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* algorithms (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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http://www.springer.com/978-1-4614-3231-9

Hamiltonian Cycle Problem and Markov Chains
Borkar, V.S.; Ejov, V.; Filar, J.A.; Nguyen, G.T.
2012, XIV, 202 p., Hardcover
ISBN: 978-1-4614-3231-9