

We also trivially know a right eigenvector of G with eigenvalue 1. Indeed, the vector e whose entries are all equal to 1 works fine. This is a consequence of the fact that G is (row-) stochastic. With our normalized vector Π^T , we also have $\Pi^T e = 1$. This is another formulation of [10.4].

From the asymptotic formula [9.3], we have

$$G^k = \mathbf{e} \Pi^T + o(1)$$

or equivalently

$$\lim_{k \to +\infty} G^k = \mathbf{e} \, \Pi^T = \begin{pmatrix} \pi_1 \, \pi_2 \, \cdots \, \pi_n \\ \pi_1 \, \pi_2 \, \cdots \, \pi_n \\ \vdots & & \vdots \\ \pi_1 \, \pi_2 \, \cdots \, \pi_n \end{pmatrix}.$$

We can estimate Π iteratively. Start with an initial distribution $p_{(0)}^T=\left(1/n\ \cdots\ 1/n\right)$ and, for all $k\geq 1$, set

$$p_{(k)}^T := p_{(0)}^T \mathbf{G}^k = p_{(k-1)}^T \mathbf{G}.$$
 [10.5]

Observe that it is easily seen by induction on k that the sum of the components of $p_{(k)}^T$ is equal to 1 for all k.

PROPOSITION 10.13.— We have

$$\lim_{k \to \infty} p_{(k)}^T = \Pi^T.$$

PROOF.- From [9.3], we directly have

$$\lim_{k \to +\infty} (1/n \cdots 1/n) G^k = \underbrace{(1/n \cdots 1/n)}_{-1} \mathbf{e} \Pi^T$$

Starting with an initial distribution whose components are all positive and sum to 1, we decide to stop computation when a sufficient precision is reached to discriminate scores, for instance measured by the norm $\left|\left|p_{(k)}^T-p_{(k-1)}^T\right|\right|$ that should be less than a specified threshold.

EXAMPLE 10.14.— Continuing examples 10.4 and 10.11. We have computed powers of the matrix G obtained in example 10.11. We only indicate the first line of G^n for some values of n in Table 10.2.

n	π_1	π_2	π_3	π_4	π_5
		0.18196			
10	0.13568	0.18801	0.26173	0.17304	0.24155
20	0.13556	0.18804	0.26163	0.17316	0.24162
200	0.13556	0.18804	0.26163	0.17316	0.24162

Table 10.2. Some powers of the Google matrix

On this very small example, it is already enough to compute \mathbf{G}^5 to rank the Webpages. For bigger cases and more pages, we need to go up to 200 iterations to reach a sufficient precision (here a few iterations are enough, the first two decimal digits are correct after 10 iterations but two digits will not be enough to rank billions of pages).

EXAMPLE 10.15.— I am not a great soccer fan but I have considered all the matches played in the Belgian first league during the 2009–2010 season (Wikipedia records all kinds of results). Every team plays against every other team twice (victory gives 3 points to the winner and none for the other team, in case of a draw both teams get 1 point). In our model, if A wins twice against B, then we consider an edge of weight 6 from B to A (i.e. B gives six points to A). If A wins one confrontation and loses the other one, then we consider an edge of weight 3 from A to B and another one from B to A. If A wins a game and the other one is a draw, then there is an edge of weight 4 from B to A and an edge of weight 1 from A to B. If the two games are draws, then we consider an edge of weight 2 from A to B and another one from B to A. Fifteen teams were competing. We list them in alphabetical order (in French): Anderlecht, Cercle de Bruges, Club de Bruges, Charleroi, Courtrai, (La) Gantoise, Genk, Germinal Beerschot, Lokeren, Malines,

Roulers, Saint-Trond, Standard de Liège⁷, Westerlo, Zulte-Waregem. We get the matrix S given in Table 10.3.

```
\begin{pmatrix} 0 & 0 & \frac{1}{4} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{12} & 0 & 0 \\ \frac{1}{7} & 0 & \frac{1}{7} & 0 & \frac{2}{21} & \frac{1}{7} & \frac{1}{14} & \frac{1}{14} & \frac{1}{42} & \frac{1}{42} & \frac{1}{14} & \frac{1}{42} & \frac{1}{42} & \frac{1}{14} & \frac{2}{12} \\ \frac{1}{7} & 0 & 0 & 0 & \frac{1}{21} & \frac{1}{21} & \frac{1}{21} & \frac{1}{7} & 0 & \frac{4}{21} & 0 & \frac{1}{21} & \frac{1}{7} & 0 & \frac{1}{21} \\ \frac{6}{53} & \frac{6}{53} & \frac{6}{53} & 0 & \frac{4}{53} & \frac{6}{53} & \frac{3}{53} & \frac{3}{53} & \frac{1}{53} & \frac{3}{53} & \frac{6}{53} & 0 & \frac{2}{53} & \frac{4}{53} & \frac{4}{53} & \frac{2}{53} \\ \frac{2}{11} & \frac{1}{33} & \frac{4}{33} & \frac{3}{33} & 0 & \frac{1}{33} & \frac{1}{33} & \frac{1}{11} & \frac{1}{33} & \frac{3}{33} & 0 & \frac{1}{11} & \frac{1}{21} & \frac{2}{33} & \frac{1}{11} \\ \frac{1}{4} & 0 & \frac{1}{7} & 0 & \frac{1}{7} & 0 & \frac{1}{28} & \frac{1}{7} & 0 & 0 & 0 & \frac{3}{28} & 0 & \frac{1}{7} & \frac{3}{14} \\ \frac{3}{20} & \frac{3}{40} & \frac{1}{40} & \frac{3}{40} & \frac{1}{10} & \frac{1}{10} & 0 & \frac{1}{10} & 0 & \frac{3}{20} & \frac{1}{20} & \frac{1}{40} & \frac{3}{40} & \frac{1}{40} & \frac{1}{20} \\ \frac{6}{41} & \frac{3}{41} & \frac{4}{41} & \frac{4}{41} & \frac{1}{41} & \frac{1}{41} & 0 & \frac{3}{41} & \frac{6}{41} & \frac{1}{41} & \frac{4}{41} & \frac{4}{41} & \frac{4}{41} \\ \frac{2}{21} & \frac{6}{63} & \frac{2}{21} & \frac{1}{21} & \frac{6}{63} & \frac{2}{21} & \frac{2}{21} & \frac{1}{21} & 0 & \frac{1}{21} & \frac{1}{21} & \frac{2}{21} & \frac{1}{21} & \frac{4}{63} \\ \frac{3}{20} & \frac{1}{10} & \frac{1}{40} & 0 & \frac{1}{10} & \frac{3}{20} & 0 & 0 & \frac{3}{40} & 0 & 0 & \frac{3}{30} & \frac{1}{10} & \frac{3}{40} & \frac{3}{40} \\ \frac{1}{10} & \frac{1}{20} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} & \frac{1}{30} & \frac{1}{15} & \frac{1}{20} & \frac{1}{10} & 0 & \frac{1}{10} & \frac{1}{20} & \frac{1}{30} & \frac{1}{60} \\ 0 & \frac{1}{9} & \frac{1}{9} & \frac{1}{18} & \frac{1}{12} & \frac{1}{12} & \frac{1}{9} & \frac{1}{12} & 0 & 0 & 0 & 0 & \frac{3}{34} & 0 & \frac{1}{22} & \frac{1}{22} & \frac{1}{23} \\ \frac{3}{22} & \frac{3}{44} & \frac{3}{22} & \frac{1}{44} & \frac{1}{21} & \frac{1}{11} & \frac{1}{11} & \frac{3}{44} & \frac{3}{44} & \frac{1}{22} & 0 & 0 & 0 \\ \frac{1}{9} & \frac{1}{9} & \frac{1}{18} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{20} & 0 & 0 & 0 & \frac{3}{24} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{9} & \frac{1}{9} & \frac{1}{22} & \frac{3}{29} & 0 & \frac{2}{29} & \frac{1}{29} & \frac{1}{29} & \frac{3}{29} & 0 & \frac{2}{29} & 0 & 0 \end{pmatrix}
```

Table 10.3. The matrix encoding the soccer 2009–2010 season

We can compute the PageRank associated with these teams and compare the ranking with the usual one (obtained by adding the points corresponding to the matches) (see Table 10.4). You will spot some differences. Remember that it is important to win a match. But PageRank gives more importance when the victory is against a good team.

REMARK 10.16.— Of course, the ranking obtained in Table 10.4 depends on the chosen model. For instance, if we replace weight 6 with 7 and weight 4 with 5 (it gives a small advantage to the offensive teams), we obtain some permutation in the middle of the list. After Standard and before Westerlo, using these new weights, the teams are ranked in Table 10.5.

⁷ I should have picked a year where my local team won the championship! But in 2008–2009, when Liège won the championship, the decision was made after a playoff. So it does not really fit with our ranking story. Moreover, I imagine that PageRank would not go well for my favorite team!

PageRank	corresp. ranking	VS	classical ranking	points
0.1038	Anderlecht	_	Anderlecht	69
0.1006	Club Bruges	-	Club Bruges	57
0.0984	Saint-Trond	+2	La Gantoise	49
0.0788	La Gantoise	-1	Courtrai	45
0.0772	Zulte	+1	Saint-Trond	42
0.0695	Standard	+2	Zulte	41
0.0661	Beerschot	+3	Malines	39
0.0658	Courtrai	-4	Standard	39
0.0648	Malines	-2	Cercle Bruges	38
0.0632	Genk	+1	Beerschot	35
0.0565	Westerlo	+1	Genk	34
0.0534	Cercle Bruges	-3	Westerlo	32
0.0372	Charleroi	_	Charleroi	23
0.0347	Roulers	+1	Lokeren	18
0.0298	Lokeren	-1	Roulers	18

Table 10.4. Comparing sport ranking with PageRank

PageRank	corresp. ranking
	:
0.06750	Standard
0.06642	Malines
0.06605	Courtrai
0.06485	Genk
0.06468	Beerschot
	:

Table 10.5. Changing the weights changes the ranking

Another topic discussed in [LAN 12, Chapter 10] is to consider products p_1, \ldots, p_n bought by customers and to build a *preference graph* whose vertices are the p_j 's. Let C_i be the set of customers who evaluated the product p_i . If there exists a customer in C_i who prefers the product p_j (i.e. this customer has ranked all the products he/she has bought, his first choice is p_j and his/her list contains p_i), then there is an edge from p_i to p_j with weight equal to the number of customers in C_i preferring p_j divided by $\#C_i$.

10.3. Computation

The matrices we are dealing with have billions of entries. It is challenging to compute powers of \mathbf{G} . Nevertheless, we can make use of the fact that the matrix \mathbf{H} is extremely sparse: each Webpage has references only to a few pages comparing with the billion of existing pages. We take this into account to avoid computation of powers of \mathbf{G} or \mathbf{S} . With the same notation as in the previous sections, we have from [10.5], [10.3] and $p_{(k-1)}^T \mathbf{e} = 1$ for all k, we get

$$p_{(k)}^{T} = p_{(k-1)}^{T} \mathbf{G} = p_{(k-1)}^{T} \left(\alpha \mathbf{S} + (1 - \alpha) \frac{\mathbf{J}}{n} \right)$$

$$= \alpha p_{(k-1)}^{T} \mathbf{S} + (1 - \alpha) \frac{\mathbf{e}^{T}}{n}$$

$$= \alpha p_{(k-1)}^{T} \left(\mathbf{H} + \mathbf{a} \frac{\mathbf{e}^{T}}{n} \right) + (1 - \alpha) \frac{\mathbf{e}^{T}}{n}$$

$$= \alpha p_{(k-1)}^{T} \mathbf{H} + \left(\alpha p_{(k-1)}^{T} \mathbf{a} + (1 - \alpha) \right) \frac{\mathbf{e}^{T}}{n}$$

where

$$\mathbf{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

is such that $a_i = 1$ if $\deg^+(i) = 0$ and $a_i = 0$ if $\deg^+(i) > 0$.

Thus, one iteration only requires a single vector-matrix multiplication $p_{(k-1)}^T \mathbf{H}$ with \mathbf{H} extremely sparse (which is much better than the multiplication of two matrices). Hopefully, the matrices \mathbf{S} and \mathbf{G} are not needed. Thus, Google does not even build these two matrices. We only need the vector \mathbf{a} of dimension n. For a deeper discussion, see [LAN 06, p. 40–43].

10.4. Probabilistic interpretation

We can also give a probabilistic interpretation of the PageRank. Indeed, stochastic matrices are also called Markov matrices. In this setting, the solution vector Π is sometimes called the *stationary vector*. We can interpret the positive quantity \mathbf{G}_{ij} as the probability that a surfer on page i has to go in

one step to page j. The model is such that, most of the time, i.e. $\alpha=85\%$ of the time, he/she randomly and uniformly chooses one of the links existing on page i. Otherwise, $1-\alpha=15\%$ of the time, he/she randomly and uniformly goes on any Webpage.

How can we interpret powers of G? If you remember theorem 8.17, about powers of the adjacency matrix of a graph counting paths, then $[G^k]_{ij}$ is the probability of a surfer on page i to end up on page j in k steps. Thus $\lim_{k\to+\infty}G^k$ gives a limiting behavior: in the long run, we have that π_j is the probability of a surfer being on page j (whatever was the origin). Otherwise stated, π_j is the average time spent on page j, when a surfer goes forever from page to page randomly choosing a new page with respect to the distribution of probability encoded by G.

10.5. Dependence on the parameter α

We refer the reader to [LAN 06, Chapter 6] where several results are discussed (taking the derivative of Π with respect to α). We take verbatim their concluding remark: "Larger values of α give more weight to the true link structure of the Web while smaller values of α increase the influence of the artificial probability⁸ vector \mathbf{v}^T . Because the PageRank concept is predicated on trying to take advantage of the Web's link structure, it's more desirable to choose α close to 1. But this is where PageRank become most sensitive, so moderation is necessary — it has been reported that Google uses $\alpha \sim .85$."

We mention only a few recent references (hundreds of entries can be found on MathSciNet). For generalization to undirected graphs, see [GRO 15]. For applications of PageRank techniques to other domains, see [GLE 15, LON 15, CHU 14]. For PageRank in a game-theoretic setting, see [AVI 11]. For a system and control point of view, see [ISH 14]. For computational issues, we mention [DAS 15, GU 15, CSÁ 14, LOF 14].

The survey papers [LAN 05] and [BIA 05] give also quick information on issues (stability, critical parameters) and solutions associated with PageRank.

⁸ See remark 10.10.

10.6. Comments

Now that you have read this chapter, do you think that it is useful to create thousands of new fresh pages (with a null score) pointing to your personal Website? Will it increase the PageRank of that particular Webpage?

Observe that the ranking that we have computed does not depend on the content of the Webpages but only on the structure of the Web (links between pages). When a user makes a query, we just have to extract, from the global ranking, the pages relevant with the given keywords. For instance, we have ranked Belgian soccer teams from the total number of games played between the teams. From that ranking, we can effortlessly extract two subrankings for the teams in Wallonia and Flanders, respectively, but keeping the scores computed globally.

As said at the beginning of this chapter, Google does not follow blindly the ranking computed with the PageRank. Not only are other parameters are taken into account but also independent pages may be conveniently added. For instance, it could be relevant to include Wikipedia pages or news feed (whatever is the associated score) because it could help the user. Also, the ranking can be tweaked to include pay-per-click advertisements to maximize the revenue of the SE.

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