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Hamiltonian Cycle Problem and Markov Chains

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Hamiltonian Cycle Problem and Markov Chains

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To the new generation of mathematicians from developing countries who will, undoubtedly, have a profound influence on the discipline in the coming decades.

Preface

Graphs and networks have been studied extensively in recent decades by mathematicians, computer scientists, engineers, operations researchers as well as physicists, biologists, chemists, and even linguists and sociologists. Their two key elements, vertices and edges, are extremely useful as representations of a wide spectrum of phenomena ranging from transportation networks, through topology of atoms to social networks. Furthermore, many problems modelled with graphs and networks naturally lend themselves to algorithmic analysis and ultimate solutions with the help of modern high-speed computers. The shortest path, maximal spanning tree and max-flow/min-cut problems are just three examples out of a large collection of well-solved important problems.

Nonetheless, there is also a large collection of graph theoretic and network optimisation problems that are fundamentally difficult in the sense of belonging to the very challenging computational complexity classes such as the NP-complete and NP-hard classes. Indeed, the famous Hamiltonian cycle problem (HCP) is known to be NP-complete. The now extensive body of research into the HCP was, perhaps, stimulated by investigations of interesting instances of that problem by great mathematicians such as Euler in the 18th and Hamilton in the 19th century, respectively.

The essence of the Hamiltonian cycle problem is contained in the following—deceptively simple—single sentence statement:

Given a graph, find a cycle that passes through every single vertex exactly once, or determine that this cannot be achieved.

Such a cycle is called a Hamiltonian cycle. The HCP has become a challenge that attracts mathematical minds both in its own right and because of its close relationship to the famous travelling salesman problem (TSP), that calls for the identification of a Hamiltonian cycle with the lowest cost possible in a graph where every edge has a known cost associated with "travelling" along

that edge. An efficient solution of the TSP would have an enormous impact in operations research, optimisation and computer science. However, from a mathematical perspective, the underlying difficulty of the TSP is, perhaps, hidden in the Hamiltonian cycle problem. Hence, in this monograph, we focus on the Hamiltonian cycle problem.

Arguably, the inherent difficulty of many problems in graph theory and combinatorial optimisation stems, precisely, from the discrete nature of the domains in which these problems are posed. Consequently, this monograph is devoted to a line of research that maps such problems into convex domains where continuum analysis can be easily carried out. This convexification of domains is achieved by assigning probabilistic interpretation to the key elements of the original problems even though these problems are deterministic.

While there are other instances of similar ideas being exploited elsewhere, our approach builds on the innovation introduced in Filar and Krass [49] where the Hamiltonian cycle problem and the travelling salesman problem are embedded in a structured singularly perturbed Markov decision process (MDP). The unifying idea of [49] is to interpret subgraphs traced out by deterministic policies (including Hamiltonian cycles, if any) as extreme points of a convex polyhedron in a space filled with randomised policies.

This approach was continued by Chen and Filar [22] and, independently, by Feinberg and Shwartz [46] and Feinberg [44]. Further results were obtained by Filar and Liu [51], Andramonov *et al.* [4], Filar and Lasserre [50], Ejov *et al.* [30]–[38] and Borkar *et al.* [17]–[18]. In addition, three recent (but not readily accessible) PhD theses by Nguyen [81], Haythorpe [62] and Eshragh [41] contain some of the most recent results. Thus, there is now an active group of researchers in various countries interested in this approach to discrete problems. Majority of these contributions focused on the classical Hamiltonian cycle problem, but in principle many of the techniques used could be adapted to other problems of discrete mathematics (as, indeed, was done by Feinberg [45]).

To indicate the flavour of the results reported in the present monograph, consider a key observation that led to the recent results presented in Borkar *et al.* [17] and [18]: the "natural" convex domain where Hamiltonian cycles should be sought is the set of doubly stochastic matrices induced by a given graph. This observation is nearly obvious, once we recall the famous Birkhoff-von Neumann theorem, which states that the set of all $N \times N$ doubly stochastic matrices is the convex hull of permutation matrices. Of course, in searching for a Hamiltonian cycle of a given graph, we need to restrict ourselves to the convex hull of only those permutation matrices that correspond to subgraphs of that graph. Results in Chapter 3 (based on Borkar *et al.* [17] and [18]) imply, that after a suitable perturbation and defining the random

variable τ_1 to be the first hitting time of the home vertex 1 (after time 0), the Hamiltonian cycle problem essentially reduces to "merely" minimising the variance-like functional $\mathbb{E}[(\tau_1 - N)^2]$ over the space of doubly stochastic matrices. This probabilistic, almost statistical, interpretation enables us to exploit a wide range of both analytical and algorithmic tools on the HCP.

More generally, this monograph summarises results of both theoretical and algorithmic investigations. The theoretical aim of this line of research is to explain the essential difficulty of the Hamiltonian cycle problem in analytic terms such as a measure of variability, or the size of a gap between certain optimisation problems, or by the nature of certain singularities. The algorithmic aim of the approach is to construct either exact or heuristic methods to obtain numerical solutions of the HCP. It is based on the belief that some classical "static" optimisation problems can be well analysed by embedding them in suitably constructed Markov decision processes.

In our setting, the theoretical and algorithmic aims are not separate. Indeed, results on one aim seem to influence progress on the other. For instance, the optimisation algorithms presented in Chapters 7 and 8 follow directly from the theoretical developments presented in Chapters 3–5 and have identified difficulties that some of the theoretical developments reported in Chapters 6, 9 and 10 are trying to resolve.

The general approach constitutes one of the few instances where probabilistic, continuous optimisation and dynamic control methods are combined to deal with a hard problem of discrete mathematics. Arguably, simulated annealing could be seen as a precursor of this approach. However, it should be mentioned that relationships between Markov chains and graphs are also of recent interest to other researchers, notably Aldous and Fill [2] and Hunter [67].

Next we shall, briefly, differentiate between our approach and some of the best known, well established, approaches to the HCP. We first note that the present line of research is essentially different from that adopted in the study of *random graphs*, where an underlying random mechanism is used to generate a graph (see, for example, Karp's seminal paper [69]). In our approach, the graph to be studied is given and fixed but a *controller* can choose edges according to a probability distribution, and with a small probability (due to a perturbation) an edge may take you to a vertex. Random graphs have played an important role in the study of Hamiltonicity, a striking result to quote is that of Robinson and Wormald [92] who show that *with high probability* k-regular graphs are Hamiltonian, for $k \geq 3$.

Typical general purpose heuristic algorithms can perhaps be classified—we cite only few representative papers—as *rotational transformation* algorithms (Posa [86]), *cycle extension* algorithms (Bollobas *et al.* [13]), *long path* algo-

rithms (Kocay and Li [71]), *low degree vertices* algorithms (Broder *et al.* [20] and Brunacci [21]), *multipath search* or *pruning* algorithms (Christofides [23]). Of course, much research has been done on algorithms for finding a Hamiltonian cycle on various restricted graph classes (see, for example, Parberry [84]). Clearly, algorithms designed for particular classes of graphs tend to outperform the best general purpose algorithms when applied to graphs from these classes.

In the operations research and optimisation communities, many of the successful, now classical, approaches to the HCP and TSP focus on solving a linear programming relaxation followed by heuristics that prevent the formation of sub-cycles (see, for example, Lawler *et al.* [76]). In the present approach, we embed a given graph in a singularly perturbed MDP in such a way that we can identify Hamiltonian cycles with irreducible Markov chains and sub-cycles with non-exhaustive ergodic classes. This permits a search for a Hamiltonian cycle in either (i) the policy space of an MDP, or (ii) the space of the occupational measures of the MDP that is a polytope with a non-empty interior. In both cases, the original discrete optimisation problem is converted to a continuous one. The Branch and Fix, Wedged-MIP and Cross-Entropy heuristics reported in Chapters 7 and 8 can be seen as belonging to (ii), as they all exploit properties of the spaces of occupational measures. They are performing competitively with alternative—general purpose—algorithms on various test problems including the Knight's Tour problem on chessboards of the size up to 32×32. The Interior Point heuristic discussed in Chapter 8 belongs to (i) and should be properly seen as being still under development. However, it opens up promising opportunities for a lot of further research, as it exploits numerically attractive algebraic factorisation properties of irreducible generator matrices of Markov chains.

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This survey summarises a line of research initiated in 1985 when the third author proposed a stochastic approach to the Hamiltonian cycle problem as a thesis topic for his former PhD student, Dmitry Krass. Since then investigations continued, albeit with numerous interruptions, but with important contributions from many collaborators, colleagues and research students. The authors gratefully acknowledge invaluable assistance and insights gained from collaboration or merely from discussions with Michael Andramonov, Konstantine Avrachenkov, Pouya Baniasadi, Ming Chen, Eric Denardo, Eugene Feinberg, Jacek Gondzio, Arie Hordijk, Lodewijk Kallenberg, Jean-Bernard Lasserre, Ke Liu, Nelly Litvak, Stephen Lucas, Wayne Lobb, Walter Murray, Kien Ming Ng, Jessica Nelson, Minh Nguyen, Panos Pardalos, Ulrich Rieder, Serguei Rossomakhine, the late Alex Rubinov, Floske Spieksma, Peter G. Taylor, Jane Thredgold and Peter Zograf.

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Contents

Part I
Motivating Phenomena

Chapter 1
Illustrative Graphs

1.1 The Graph That Started It All

Sir William Rowan Hamilton (1805–1865) was a famous mathematician and physicist, well-known for his vast contribution in various fields such as optics, classical mechanics and algebra. However, it is a lesser known fact that Sir William was the inventor of a commercial game, the mathematically generalised version of which later became one of the most difficult graph theoretic problems. Towards the end of his life, in 1857, Sir William Rowan Hamilton designed a game called *Icosian*. Its name derived from a Greek word *Icosa*, meaning twenty, the Icosian Game featured twenty connected cities, each represented by a hole on a wooden pegboard. Deceptively simple, the player was to visit every city exactly once and return to where he or she started. If we represent each city in this game by a vertex and each connection between two cities by an edge, then the resulting map of cities in the Icosian game is the Dodecahedron graph (Figure 1.1).

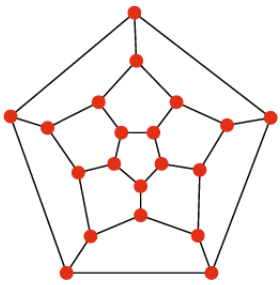

Fig. 1.1: The dodecahedral graph [102], which represents the city map of Icosian game, is the planar projection of a dodecahedron (a polyhedron with twelve faces)

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A mathematically generalised version of the Icosian game, the *Hamiltonian cycle problem* (HCP) can be succinctly stated as:

Given a graph, find a cycle that passes through every single vertex exactly once, or determine that this cannot be achieved.

Such a cycle is called a *Hamiltonian cycle* (HC). A graph is said to be *Hamiltonian* if it possesses at least one Hamiltonian cycle, and is otherwise *non-Hamiltonian*. There might be, and usually are, multiple Hamiltonian cycles in a Hamiltonian graph. The dodecahedron graph is Hamiltonian and has multiple Hamiltonian cycles. The property of a graph possessing a Hamiltonian cycle is called *Hamiltonicity*.

In 1859, Sir William sold the game to an Irish toy manufacturer for 25 British pounds, approximately equivalent to today's 2770 US dollars. The Icosian game was later commercially distributed as the *Traveller's Dodecahedron*. In 2000, the Clay Mathematics Institute announced their list of seven *Prize Problems*, and offered a one million US dollar prize for a solution to each problem. One listed problem is the long-standing question on the relationship between two complexity classes P and NP (see Cook [26] for the formal problem description), an answer to which can be found by determining whether there exists a polynomial-time algorithm to solve the Hamiltonian cycle problem.

In the even better known travelling salesman problem, where we assign a cost for each edge in a given graph, the objective is essentially to determine *which* Hamiltonian cycle on the graph is the most cost-efficient. Thus, the Hamiltonian cycle problem is a special case of the travelling salesman problem, and both are computationally difficult to solve. An efficient solution to the Hamiltonian cycle problem would help solve the travelling salesman problem effectively, and therefore would have a great impact in various fields such as computer science, operations research and cryptology.

1.2 A Sample of Distinctive Graphs

A simple indication of the complexity of the Hamiltonian cycle problem is, that it is not easy to determine whether or not a graph is Hamiltonian by inspection even for small-sized problems. For example, it might take several minutes for a person to determine whether the famous 10-vertex Petersen graph (Figure 1.2) is Hamiltonian. A larger, but still reasonably small in terms of computer science instances, problem that has challenged many HCP algorithms is the 96-vertex Horton graph (Figure 1.3). In both graphs, there is no Hamiltonian cycle.

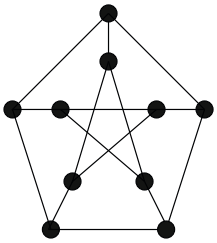

Fig. 1.2: Petersen graph

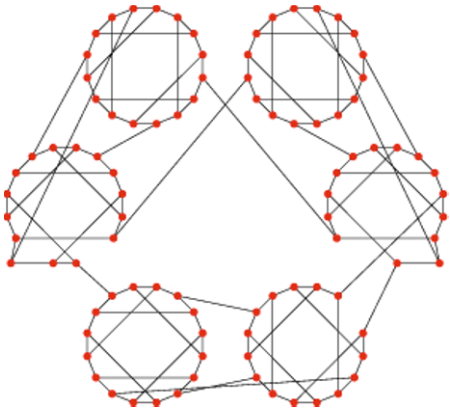

Fig. 1.3: Horton graph [103]

The dodecahedral graph, the Petersen graph and the Horton graph are all *cubic* graphs. A graph is *cubic* or *3-regular* if every vertex in the graph is connected to exactly three other vertices. In general, a graph is *k-regular* if every vertex in the graph is connected to exactly k other vertices. Despite this regularity constraint which seemingly simplifies things, the Hamiltonian cycle problem when restricted to cubic graphs retains its full complexity and hence remains NP-complete [53]. Consequently, cubic graphs are one of the simplest classes of graphs frequently chosen for analysis, in regards not only to the Hamiltonian cycle problem but also to many other graph theoretic problems [57].

In Figure 1.4, we list all 19 connected 10-vertex cubic graphs, 17 of which are Hamiltonian and two are non-Hamiltonian, including the Petersen graph. We enumerate these graphs using the graph-generating GENREG software (Meringer [79]). For the Hamiltonian 10-vertex cubic graphs (numbered 2 to 18), all vertices are drawn in a circle to highlight the Hamiltonicity of these graphs. Indeed, each of these Hamiltonian graphs has at least one Hamilto-

nian cycle that is the circle circumscribing the graph. However, both non-Hamiltonian graphs (numbered 1 and 19) are drawn with a different vertex arrangement. This diagrammatic version of the first graph highlights a *bridge* connecting two subgraphs, consequently indicating the lack of Hamiltonian cycles in the graph.

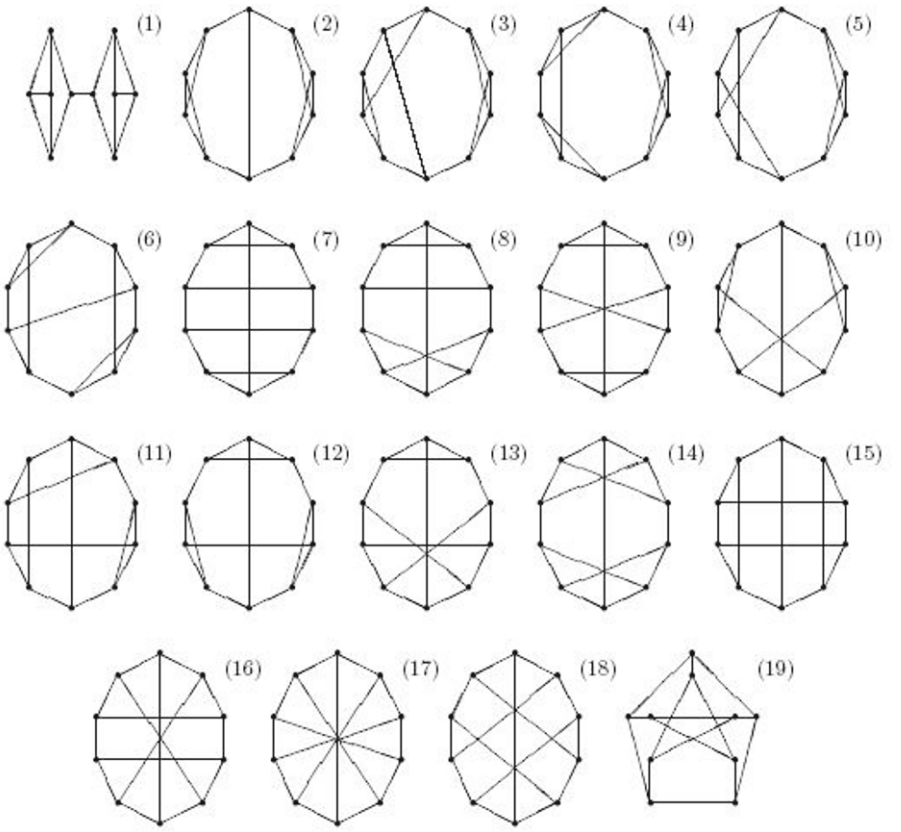

Fig. 1.4: All 19 connected 10-vertex cubic graphs

For any given graph, there are many different graphical representations. A *planar* graph is a graph that can be drawn in the plane in such a way that its edges intersect only at the vertices. A *nonplanar* graph is a graph that is not planar. Garey *et al.* [53] show that, even when restricted to planar cubic graphs, the Hamiltonian cycle problem is NP-complete.

In addition to the quest for finding an efficient algorithm to solve the Hamil-

tonian cycle problem for generic graphs, a lot of focus is on determining whether classes of graphs with certain properties are always Hamiltonian. Before stating a famous conjecture on a particular class of graphs, we need to introduce a few definitions. A graph is *bipartite* if its set of vertices can be divided in two disjoint subsets such that no pair of vertices in the same subset are connected to each other. In general, a graph is *k-partite* if its set of vertices can be divided into k disjoint subsets such that no two pair of vertices in same subset are connected to each other. A graph is *k-connected* if it remains connected after we remove any set of $k-1$ vertices from the graph. Of course, a cubic graph can be at most 3-connected, since removing the three vertices adjacent to any vertex isolates it.

Among the aforementioned graphs, the dodecahedral graph is planar and 3-connected; the Petersen graph is nonplanar, 3-partite and 3-connected; the Horton graph is nonplanar, bipartite and 3-connected. Out of 19 connected 10-vertex cubic graphs in Figure 1.4, only the graph numbered 1 is 1-connected, as the removal of either vertex at the endpoints of the bridge disconnects the graph, and this graph is non-Hamiltonian. In fact, it was shown almost a century ago that every 1-connected graph is non-Hamiltonian [72]. It is easy to verify that 1-connected graphs can be detected in polynomial time.

A famous, long-standing and still open conjecture on Hamiltonicity of graphs is the following conjecture, which relates Hamiltonicity to connectivity, regularity and planarity.

Conjecture 1.1. ***Barnette's Conjecture*** [100]. *Every 3-connected bipartite cubic planar graph is Hamiltonian.*

1.3 Co-spectral Graphs

A common way to represent a graph with N vertices is using an $N \times N$ *adjacency matrix*, of which the (i,j)th entry is 1 if edge (i,j) is present in the graph and 0 otherwise. Two graphs are *co-spectral* if their adjacency matrices share the same set of eigenvalues. In various texts, associated with a graph eigenvalues could also be the *Laplacian matrix* or the *normalised Laplacian matrix* of the graph (see Chapter 2 for precise definitions of these matrices).

Consider two graphs G and H, and let $V(G)$ and $V(H)$ be the sets of vertices, and $E(G)$ and $E(H)$ be the sets of edges in G and H, respectively. For brevity, we drop the dependency on graphs and simply write E and V when no confusion can arise. The graphs G and H *isomorphic* if there exists a bijection $f : V(G) \mapsto V(H)$ such that for every edge $(u,v) \in E(G)$, the edge $(f(u), f(v)) \in E(H)$. They are *non-isomorphic* otherwise. An automorphism

of a graph G is an *isomorphism* of G with itself. Isomorphic graphs are co-spectral. Cvetkovic [27] shows that there exist non-isomorphic graphs that are co-spectral, and van Dam and Haemers [28] discuss the types of graphs that are uniquely determined by their spectrum. More directly related to the Hamiltonian cycle problem, Filar *et al.* [47] construct two 20-vertex cubic, isomorphic and co-spectral graphs, one of which is Hamiltonian and the other non-Hamiltonian.

This indicates that we cannot rely on the spectrum of a graph alone to determine whether the graph is Hamiltonian or not. However, the eigenvalues and consequently the determinant of the adjacency matrix of a graph still contain a lot of useful insights that could help us with determining Hamiltonicity. For example, in an N-vertex Hamiltonian graph, it is well-known that the characteristic polynomial of an adjacency matrix of a subgraph corresponding to any Hamiltonian cycle on the graph is $\lambda^N - 1$. Moreover, Ejov *et al.* [32] show that, for a given N-vertex Hamiltonian graph, any Hamiltonian cycle is equivalent to a solution of the following system of polynomial equations:

$$\begin{aligned} x_{ij}(1 - x_{ij}) &= 0 \quad \text{for all } (i,j) \in E, \\ \sum_j x_{ij} - 1 &= 0 \quad \text{for all } i \in V, \\ \sum_i x_{ij} - 1 &= 0 \quad \text{for all } j \in V, \\ \det(\lambda \mathbf{I} - \mathbf{X}) - \lambda^N + 1 &= 0, \end{aligned}$$

where $\det \mathbf{A}$ denotes the determinant of a matrix $\mathbf{A}$, $\mathbf{I}$ is an $N \times N$ identity matrix, and $\mathbf{X}$ is the *modified adjacency matrix*, defined to be the adjacency matrix with every non-zero (i,j)th entry replaced by the variable x_{ij}, for all $i, j \in V$.

In Chapter 2, we discuss a few motivating numerical observations about eigenvalues and determinants of subgraphs that lead to theoretical results presented in the subsequent chapters.

Chapter 2
Intriguing Properties

2.1 Preliminaries and Notation

In this book, all graphs are connected and undirected, unless otherwise stated. We follow the graph terminology and conventions from Harary [59], where the reader can find an excellent introduction to graph theory. Consider a graph $G = (V(G), E(G)) = (V, E)$, where V is the set of vertices of G, $|V| = N$, and E is the set of edges of G. A graph with N vertices is said to be a graph of *order* N. As the graph G is undirected, for every edge $(i, j) \in E$ there exists an opposite edge $(j, i) \in E$, where $i \neq j$. A *loop* is an edge (i, i) joining a vertex to itself. We do not consider *multi-edges*, which are distinct edges that connect the same pair of vertices, and we use the terms *edge* and *arc* interchangeably.

Subgraphs and Regularity Consider a graph G', and let $V(G')$ be the set of its vertices and $E(G')$ be the set of its edges. Then G' is a *subgraph* of G if $V(G') \subseteq V(G)$ and $E(G') \subseteq E(G)$. A subgraph G' is a *spanning subgraph* if $V(G') = V(G)$. From now on, the term *subgraph* refers to a spanning subgraph, unless otherwise stated. A vertex j is a *neighbour* of i, or vertex j is *adjacent* to i, if there exists an edge between them, that is, $(i, j) \in E(G)$. A vertex v has a *degree* d if it has d neighbours, and we write $\deg(v) = d$. A graph is *k-regular* if every vertex $i \in V$ has the same degree k, and a *cubic* graph is a 3-regular graph.

Walks, Paths and Cycles A *walk* is a sequence of vertices $(v_0, v_1, \ldots, v_n)$ where each edge $(v_i, v_{i+1}) \in E$ for $i = 0, \ldots, n-1$. A walk is said to be *closed* if $v_0 = v_n$, and *open* otherwise. A walk is a *path* if all vertices in the sequence are distinct, that is, $v_i \neq v_j$ for all $i \neq j$. A path is a *cycle* if it is closed. The *length* of a walk, a path or a cycle is the number of edges on the walk, the path or the cycle, respectively. The *girth* of a graph is the length of a shortest cycle on the graph, excluding cycles of length two. On the other hand, the

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circumference of a graph is the length of a longest cycle on the graph. The circumference of a Hamiltonian graph of order N is N, as any Hamiltonian cycle is a longest cycle of the graph.

Example 2.1 *We give examples of an open walk (Figure 2.1), an open path (Figure 2.2) and a cycle (Figure 2.3).*

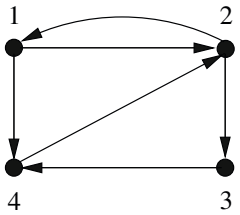

Fig. 2.1: An open walk $(1, 2, 3, 4, 2, 1, 4)$

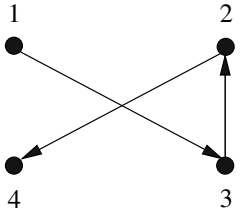

Fig. 2.2: An open path $(1, 3, 2, 4)$

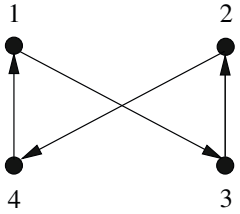

Fig. 2.3: A cycle $(1, 3, 2, 4, 1)$

Adjacency Matrices The *adjacency matrix* $\mathbf{A} = [a_{ij}]$ of a graph G has elements

$$a_{ij} = \begin{cases} 1 & \text{for } (i,j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$