

DETECTING NON-HAMILTONIAN GRAPHS
BY IMPROVED LINEAR PROGRAMS AND
GRAPH REDUCTIONS

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Doctor of Philosophy

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To my mother Gina for her immeasurable support.

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Summary

In this thesis, we continue a recent line of research that seeks to solve the Hamiltonian cycle problem (HCP). In particular, the research is aimed at providing certificates of non-Hamiltonicity. The approaches described fall broadly into two categories. First, we can detect non-Hamiltonicity by formulating HCP as a linearly-constrained integer program, and subsequently relaxing it to a linear program (LP). Infeasibility of such an LP implies non-Hamiltonicity. Second, we can attempt to identify edges or vertices that can be removed from a graph without altering its Hamiltonicity, resulting in a reduced graph which may be easier to solve. In order to test the effectiveness of our approaches, we will consider all non-Hamiltonian non-bridge cubic graphs with up to 20 vertices, the set of which we call NHNB20.

Following an introduction of the relevant background in Chapter 1, in Chapter 2 we consider several notable formulations of HCP, and compare their effectiveness on NHNB20. In Section 2.1 we introduce four LP models from literature to which we assign the names MCF, MCF+, SST, and the Base Model. In Section 2.2.2 we find that the first three of these models are similarly effective, solving 399 out of the 2099 instances of NHNB20. The Base Model is found to be somewhat more effective, solving 477 out of the 2099 instances. To achieve a finer comparison, in Section 2.2.5, we consider these four models in the context of the travelling salesman problem (TSP), a problem closely related to HCP. We introduce Algorithm 2.1, a technique for producing small but difficult instances of TSP, and use this technique to

produce two TSP problem sets which we call ATSP16A and ATSP16AC. In Section 2.2.5 we report on experiments on these TSP problem sets, which indicate that the Base Model is the strongest of the considered models on average. Based on the empirical evidence, in Section 2.2.6, we conjecture that the Base Model is stronger than MCF and MCF+, and provide a partial proof of this conjecture. Next, in Section 2.3, we consider classifications of the non-Hamiltonian graphs that are not identified by these methods. Notably, in Section 2.3.2 we consider non-tough graphs, and prove that MCF, MCF+ and SST are infeasible for any non-tough graph. We conjecture that the same result holds for the Base Model. The problem sets considered in Chapter 2, and in the remainder of the thesis, are given in Appendices A and B.

In Chapter 3, we develop a framework for reducing a given graph without altering its Hamiltonicity. In Section 3.1 we consider particular subgraphs that, if present in a graph, may be replaced by a vertex. Next, in Section 3.2 we examine the effect of forced edges on a graph, and use this to identify other edges that may be removed. Then, in Section 3.3 we consider the automorphism group of a graph, and use this information about the symmetries of the graph to identify redundant edges that are not otherwise obvious. Combining these approaches, in Section 3.5 we introduce Algorithm 3.1 to search for applicable reductions and show, in Section 3.6, that the algorithm successfully reduces many of the graphs in NHNB20 to trivial instances of HCP. Of those graphs in NHNB20 not reduced to a trivial graph, a majority are at least partially reduced. We also demonstrate that the Base Model is more effective on these partially reduced graphs than on the original graphs. In addition to the pseudocode of Algorithm 3.1 given in Section 3.5, an implementation of the algorithm is presented in Appendix C.

In Chapter 4, we seek to improve upon the Base Model by augmenting it with new constraints that take advantage of particular graph features. First, in Section 4.1, we combine the Base Model with SST by expressing the latter

in the variables of the former. We then extend this model further by taking advantage of the Base Model's built-in capacity to handle different starting vertices. Next, in Sections 4.2 and 4.3, we introduce constraints based on the presence of forced edges, as well as the presence of non-trivial 3-cuts, and show that both of these are very strong constraints in graphs that contain these features. Then, in Section 4.4 we introduce constraints based on an eigenvalue of permutation matrices corresponding to Hamiltonian cycles, and demonstrate that a small improvement results. In Section 4.5 we combine all of these constraints into a single model, which we call Base-Combined. We show that Base-Combined is stronger than taking the best result of any of its constituent models. Finally, in Section 4.6 we introduce a technique, which we call the subgraph method, that uses Base-Combined on a set of subgraphs of a given graph to test necessary conditions for Hamiltonicity of the original graph. We show that this technique is often effective at detecting non-Hamiltonicity.

We conclude in Chapter 5 by considering, in turn, the application of each of the developed approaches, to the 2099 instances of NHNB20, and show that we can now provide certificates of non-Hamiltonicity for 2087 instances. This is significantly more than the 477 instances solved by the unaugmented Base Model. We note that although our focus was often limited to cubic graphs, the approaches considered are applicable to more general HCP instances. The dramatic improvements obtained inspire great hope that further investigations in this direction will constitute a successful line of research. To this end, in Sections 5.2 to 5.4 we outline the most promising future directions arising from this thesis.

Declaration

I certify that this thesis does not incorporate without acknowledgment any material previously submitted for a degree or diploma in any university; and that to the best of my knowledge and belief it does not contain any material previously published or written by another person except where due reference is made in the text.

Kieran Clancy

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Glossary of terms

The following notations are commonly used in this thesis.

$G = (V, E)$	A simple graph with vertices V and edges E
n	The number of vertices $ V $ of a graph G
G_n^k	The cubic graph on n vertices with GENREG ID k
C_n	The cycle graph with n vertices
K_n	The complete graph with n vertices
P_r	The path graph with r edges
S_r	The star graph with r edges
$\Gamma(G)$	The automorphism group of a graph G
$L(G)$	The line graph of G
$N(i)$	The set of vertices adjacent to $i \in V$
$\deg(i)$	The degree of a vertex $i \in V$
uv	The edge with endpoints u and v in V
$u \rightarrow v$	The arc from u to v , using the edge uv
$x_1 \neq \dots \neq x_k$	$x_i \neq x_j$ for all $i \neq j$ in $1, \dots, k$
$\mathcal{O}(f(n))$	A function bounded from above by a constant positive multiple of $f(n)$ for all $n > n_0$ for some n_0
G_S	The subgraph of G induced by the vertices S if $S \subseteq V$, or by the edges S if $S \subseteq E$

The following acronyms are commonly used in this thesis.

ATSP	Asymmetric travelling salesman problem
DFJ	Dantzig, Fulkerson and Johnson formulation/model
HC	Hamiltonian cycle
HCP	Hamiltonian cycle problem
LP	Linear program
MCF	Multi-commodity flow formulation/model
MCF+	Multi-commodity flow, improved formulation/model
NH	Non-Hamiltonian
NHNB	Non-Hamiltonian non-bridge
NP	Nondeterministic polynomial time
SAT	Boolean satisfiability problem
SST	Sherali, Sarin and Tsai ATSP6 formulation/model
TSP	Traveling salesman problem

Archive of problem sets and algorithms

An archive of the most commonly considered problem sets in this thesis, and of a GNU Octave / MATLAB implementation of the graph reduction algorithm Algorithm 3.1, is available for download on the *FHCP Dissertations* page on the Flinders Hamiltonian Cycle Project website:

<http://fhcp.edu.au>.

The two archives are as follows.

- (i) `GraphReduction.zip` contains the GNU Octave / MATLAB implementation of `GRAPHREDUCTION` (Algorithm 3.1), as well as the sub-algorithms Algorithms 3.2 to 3.4.
- (ii) `ProblemSets.zip` contains each instance of the following problem sets.
 - *NHNB20*, introduced in Section 2.2.2.
 - *NHNB20PR*, introduced in Section 3.6.
 - *ATSP16A* and *ATSP16AC*, introduced in Section 2.2.4.

`README` files with further details may be found in the archives. The implementation of the graph reduction algorithm as well as an index of the above problem sets may also be found in Appendices A to C.

Chapter 1

Introduction and background

1.1 Hamiltonian cycle problem

The Hamiltonian cycle problem (HCP) is a famous problem in graph theory that has the following, deceptively simple, definition.

Definition 1.1 (Hamiltonian cycle problem). Given a graph $G = (V, E)$, determine whether any cycle of length $|V|$ exists in G .

Such cycles of length $|V|$ are known as *Hamiltonian cycles*. HCP could thus more succinctly be defined as determining whether a given graph contains a Hamiltonian cycle.

The concept of a Hamiltonian cycle was formalised independently by two authors. While the concept was named after Sir William Rowan Hamilton who posed a single instance of the problem in 1856, in fact it was Kirkman who had written a more general paper on the matter a year prior in 1855 [6]. Unfortunately, this and many of Kirkman's other results were not recognised until much later. Credit is due to Hamilton, however, for having popularised HCP with a board game based on the planar embedding of the dodecahedron, the graph of which is displayed in Figure 1.1 [7].

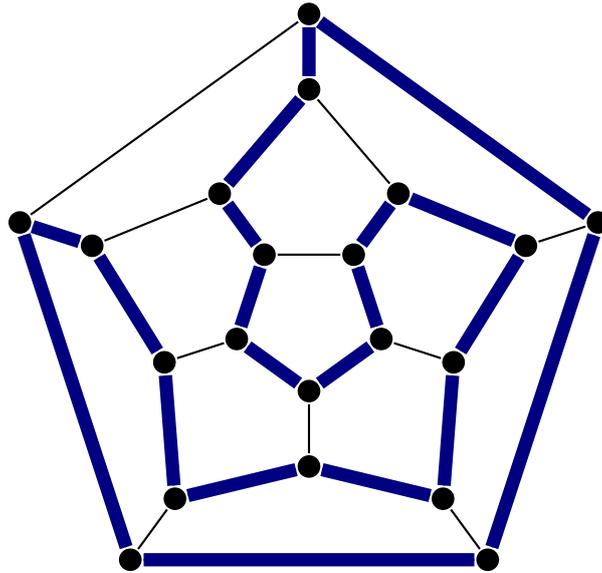


Figure 1.1: An example of a Hamiltonian cycle in the 20 vertex dodecahedral cubic graph.

Although the Hamiltonian cycle problem was not formally defined until the nineteenth century, particular instances of HCP, albeit by other names, had been considered in other contexts for centuries. The most notable of these instances is the problem of finding *knight's tours* on square chessboards. This centuries-old problem involves finding a way for a knight to start on one square of a vacant 8×8 chessboard and visit each of the squares exactly once before returning to the start location, using only valid “L-shaped” moves (1 square in one direction and 2 squares in a perpendicular direction). Euler was fascinated by the problem and in 1766 published several solutions [25], the first of which is shown in Figure 1.2. Solutions to the knight's tour problem correspond directly to Hamiltonian cycles where each square of the chessboard is considered to be a vertex of a graph.

For the most part, however, HCP did not begin to be widely explored until its close relationship with other problems became apparent. In particular, there has been renewed interest in HCP due to its importance in complexity theory. A key set of problems in complexity theory is the set of *decision problems*, which is the set of all problems having a YES or NO answer. Indeed, HCP is a decision problem; the answers can be that YES, the graph contains

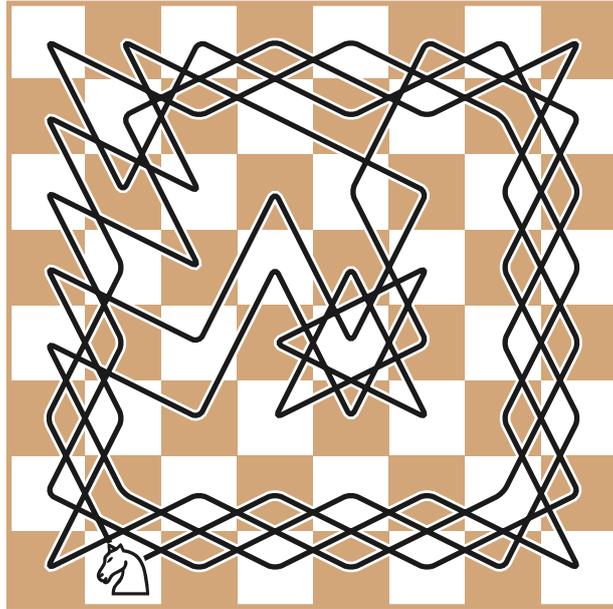


Figure 1.2: The first of Euler's solutions to the knight's tour problem [25].

at least one Hamiltonian cycle, or NO, it does not. A special class of decision problems is the set of *NP* problems defined as follows.

Definition 1.2 (NP problems). A decision problem is said to be in the set of *nondeterministic polynomial time* (NP) problems if for any instance that has the answer YES, it is possible to provide a proof of that answer that can be verified in polynomial time. We call any such proof a *certificate* of that YES answer.

In the case of HCP, a certificate of the answer YES typically takes the form of a discovered Hamiltonian cycle, which can be verified to exist in the given graph in linear time. Note that the definition of NP does not require instances with a NO answer to have any certificate. It is for this very reason that the problem of providing certificates of NO answers for NP problems is a fascinating area of research. For HCP, one approach for providing such a certificate is to establish that a necessary condition for Hamiltonicity is violated by the instance, where this violation can be established by some algorithm that terminates in polynomial time. This thesis considers a number of such necessary conditions and polynomial time algorithms.

We say that an algorithm has *time complexity* $\mathcal{O}(f(n))$ if, for an input of size n , the algorithm is guaranteed to terminate within $\mathcal{O}(f(n))$ time steps of some fixed duration. Notably, an algorithm is said to be *polynomial-time* if it has a time complexity of $\mathcal{O}(n^c)$ for some constant c .

In a seminal paper in 1971, Cook [18] proved that any instance of any problem from NP can be converted to an instance of *boolean satisfiability* (SAT) with only polynomial growth in the size of the instance, implying that, in general, SAT is at least as difficult to solve as any problem from NP. Then, in 1972, Karp [46] investigated a set of twenty NP problems, including HCP, to which SAT can be converted, implying that each of these problems must be at least as difficult as SAT. However, since Cook's result implies that SAT is at least as difficult as any of those problems, the problems considered by Karp are therefore equally difficult in a complexity sense. Problems of this type are called *NP-complete* and are, by definition, the most difficult problems in NP. For more on this fascinating topic, the interested reader is referred to the seminal book by Garey and Johnson [30].

One of the most important open problems in mathematics and computer science is the so-called *P vs NP* problem, which is now famous as one of the Clay Institute Millennium Prize problems [13]. The P vs NP problem asks whether P, the set of decision problems that can be solved in polynomial time, is equal to NP, the set of decision problems for which a certificate exists for every YES answer. Since every NP problem is at most as difficult as a problem in NP-complete, then if a polynomial time algorithm were found to solve any one problem from NP-complete, such as HCP, it would imply the existence of polynomial time algorithms to solve every other problem in NP. It is perhaps this prospect that has prompted much of the research on HCP in recent years. For more history on the P vs NP problem, refer to Cook [17].

In addition to being famous as one of the first discovered NP-complete problems, HCP is also well-known for its close relationship with the *travelling*

salesman problem (TSP). In this problem, a salesman must visit n cities using roads of given distance between pairs of cities, by starting at one city and visiting every other city exactly once before returning, such that the total distance travelled is minimised. The observant reader will notice that HCP is embedded in this problem since a valid travel itinerary necessarily constitutes a Hamiltonian cycle. Formally, the travelling salesman problem can be defined as follows.

Definition 1.3 (Travelling salesman problem). Given a graph $G = (V, E)$ and an associated cost c_{ij} for each arc $i \rightarrow j$ with $i, j \in V$, find a Hamiltonian cycle or *tour*, if one exists, such that the sum of the costs on the arcs used, called the *tour cost*, is minimised. If $c_{ij} = c_{ji}$ for all i and j , then the instance is said to be *symmetric*, otherwise the instance is said to be *asymmetric*. The latter is sometimes distinguished by the abbreviation ATSP.

The travelling salesman problem is a member of the *NP-hard* set of problems, which is the set of problems that are at least as difficult as any problem in NP. Note that although TSP as defined in Definition 1.3 is not a decision problem, there is a decision variant in which the question is whether any Hamiltonian cycles exist that have a tour cost below a given threshold.

There is a myriad of different approaches for solving HCP and TSP. For HCP, these include fast heuristics [2], as well as exhaustive algorithms that find every Hamiltonian cycle in a graph [14]. For HCP and TSP restricted to graphs of certain types there are more efficient algorithms such as [23, 43, 75]. Finally, for TSP in general, there are various approaches, including simulated annealing [49], edge-exchange heuristics [52, 37], and approaches based on relaxations of integer programming formulations [1, 19]. Much of this thesis is focused on linear programming relaxations of integer programming formulations for HCP and TSP. A further discussion of this topic is included in Section 1.3. For more information about the TSP in general, the reader is referred to [50].

The heuristics for solving HCP are often quick to find a Hamiltonian cycle in a Hamiltonian graph, and this Hamiltonian cycle constitutes a certificate that can be efficiently verified. However, for non-Hamiltonian graphs, these algorithms are not able to provide any evidence of that non-Hamiltonicity other than their failure to find a Hamiltonian cycle in a reasonable time. In this thesis, we seek to continue a relatively new line of research, initiated in Haythorpe [36] and continued in Eshragh [24] and Filar et al. [28], aimed at providing certificates of non-Hamiltonicity.

1.2 Graph theory

As this thesis is primarily concerned with the investigation of graphs, we now include a brief introduction of some relevant concepts from graph theory.

Definition 1.4 (Graph). A graph $G = (V, E)$ is defined as a finite set V , called the *vertices* of G , and a set E , called the *edges* of G , where each edge $uv \in E$ is an unordered pair of distinct vertices $u, v \in V$. Two vertices $u, v \in V$ are said to be *adjacent* if the edge $uv \in E$. An edge $uv \in E$ is said to be *incident* to the endpoint vertices u and v . Also, two distinct edges $uv, wx \in E$ are said to be *adjacent* if both are incident to a common vertex.

More general definitions of graphs do exist, for example permitting directed edges (directed graphs) or multiple edges between the same pair of vertices (multigraphs). However, in this thesis we restrict our consideration to *simple, undirected* graphs with finitely many vertices. A graph is said to be *simple* if it contains no loops and no multi-edges; that is, $vv \notin E$ for any v , and E is not a multiset. A graph is said to be *undirected* if its edges are unordered pairs of vertices; that is, uv and vu are considered to be the same edge for any u and v . As given, Definition 1.4 already excludes these possibilities, but we provide this clarification for readers familiar with a more general definition of graphs. Further, unless otherwise stated, all graphs considered in this thesis are *connected*; that is, every pair of vertices in G has

some path of edges in E between them.

We refer to the number of vertices $|V|$ of a graph $G = (V, E)$ as the *order* of G and, where no confusion is possible, denote this simply by n . Although we only consider undirected graphs, in the context of Hamiltonian cycles it is often necessary to consider an edge uv of a graph used in some particular direction; such an ordered pair of vertices is called an *arc*. If u precedes v we denote the arc by $u \rightarrow v$, otherwise, by $v \rightarrow u$.

Since we are primarily interested in graphs from the perspective of HCP, we will mostly consider graphs with relatively few edges. Indeed, graphs with many edges are usually trivial instances of HCP. It is therefore desirable to consider *sparse* graphs. Technically speaking, it is difficult to define whether a given graph is sparse on its own. Rather, a graph must be considered in the context of a family of graphs to which it belongs. One definition is that a graph is sparse if it is contained in a family of graphs satisfying the property that the number of edges is bounded from above by some constant multiple of the number of vertices.

One method of describing a graph is via its *adjacency matrix*, which for a graph $G = (V, E)$ with vertices $V = \{1, \dots, n\}$ is an $n \times n$ matrix containing a 1 in row i and column j if $ij \in E$, and 0 otherwise. Figure 1.3 shows an example of the adjacency matrix of the Petersen graph, a non-Hamiltonian graph famous as a counterexample to many conjectures [40].

We now define some common graph theoretic terms and concepts that will be important throughout this thesis. More specialised concepts will be introduced in later chapters as they arise. For a more detailed introduction to graph theory, the reader is directed to Bondy and Murty [9].

Definition 1.5 (Degree). Given a graph $G = (V, E)$, the *degree* of a vertex $v \in V$, denoted by $\deg(v)$, is defined as the number of vertices adjacent to v .

Definition 1.6 (k -regular graph). A graph $G = (V, E)$ is said to be *k -regular* if every vertex in V has degree k .

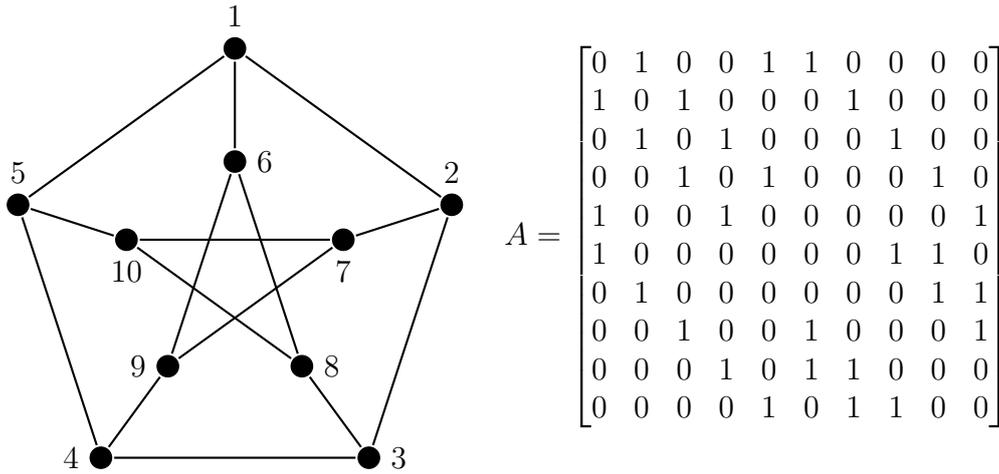


Figure 1.3: The Petersen graph and its corresponding adjacency matrix.

Definition 1.7 (Cubic and subcubic graphs). A graph $G = (V, E)$ is said to be *cubic* if it is 3-regular. G is said to be *subcubic* if no vertex in V has degree greater than 3.

Definition 1.8 (Bipartite graph). A graph $G = (V, E)$ is said to be *bipartite* if there is a partition of V into two subsets V_1 and V_2 such that every edge $e \in E$ is incident to exactly one vertex in V_1 and one vertex in V_2 .

Definition 1.9 (Subgraph). A graph $H = (V', E')$ is said to be a *subgraph* of a graph $G = (V, E)$ if $V' \subseteq V$ and $E' \subseteq E$.

Definition 1.10 (Vertex-induced subgraph). For any graph $G = (V, E)$, and a subset $U \subseteq V$ of its vertices, the subgraph of G *induced* by U is the graph $G_U = (U, E')$, where $E' = \{uv \in E \mid u, v \in U\}$. That is, $G_U = (U, E')$ is the subgraph of G containing only vertices U and any edges that are incident only to vertices in U . The subgraph G_U is called a *vertex-induced subgraph*.

Definition 1.11 (Edge-induced subgraph). For any graph $G = (V, E)$, and a subset $D \subseteq E$ of its edges, the subgraph of G *induced* by D is the graph $G_D = (V', D)$, where $V' = \{v \in V \mid \exists u \in V \text{ such that } uv \in D\}$. That is, $G_D = (V', D)$ is the subgraph of G containing only edges D and the vertices to which those edges are incident. The subgraph G_D is called an *edge-induced subgraph*.

Where no confusion is possible, we will use the term *induced subgraph* to refer to either a vertex-induced subgraph or edge-induced subgraph as the context dictates.

Definition 1.12 (Connected component). Given a graph $G = (V, E)$, a subgraph $H = (V', E')$ of G is said to be a *connected component* of G if H is connected, H is the subgraph of G induced by the vertices V' , and no edge in E is incident to both a vertex in V' and a vertex not in V' .

Definition 1.13 (k -connected graph). A graph $G = (V, E)$ with at least $k + 1$ vertices is said to be *k -connected* if it cannot be disconnected by the removal of $k - 1$ vertices. In other words, at least k vertices must be removed to disconnect the graph or to obtain a 1-vertex graph.

Definition 1.14 (k -edge-connected graph). A graph $G = (V, E)$ with at least $k + 1$ vertices is said to be *k -edge-connected* if it cannot be disconnected by the removal of $k - 1$ edges. In other words, at least k edges must be removed to disconnect the graph.

Definition 1.15 (k -cut). Given a graph $G = (V, E)$, we define a *k -cut* (also known as a *disconnecting set* of size k) to be a subset of k edges from E whose removal disconnects the graph. A k -cut is said to be *minimal* if the removal of no proper subset of the edges in the k -cut leaves the graph disconnected.

Definition 1.16 (Bridge graph). A graph $G = (V, E)$ is called a bridge graph if it contains at least one minimal 1-cut.

Definition 1.17 (Path). A *path* of length k in a graph $G = (V, E)$ is an ordered subset of sequentially adjacent edges $\{v_1v_2, v_2v_3, \dots, v_kv_{k+1}\} \subseteq E$ such that the vertices v_1, \dots, v_{k+1} are all distinct.

Definition 1.18 (Cycle). A *cycle* of length $k \geq 3$ in a graph $G = (V, E)$ is a path of length $k - 1$ with an additional edge that closes the path in G . That is, a cycle is a path $\{v_1v_2, \dots, v_{k-1}v_k\} \subset E$ with the additional edge $v_kv_1 \in E$.

Similarly to individual edges, which we sometimes consider as arcs in a particular direction, there are occasions where we must also consider paths or cycles in a directed sense. That is, we may consider a path or cycle as a sequence of arcs end-to-end $v_1 \rightarrow v_2, v_2 \rightarrow v_3, \dots$, which we abbreviate by $v_1 \rightarrow v_2 \rightarrow v_3 \rightarrow \dots$.

Definition 1.19 (Hamiltonian path). A *Hamiltonian path* in a graph $G = (V, E)$ is a path of length $|V| - 1$; that is, a path that traverses all vertices of V .

Definition 1.20 (Hamiltonian cycle). A *Hamiltonian cycle* (HC) in a graph $G = (V, E)$ is a cycle of length $|V|$; that is, a cycle that traverses all vertices of V .

Definition 1.21 (Graph isomorphism). Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are said to be *isomorphic* if there exists a one-to-one mapping $\varphi : V_1 \rightarrow V_2$ such that for any $u, v \in V_1$, $uv \in E_1$ if and only if $\varphi(u)\varphi(v) \in E_2$. To consider a set of graphs *up to isomorphism* is to consider all pairwise isomorphic graphs in the set as the same element.

We now define some common graph families used in this thesis.

Definition 1.22 (Complete graph K_n). The *complete graph* K_n is the n -vertex graph in which any two distinct vertices are adjacent.

Definition 1.23 (Path graph P_r). A *path graph* $P_r = (V, E)$ is a graph comprising just the vertices and edges to trace out a path of length r . In P_r , $|V| = r + 1$ and $|E| = r$.

Definition 1.24 (Cycle graph C_n). A *cycle graph* $C_n = (V, E)$ is a graph comprising just the vertices and edges to form a cycle of length n . In C_n , $|V| = |E| = n$.

Definition 1.25 (Star graph S_r). A *star graph* $S_r = (V, E)$ is a graph comprising just a central vertex $v \in V$ and r degree-1 vertices each of which is adjacent to v . In S_r , $|V| = r + 1$ and $|E| = r$.

1.2.1 Hamiltonian cycle problem for cubic graphs

If it were necessary to consider all simple connected graphs for HCP, the task would be unmanageable if only due to the astronomical number of possible graphs for a given order n . For example, there are on the order of 10^7 unique simple connected graphs with 10 vertices, 10^{38} with 20 vertices and 10^{98} with 30 vertices [67]. It is a natural question, then, to ask whether we can consider a subset of the problem space for which HCP remains NP-complete.

Fortunately, there are indeed several considerably smaller subsets of simple connected graphs to which HCP may be restricted while retaining NP-completeness. The first paper to show this was by Garey et al. [31] in 1976; they showed that the problem space may be restricted to graphs that are planar, cubic, and 3-connected, with HCP still being NP-complete on this subspace. Since the intersection of these three subsets of simple graphs provides an NP-complete problem space, it follows that HCP restricted just to any one of those individual sets is also NP-complete. Following Garey et al.'s result, many other subsets of the problem space have been found to fulfill this condition, including planar, cubic, 2-connected, bipartite graphs; cubic, 3-connected, bipartite graphs; maximal planar graphs; and 4-connected, 4-regular graphs, as summarised in [38]. Perhaps the most practical subset of these is the set of cubic graphs, which can be identified and enumerated efficiently and have fascinating structural properties. There are also far fewer of them for a given number of vertices n than planar graphs or 3-connected graphs with the same number of vertices, making them ideal for use in computation. Furthermore, it was shown recently that any non-cubic graph can be converted to an equivalent cubic instance of HCP with only linear growth in the order of the problem [22].

Cubic graphs have also been the subject of a number of conjectures, such as the disproved conjectures by Tait [68] and Tutte [69], as well as Bar-

nette's conjecture [3] that every 3-connected, planar, bipartite cubic graph is Hamiltonian, which remains open. There are numerous extremely efficient algorithms for enumerating all cubic graphs satisfying certain properties, such as GENREG [56], Plantri [10], and Snarkhunter [11]. Throughout this thesis, it will often be convenient to refer to particular cubic graphs by the ID number given to them by GENREG. In such a case we will refer to a cubic graph with n vertices and ID k as G_n^k .

In 1992, Robinson and Wormald [64] proved that almost all cubic graphs are Hamiltonian. Later, Filar et al. [27] conjectured that, of the remaining, non-Hamiltonian, cubic graphs, almost all are bridge graphs, and as such can be identified as non-Hamiltonian in linear time. However, there are difficult and interesting examples of non-Hamiltonian cubic graphs. Snarks, which are cubic graphs that are not 3-edge-colourable [62], are perhaps the most well-known of these. The smallest snark is the Petersen graph displayed in Figure 1.3, which was proved to be a minor of every snark [58].

There is a variety of research into HCP restricted to cubic graphs. Currently, one of the state-of-the-art algorithms for solving HCP and TSP on cubic instances, due to Xiao and Nagamochi [75], can solve HCP on cubic graphs in $\mathcal{O}(1.2312^n)$ time. This is significantly better than brute-forcing combinations of vertices, requiring $\mathcal{O}(n!)$ time, and still better than a depth-first search of paths in the graph, requiring $\mathcal{O}(2^n)$ time.

1.3 Linear programming relaxations

One approach to solving HCP or TSP is to formulate the problem as an integer program such that the set of feasible solutions and the set of Hamiltonian cycles is in one-to-one correspondence. Note that if the graph under consideration does not contain any Hamiltonian cycle, then such an integer program will be infeasible. Unfortunately, integer programming is NP-hard,

and as such, difficult to solve. A common technique, then, is to relax the integer requirement to obtain a linear program (LP). Linear programming is a powerful platform for solving many problems and has polynomial-time implementations [48, 45]. The continuation of research into linear programs for HCP and TSP is a key component of this thesis.

Definition 1.26 (Linear program). A *linear program* consists of a set of variables and a set of linear constraints on those variables, which may be equalities or inequalities. A linear program typically also has a linear objective function to be optimised. For example, suppose there are n variables x_1, x_2, \dots, x_n for which we have an objective function

$$\text{Minimise } c_1x_1 + c_2x_2 + \dots + c_nx_n,$$

and which are subject to l inequality constraints and m equality constraints:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &\leq b_1 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n &\leq b_2 \\ &\vdots \\ a_{l1}x_1 + a_{l2}x_2 + \dots + a_{ln}x_n &\leq b_l \\ \\ a_{(l+1)1}x_1 + a_{(l+1)2}x_2 + \dots + a_{(l+1)n}x_n &= b_{l+1} \\ a_{(l+2)1}x_1 + a_{(l+2)2}x_2 + \dots + a_{(l+2)n}x_n &= b_{l+2} \\ &\vdots \\ a_{(l+m)1}x_1 + a_{(l+m)2}x_2 + \dots + a_{(l+m)n}x_n &= b_{l+m}. \end{aligned}$$

If the system of constraints is inconsistent, that is, if there are no feasible solutions, then the linear program is said to be *infeasible*. Otherwise, the LP is said to be *feasible*, and any solution that minimises the objective function is called *optimal*.

Definition 1.27 (Integer program). A *linearly-constrained integer program*, or simply *integer program*, is an extension of a linear program in which some or all of the variables are required to take integer values.

As mentioned earlier, linear programs can arise from relaxing linearly-constrained integer programs by simply replacing the integer requirements with appropriate bounds. For example, if a variable is constrained in the integer program to be 0 or 1, the appropriate relaxation is for it to lie on the interval $[0, 1]$. In such a case, the optimal solution to the relaxed program, provided that one exists, cannot have a higher objective function value than that of the integer program. For this reason, the optimal objective function value for the LP in such a case is called a *lower bound*. The following definition will be used as one of the primary measures of effectiveness throughout this thesis.

Definition 1.28 (Gap). For an integer programming formulation, and its associated linear programming relaxation, the *gap* is defined to be the difference between the lower bound from the linear program and the optimal objective value for the integer program.

If a linear programming relaxation of an integer program has a relatively small gap, then it implies that the relaxation is relatively tight. Throughout this thesis we compare several such relaxations by considering the gaps over a number of instances of TSP. In the case where an integer programming formulation has no feasible solutions, the linear programming relaxation may or may not be infeasible. If the linear program has polynomially many variables and constraints and is infeasible, then this constitutes a polynomial-time certificate that the corresponding integer program has no solution.

Chapter 2

Identifying non-Hamiltonian graphs by linear programming

In this chapter we consider linear programming formulations of TSP and HCP from literature. Three of the considered models, MCF [16], MCF+ [34] and SST [66], were designed to solve the traveling salesman problem (TSP), while the most recent model considered, the Base Model [28], was designed specifically to solve HCP. These four models along with another, equivalent to MCF, will be detailed in Section 2.1.

Each of the aforementioned models, when expressed as integer programs, are exact formulations of HCP and TSP in the sense that the set of each model's feasible points corresponds exactly to the set of Hamiltonian cycles. However, their linear relaxations, which we consider here, may permit feasible solutions outside the convex hull of solutions corresponding to Hamiltonian cycles. Ideally, the feasible region of a relaxed model should be as close an approximation as possible to the convex hull of integer solutions, which in this case correspond to Hamiltonian cycles. Figure 2.1 provides a visualisation of this concept.

In Section 2.2 we compare the performance of the four linear programming models. For comparisons of the models on HCP instances, we first modify the

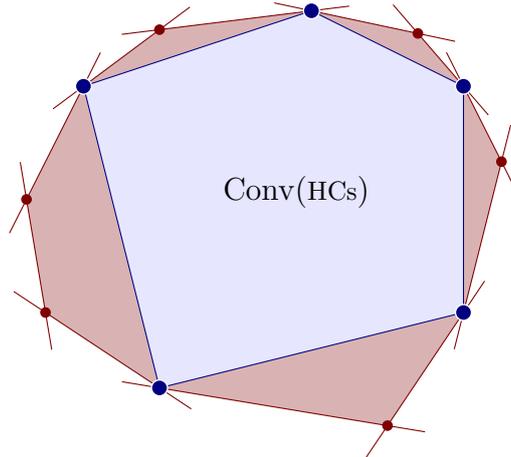


Figure 2.1: A two-dimensional visualisation of the feasible region of a relaxed model for HCP. The desired solutions will be at one of the blue vertices corresponding to Hamiltonian cycles. The light-blue shaded convex hull of these blue vertices represents the feasible region of a theoretical set of ideal linear constraints. Red lines represent the (non-ideal) constraints of the relaxed model.

three TSP models in Section 2.2.1 so that they may be applied directly to non-complete graphs, with infeasibility implying the graph is non-Hamiltonian. We show in Section 2.2.2 that considering only the feasibility of the generated linear programs does not provide a very precise comparison of the models.

To obtain a finer comparison of the models, we seek to also compare the models in a TSP context. To this end, in Section 2.2.3 we augment the Base Model with an appropriate objective function so that it can be used to find lower bounds for TSP instances. Then, in Section 2.2.4, we introduce a new technique for producing instances of TSP based on cubic instances of HCP, and construct two problem sets that will be valuable for comparing models throughout the thesis. Results on these problem sets, presented in Section 2.2.5, will lead naturally to a conjecture in Section 2.2.6 that the Base Model is stronger than both MCF and MCF+. We give a partial proof of this conjecture. It will also be seen that, although the Base Model performs better than SST in the average case, there are some instances for which SST outperforms the Base Model.

In Section 2.3 we will consider the classifications of graphs whose non-Hamiltonicity cannot be identified by this approach and summarise our findings. The results of this section suggest that the considered models are always infeasible for non-tough graphs, which is proved for MCF, MCF+ and SST, and stated as a conjecture for the Base Model.

Finally, in Section 2.4, we outline the approaches we will take in the following chapters to improve upon the detection of non-Hamiltonian graphs currently offered by the Base Model.

2.1 Existing models to solve TSP and HCP

2.1.1 Subtour elimination model and MCF

Some of the earliest models that could be used to solve HCP were based on formulations of the traveling salesman problem (TSP, Definition 1.3).

In a seminal article in 1954, Dantzig et al. formulated TSP as an assignment problem with $\mathcal{O}(2^n)$ linear constraints designed to eliminate subtours [19]. A subtour is where a path prematurely returns to a previously visited vertex rather than completing a cycle of all n vertices in the graph. Figure 2.2 shows an example of two candidate solutions to a TSP instance; the left candidate has a total cost of just 6 but contains subtours, whereas the candidate on the right has a total cost of 8 and is the correct solution. Dantzig et al.'s formulation of TSP may be expressed as:

Definition 2.1 (Dantzig, Fulkerson and Johnson (DFJ) formulation [19]).

Given a graph with vertices $1, \dots, n$ and a cost c_{ij} of using each arc $i \rightarrow j$ for $i, j \in \{1, \dots, n\}$,

$$\text{minimise} \quad \sum_{i=1}^n \sum_{j=1}^n c_{ij} x_{ij},$$

$$\text{subject to } \sum_{j=1}^n x_{ij} = 1 \quad \forall i = 1, \dots, n \quad (2.1)$$

$$\sum_{i=1}^n x_{ij} = 1 \quad \forall j = 1, \dots, n \quad (2.2)$$

$$\sum_{i \in S} \sum_{j \notin S} (x_{ij} + x_{ji}) \geq 2 \quad \forall S \subset V, 0 < |S| < n \quad (2.3)$$

$$x_{ij} \in \{0, 1\} \quad \forall i, j = 1, \dots, n. \quad (2.4)$$

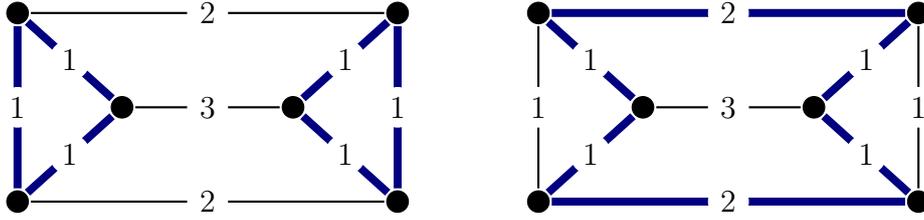


Figure 2.2: An invalid and a valid candidate solution to the same TSP instance. Costs are shown on the edges, and edges used in the path are highlighted in blue.

In the DFJ formulation, x_{ij} is 1 if the arc $i \rightarrow j$ is used in the Hamiltonian cycle, and 0 otherwise. For a binary solution, the LHS of (2.3) counts the number of edges in the cycle connecting a subset S to the rest of the graph. In particular, the x_{ij} terms in the equation count the number of arcs leaving the subset, and the x_{ji} terms count the number of arcs entering the subset. If the solution contains a subtour comprising just the vertices of S , there will not be any arc leaving S and the LHS will be less than 2, violating (2.3). As this constraint is present for every proper subset S , it follows that all subtours are prevented. Figure 2.3 shows an example of a subtour elimination constraint that would prevent the subtour seen in the left side of Figure 2.2. Note that (2.3) may be replaced with constraints counting only the arcs in one direction (for instance, those leaving the subset), so the DFJ constraints are often reported using (2.5) below rather than (2.3):

$$\sum_{i \in S} \sum_{j \notin S} x_{ij} \geq 1 \quad \forall S \subset V, 0 < |S| < n. \quad (2.5)$$

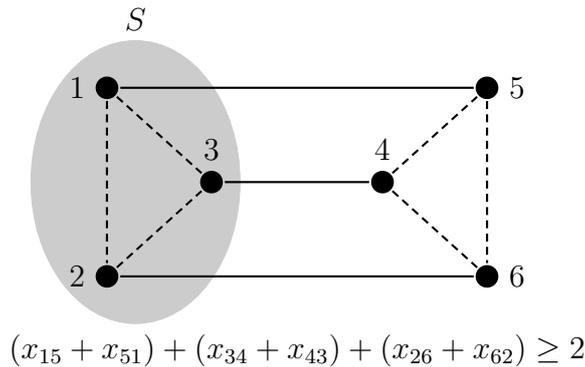


Figure 2.3: Example of a DFJ subtour elimination constraint (2.3) for a graph with vertices and a subset S as labelled. Edges with exactly one endpoint in S are shown in solid black, with other edges of the graph dashed.

Since solving a general integer programming problem, such as the DFJ integer program, is NP-hard, the binary condition (2.4) is typically relaxed so that $x_{ij} \in [0, 1]$ for all $i, j \in \{1, \dots, n\}$. The relaxed version of DFJ is a linear program, and as mentioned in Section 1.3, linear programs can be solved in polynomial time. The downside of relaxing (2.4) is that this may introduce new extreme points (with fractional values) that do not correspond to proper solutions of TSP. Therefore, the relaxed version of DFJ is no longer an exact formulation and will hereafter be referred to as the DFJ *model*. After relaxation, we may think of the x_{ij} variables as being elements of a doubly-stochastic matrix due to (2.1) and (2.2). Then, the well-known Birkhoff–von Neuman Theorem [8] implies that the solution will always correspond to a convex combination of permutation matrices, of which some may, unfortunately, represent subtours.

Even after relaxing the x_{ij} variables, the main barrier to using the DFJ model is that (2.3) comprises an exponential number of constraints; if there are n vertices in the graph, then there are $2^n - 2$ non-empty proper subsets S . This precludes the DFJ model from being used to provide (polynomial

time) certificates of non-Hamiltonicity. For use in practice, Dantzig et al. introduced a heuristic approach in which the model is first solved without any subtour elimination constraints. Then, if a binary solution corresponding to a tour is obtained, that tour is optimal. Otherwise, they identify some subtour elimination constraints that the solution violates, add them to the model, and solve again, iterating until the optimal tour is found.

Many years after the introduction of DFJ, Wong [71] developed an alternative construction of the same subtour elimination model that makes use of some extra variables but has only polynomially many, $\mathcal{O}(n^3)$, constraints. Claus [16] later developed another DFJ-equivalent construction along the same approach but using fewer variables and constraints, though still $\mathcal{O}(n^3)$; a version of this model is given below as the *multi-commodity flow* (MCF) model, where $V = \{1, \dots, n\}$ and $V^* = \{2, \dots, n\}$. The equivalence to DFJ was proved by Padberg and Sung [60].

Definition 2.2 (Multi-commodity flow (MCF) model [16]).

$$\text{Minimise} \quad \sum_{i \in V} \sum_{j \in V} c_{ij} x_{ij}, \quad (2.6)$$

$$\text{subject to} \quad \sum_{j \in V} x_{ij} = 1 \quad \forall i \in V \quad (2.7)$$

$$\sum_{i \in V} x_{ij} = 1 \quad \forall j \in V \quad (2.8)$$

$$\sum_{j \in V} y_{ijk} - \sum_{j \in V} y_{jik} = 0 \quad \forall i, k \in V^*; i \neq k \quad (2.9)$$

$$\sum_{i \in V} y_{ikk} = 1 \quad \forall k \in V^* \quad (2.10)$$

$$\sum_{i \in V^*} y_{1ik} = 1 \quad \forall k \in V^* \quad (2.11)$$

$$\sum_{i \in V} y_{kik} = 0 \quad \forall k \in V^* \quad (2.12)$$

$$0 \leq y_{ijk} \leq x_{ij} \quad \forall i, j \in V; k \in V^* \quad (2.13)$$

$$0 \leq x_{ij} \leq 1 \quad \forall i, j \in V. \quad (2.14)$$

The x_{ij} variables here have precisely the same interpretation as in DFJ, while the y_{ijk} variables can be thought of as tracking the location of a number of packages (or commodities) to be delivered as the Hamiltonian cycle is traversed. Specifically, there are $n - 1$ packages to be delivered, one to every vertex except the first vertex, which is considered to be the depot from which the commodities are dispatched. Then, y_{ijk} is intended to be 1 only if both the arc $i \rightarrow j$ is used in the cycle and the package destined for vertex k is yet to be delivered after leaving vertex i ; otherwise, y_{ijk} is intended to be zero. As the model does not restrict y_{ijk} variables to integer values, it is possible to obtain extreme points with fractional values as in the relaxed DFJ model. MCF and three other models will be compared empirically in Section 2.2.

2.1.2 Tightened multi-commodity flow model

Since the relaxed subtour-elimination models such as DFJ and MCF have extreme points that do not correspond to Hamiltonian cycles, there are many potential improvements to be made through the addition of new linear constraints (see Figure 2.4 for a visualisation). If one can design additional constraints to exclude some of the unwanted points lying outside the convex hull of Hamiltonian cycles, the model will be tighter, often reducing the difference between the solution to the LP and the desired integer solution.

One such improvement to the MCF model was introduced as MCF+ by Gouveia and Pires [34] in 2001. Their approach was to take advantage of a third set of variables, v_{ij} , intended such that v_{ij} will be 1 if vertex j comes later than vertex i in the Hamiltonian cycle, and 0 otherwise. By adding these variables and some linking constraints to MCF, the resulting MCF+ can be shown to be a tighter model. Gouveia and Pires changed the notation slightly by replacing the y_{ijk} variables in MCF with equivalent variables f_{kij} . The variables f_{kij} are intended to be 1 only if both the arc $i \rightarrow j$ is used in the cycle, starting at vertex 1, and the package destined for vertex k has been

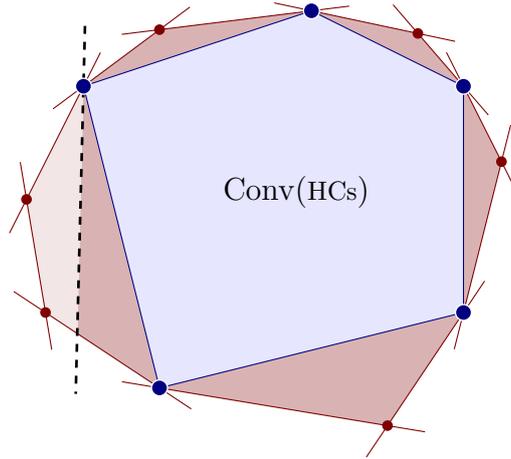


Figure 2.4: A visualisation of the feasible region from Figure 2.1 after adding additional linear constraints to obtain a tighter LP. The additional constraints are represented by a dashed line. The blue vertices corresponding to Hamiltonian cycles are all still contained in the feasible region.

delivered prior to reaching vertex j . Therefore, the linear relation between f_{kij} and the y_{ijk} variables of MCF is given by

$$y_{ijk} = x_{ij} - f_{kij}.$$

Substituting this change of variable into (2.9) – (2.13) and using (2.7), (2.8) and (2.13) for simplification, we arrive at equivalent constraints, to those of MCF, in terms of the new variables:

$$\sum_{j \in V} f_{kji} - \sum_{j \in V} f_{kij} = 0 \quad \forall i, k \in V^*; i \neq k \quad (2.15)$$

$$\sum_{i \in V} f_{kik} = 0 \quad \forall k \in V^* \quad (2.16)$$

$$\sum_{i \in V^*} f_{k1i} = 0 \quad \forall k \in V^* \quad (2.17)$$

$$\sum_{i \in V} f_{kki} = 1 \quad \forall k \in V^* \quad (2.18)$$

$$0 \leq f_{kij} \leq x_{ij} \quad \forall i, j \in V; k \in V^*. \quad (2.19)$$

The extra v_{ij} variables are then added to the model and linked with the f_{kij}

variables through the following constraints:

$$\sum_{j \in V} f_{kij} = v_{ki} \quad \forall i, k \in V^* \quad (2.20)$$

$$x_{ij} + x_{ji} + v_{ki} - v_{kj} \leq 1 \quad \forall i, j, k \in V^*; k \neq i, j \quad (2.21)$$

$$0 \leq v_{ij} \leq 1 \quad \forall i, j \in V^*. \quad (2.22)$$

We remark that the v_{ij} variables are more of a notational convenience, as they may be expressed as linear combinations of the f_{kij} variables via (2.20).

Definition 2.3 (MCF+ model [34]). Minimise the objective function (2.6) subject to (2.7), (2.8) and (2.14) – (2.22).

The key addition in MCF+ are the $\mathcal{O}(n^3)$ constraints of (2.21) which may be interpreted in the following way: Considering the case where the x variables are integers, the edge ij may be used in one direction ($x_{ij} = 1$), in the other direction ($x_{ji} = 1$), or not used at all ($x_{ij} = x_{ji} = 0$). In the last case, (2.21) becomes $v_{ki} - v_{kj} \leq 1$, which is redundant due to (2.22). However, in the first and second cases, $x_{ij} + x_{ji} = 1$ and so (2.21) becomes $v_{ki} - v_{kj} \leq 0$. Given there is no condition on the ordering of the indices i and j in the constraint, we will additionally have the constraint $v_{kj} - v_{ki} \leq 0$; together, these imply $v_{ki} = v_{kj}$. Recalling the interpretation of the v_{ij} variables, this means that if the edge ij is used in either direction, then any third vertex k is either visited before both i and j ($v_{ki} = v_{kj} = 1$), or after both i and j ($v_{ki} = v_{kj} = 0$). MCF+ is compared to the other models in Section 2.2.

2.1.3 SST model

Another model based on similar variables to those of MCF+ was presented in 2006 by Sherali, Sarin and Tsai [66], and shown to be tighter than MCF+. Sherali et al. refer to the model as ATSP6 in [66], but for clarity we will refer to it as the SST model, with its relaxed definition given below. The model uses three sets of variables; x_{ij} exactly as in DFJ, y_{ij} analogous to the

v_{ij} variables in MCF+, and f_{ij}^v with indices i, v and j analogous to the f_{ijk} variables from MCF with respective indices i, j and k . That is, in SST, f_{ij}^v is intended to be 1 if the arc $i \rightarrow v$ is used in the cycle before visiting vertex j , and 0 otherwise. One other difference in the way the indices are defined is that SST does not include any variables for which two indices are equal.

Definition 2.4 (SST model [66]).

$$\text{Minimise} \quad \sum_{i=1}^n \sum_{j=1, j \neq i}^n c_{ij} x_{ij},$$

$$\text{subject to} \quad \sum_{j=1, j \neq i}^n x_{ij} = 1 \quad \forall i = 1, \dots, n \quad (2.23)$$

$$\sum_{i=1, i \neq j}^n x_{ij} = 1 \quad \forall j = 1, \dots, n \quad (2.24)$$

$$y_{ij} + y_{ji} = 1 \quad \forall i, j = 2, \dots, n; i \neq j \quad (2.25)$$

$$y_{ij} \geq x_{1i} \quad \forall i, j = 2, \dots, n; i \neq j \quad (2.26)$$

$$y_{ji} \geq x_{i1} \quad \forall i, j = 2, \dots, n; i \neq j \quad (2.27)$$

$$0 \leq x_{ij} \leq 1 \quad \forall i, j = 1, \dots, n; i \neq j \quad (2.28)$$

$$y_{ij} \geq 0 \quad \forall i, j = 2, \dots, n; i \neq j \quad (2.29)$$

$$y_{ij} + x_{ji} + y_{jk} + y_{ki} \leq 2 \quad \forall i, j, k = 2, \dots, n; \\ i \neq j \neq k \quad (2.30)$$

$$0 \leq f_{ij}^v \leq x_{iv} \quad \forall i, j, v = 2, \dots, n; \\ i \neq j \neq v \quad (2.31)$$

$$\sum_{v=2, v \neq i, j}^n f_{ij}^v + x_{ij} = y_{ij} \quad \forall i, j = 2, \dots, n; i \neq j \quad (2.32)$$

$$x_{1v} + \sum_{i=2, i \neq v, j}^n f_{ij}^v = y_{vj} \quad \forall v, j = 2, \dots, n; v \neq j. \quad (2.33)$$

The constraints involving the variables y_{ij} and f_{ij}^v may be interpreted as follows: If i and j are distinct vertices, then (2.25) expresses that either vertex i comes before vertex j or vice versa. Next, the inequalities in (2.26) and (2.27) ensure that if vertex i is either the first vertex visited after vertex

1, or the last vertex visited before vertex 1, then all other vertices j must come respectively after or before vertex i . Considering just the y variables of (2.30), it can be seen that these inequalities express the property that three distinct vertices $i, j, k \neq 1$ should not form a subtour; for example, having started at vertex 1, if i comes before j ($y_{ij} = 1$), then it follows that k cannot be both after j and before i (at most one of y_{jk} and y_{ki} can be 1). The addition of the variable x_{ji} to the LHS of (2.30) is an insightful way to strengthen this inequality, since if vertex i immediately follows j then it still follows that k cannot be after j and before i . Bounds on the y_{ij} and f_{ij}^v variables in (2.29) and (2.31) follow logically from the interpretation of the variables. Finally, (2.32) and (2.33) express, in two different ways, the y variables as linear combinations of the other variables. The former expresses that vertex i precedes j precisely when either the arc $i \rightarrow j$ is used, or when some other vertex v immediately follows i before later visiting j . The latter is similar, expressing that a vertex v precedes j if either v is the first vertex visited after vertex 1, or if some arc $i \rightarrow v$ for $i \neq 1$ is used before j .

In 2009, Öncan et al. [57] compared several TSP formulations in this class and reported that SST was the strongest known polynomial size formulation of TSP. However, as SST uses only a combination of 2-index and 3-index variables, it is reasonable that a four index model (with more variables and constraints) may be even stronger. We next introduce a recently published four index model, following a short discussion of how the aims of this recent model may differ from those considered so far.

2.1.4 The Base Model

It may be said that solving a TSP instance comprises two separate problems. The first is to identify Hamiltonian cycles in the graph, and the second is to find an optimal tour from amongst these cycles. Previous applications of linear programming to these problems such as DFJ, MCF, MCF+ and SST,

have typically focused on complete graphs wherein identifying Hamiltonian cycles is trivial (any ordering of the vertices suffices) and thus the difficulty lies solely in determining which is optimal. Some recent research has instead focused on applying linear programming to sparse graphs, where even establishing the existence of Hamiltonian cycles is a challenging problem.

In 2015, Filar et al. [28] published a linear programming model, the feasibility of which is a necessary condition for the existence of Hamiltonian cycles in a given undirected graph. Filar et al. begin by defining the model, which they call the *Base Model*, then consider a branching algorithm with branch-specific constraints designed for cubic graphs. We will not consider that branching algorithm in this thesis, but rather focus on the Base Model itself without any branch-specific constraints. We give the linear constraints of the Base Model below.

Let G be a graph with vertices $V = \{1, \dots, n\}$. We denote by $N(i)$ the set of all vertices adjacent to $i \in V$. Unless otherwise restricted, it should be assumed that the indices i, j , and k range from 1 to n , representing the vertices of V , and that the indices r and s range from 0 to $n - 1$.

Definition 2.5 (Base Model).

$$\sum_{a \in N(i)} x_{r,ia}^k - \sum_{a \in N(i)} x_{r-1,ai}^k = 0 \quad \forall i, k, r; r \neq 0 \quad (2.34)$$

$$\sum_{a \in N(i)} x_{r,ia}^k - \sum_{a \in N(k)} x_{n-r,ka}^i = 0 \quad \forall i, k, r; r \neq 0 \quad (2.35)$$

$$\sum_{r=0}^{n-1} x_{r,ia}^k - \sum_{r=0}^{n-1} x_{r,ia}^j = 0 \quad \forall i, j, k; a \in N(i); k \neq j \quad (2.36)$$

$$\sum_{k=1}^n x_{r,ia}^k - \sum_{k=1}^n x_{s,ia}^k = 0 \quad \forall i, r, s; a \in N(i); s \neq r \quad (2.37)$$

$$\sum_{r=0}^{n-1} \sum_{a \in N(i)} x_{r,ia}^k = 1 \quad \forall i, k \quad (2.38)$$

$$\sum_{k=1}^n \sum_{a \in N(i)} x_{r,ia}^k = 1 \quad \forall i, r \quad (2.39)$$

$$x_{0,ia}^k = 0 \quad \forall i, k; a \in N(i); i \neq k \quad (2.40)$$

$$x_{r,ia}^k \geq 0 \quad \forall k, r; a \in N(i). \quad (2.41)$$

Note that the Base Model as introduced has no objective function. It is only necessary to find a feasible solution satisfying (2.34) – (2.41). In Section 2.2.3 we will consider the addition of an appropriate objective function in order to permit more effective comparisons with other models.

The intention of the Base Model is to determine the Hamiltonicity of G by attempting to find a solution corresponding to a Hamiltonian cycle in G from the complementary perspectives of n different starting points. The value of $x_{r,ia}^k$ is intended to be 1 if the arc $i \rightarrow a$ is used exactly r steps after leaving vertex k in the Hamiltonian cycle, and 0 otherwise. For example, $x_{0,34}^3 = 1$ would indicate that the arc $3 \rightarrow 4$ is used 0 steps after, that is, immediately after, leaving vertex 3. Here we give a brief summary of the constraints according to this interpretation:

(2.34) Vertex i is departed r steps after leaving vertex k if and only if i was entered by an arc during the previous step.

(2.35) Vertex i is departed r steps after leaving vertex k if and only if k is departed $n - r$ steps after leaving i .

(2.36) If arc $i \rightarrow a$ is used in the cycle for one starting vertex, it must be used in the cycle for every other starting vertex.

(2.37) For every starting vertex that uses $i \rightarrow a$ after exactly r steps, there is a starting vertex using the same arc after exactly s steps.

(2.38) For any starting vertex k , there will be precisely one step in which vertex i is departed.

(2.39) There will be precisely one starting vertex for which vertex i is departed after exactly r steps.

(2.40) Only the starting vertex itself can be departed after exactly 0 steps.

(2.41) Non-negativity follows immediately from the interpretation.

For sparse graphs, the Base Model has $\mathcal{O}(n^3)$ variables and constraints, while for non-sparse graphs such as complete graphs, the Base Model has $\mathcal{O}(n^4)$ variables and constraints. The set of all binary solutions to the Base Model corresponds precisely to the set of Hamiltonian cycles in G . Indeed, if (2.41) is replaced with binary constraints on the $x_{r,ia}^k$ variables, the resulting model is an exact formulation of HCP [28]. However, as in the relaxed DFJ, MCF, MCF+ and SST models, the Base Model is not guaranteed to find a binary solution. In the case that $0 < x_{r,ia}^k < 1$, Filar et al. instead interpret the value as the probability of, r steps after leaving vertex k , using the arc $i \rightarrow a$.

If G contains no Hamiltonian cycles, then the variables $x_{r,ia}^k$ cannot describe a Hamiltonian cycle, and hence there are no binary solutions to the Base Model for non-Hamiltonian graphs. However, there may or may not be other feasible solutions. If there are no feasible solutions, then it is certain that G is non-Hamiltonian. This situation is desirable since infeasibility of the Base Model can be verified in polynomial time, providing a certificate of non-Hamiltonicity for G .

2.2 Comparisons of LP models

Having introduced MCF¹, MCF+, SST, and the Base Model in Section 2.1, which relate to either solving TSP or HCP, we now develop methods by which the models may be evaluated. Firstly, we consider straightforward variations of MCF, MCF+ and SST that can be used on non-complete graphs, allowing us to try solving HCP instances by the LP infeasibility of those

¹As DFJ is equivalent to MCF but requires exponentially many constraints, we omit it from further consideration.

models as with the Base Model. Following that, we construct an appropriate objective function to enable the Base Model to solve TSP instances, and introduce a new method for generating TSP instances based on cubic graphs. Having created a framework by which all four models may be compared, Sections 2.2.2 and 2.2.5 then present the results of each model on a set of non-Hamiltonian cubic graphs, and on TSP instances derived from cubic graphs.

All the results from this section and the remainder of the chapter were found using CPLEXTM Optimization Studio version 12.5 [42]. The linear programs were executed on a cluster of machines with four 16-core AMD OpteronTM 6282 processors.

2.2.1 Adapting TSP models to solve HCP

Suppose there is a non-complete graph $G = (V, E)$ whose Hamiltonicity is unknown. There are three ways in which a TSP model for complete instances may be used to try to detect non-Hamiltonicity in G . One way is to set the costs c_{ij} to be zero only when the arc $i \rightarrow j$ is in E , and positive otherwise. A feasible solution using only the edges of G then exists if and only if the objective function can be minimised to zero. The advantage of this approach is that it will work for any TSP linear programming model, but it comes at the expense of potentially having many superfluous variables or constraints. A second method is to retain the original costs c_{ij} on the arcs in E and set all other costs to a suitably large penalty value. The benefit is that we can still obtain a lower bound for the minimum tour cost, as opposed to the first approach. However, a difficulty is that in order to ensure that only the variables corresponding to arcs in E have non-zero values, the penalties must in theory be infinitely large. A sensible third approach that avoids these drawbacks is to modify the model to only include variables and constraints relevant to finding a solution in G . This still allows us to use arbitrary costs c_{ij} on the arcs of G while ensuring that only these arcs are used.

We now make the appropriate variations to the objective function and constraints of MCF, using the same notation $N(i)$ as in the Base Model to denote the set of vertices adjacent to i . The objective function (2.6) becomes

$$\sum_{i \in V} \sum_{j \in N(i)} c_{ij} x_{ij}, \quad (2.42)$$

and the constraints (2.7) – (2.14) become

$$\sum_{j \in N(i)} x_{ij} = 1 \quad \forall i \in V \quad (2.43)$$

$$\sum_{i \in N(j)} x_{ij} = 1 \quad \forall j \in V \quad (2.44)$$

$$\sum_{j \in N(i)} y_{ijk} - \sum_{j \in N(i)} y_{jik} = 0 \quad \forall i, k \in V^*; i \neq k \quad (2.45)$$

$$\sum_{i \in N(k)} y_{ikk} = 1 \quad \forall k \in V^* \quad (2.46)$$

$$\sum_{i \in N(1)} y_{1ik} = 1 \quad \forall k \in V^* \quad (2.47)$$

$$\sum_{i \in N(k)} y_{kik} = 0 \quad \forall k \in V^* \quad (2.48)$$

$$0 \leq y_{ijk} \leq x_{ij} \quad \forall i \in V; j \in N(i); k \in V^* \quad (2.49)$$

$$0 \leq x_{ij} \leq 1 \quad \forall i \in V; j \in N(i). \quad (2.50)$$

Similarly, we can make the necessary variations to (2.15) – (2.21), the constraints used in MCF+:

$$\sum_{j \in N(i)} f_{kji} - \sum_{j \in N(i)} f_{kij} = 0 \quad \forall i, k \in V^*; i \neq k \quad (2.51)$$

$$\sum_{i \in N(k)} f_{kik} = 0 \quad \forall k \in V^* \quad (2.52)$$

$$\sum_{i \in N(1)} f_{k1i} = 0 \quad \forall k \in V^* \quad (2.53)$$

$$\sum_{i \in N(k)} f_{kki} = 1 \quad \forall k \in V^* \quad (2.54)$$

$$0 \leq f_{kij} \leq x_{ij} \quad \forall i \in V; j \in N(i); k \in V^* \quad (2.55)$$

$$\sum_{j \in N(i)} f_{kij} = v_{ki} \quad \forall i, k \in V^* \quad (2.56)$$

$$x_{ij} + x_{ji} + v_{ki} - v_{kj} \leq 1 \quad \begin{array}{l} \forall i \in V^*; j \in V^* \cap N(i); \\ k \in V^*; k \neq i, j. \end{array} \quad (2.57)$$

We use the subscript HCP to denote the altered models as defined below:

Definition 2.6 (MCF_{HCP} model). Minimise (2.42) subject to (2.43) – (2.50).

If the costs c_{ij} are not provided, find any solution subject to these constraints.

Definition 2.7 (MCF_{+HCP} model). Minimise (2.42) subject to (2.22), (2.43),

(2.44) and (2.50) – (2.57). If the costs c_{ij} are not provided, find any solution

subject to these constraints.

To construct SST_{HCP} in a similar manner, we provide variations of the SST constraints (2.26), (2.27) and (2.30) – (2.33). Note that (2.23), (2.24) and (2.28) from SST become equivalent to the modified constraints (2.43), (2.44) and (2.50) above.

$$y_{ij} \geq x_{1i} \quad \forall i \in N(1); j = 2, \dots, n; i \neq j \quad (2.58)$$

$$y_{ji} \geq x_{i1} \quad \forall i \in N(1); j = 2, \dots, n; i \neq j \quad (2.59)$$

$$y_{ij} + x_{ji} + y_{jk} + y_{ki} \leq 2 \quad \forall i, k = 2, \dots, n; j \in N(i); 1 \neq j \neq k \neq i \quad (2.60)$$

$$y_{ij} + 0 + y_{jk} + y_{ki} \leq 2 \quad \forall i, k = 2, \dots, n; j \notin N(i); i \neq j \neq k \neq 1 \quad (2.61)$$

$$0 \leq f_{ij}^v \leq x_{iv} \quad \forall i, j = 2, \dots, n; v \in N(i); i \neq j \neq v \neq 1 \quad (2.62)$$

$$\sum_{v \in N(i) \setminus \{1, j\}} f_{ij}^v + x_{ij} = y_{ij} \quad \forall i = 2, \dots, n; j \in N(i); j \neq 1 \quad (2.63)$$

$$\sum_{v \in N(i) \setminus \{1\}} f_{ij}^v + 0 = y_{ij} \quad \forall i = 2, \dots, n; j \notin N(i); j \neq i \neq 1 \quad (2.64)$$

$$x_{1v} + \sum_{i \in N(v) \setminus \{1, j\}} f_{ij}^v = y_{vj} \quad \forall j = 2, \dots, n; v \in N(1) \quad (2.65)$$

$$0 + \sum_{i \in N(v) \setminus \{j\}} f_{ij}^v = y_{vj} \quad \forall j = 2, \dots, n; v \notin N(1); v \neq 1. \quad (2.66)$$

Note that (2.30), (2.32) and (2.33) each become two separate constraints here; (2.60) and (2.61), (2.63) and (2.64), and (2.65) and (2.66), respectively.

SST_{HCP} is defined as follows.

Definition 2.8 (SST_{HCP} model). Minimise (2.42) subject to (2.25), (2.29), (2.43), (2.44), (2.50) and (2.58) – (2.66). If the costs c_{ij} are not provided, find any solution subject to these constraints.

2.2.2 Results of LP models on HCP instances

We now compare MCF_{HCP} , $MCF_{+\text{HCP}}$, SST_{HCP} and the Base Model on their ability to detect non-Hamiltonian graphs by the infeasibility of their linear programs. In such a case, we say that a graph *induces infeasibility* in the given LP model. In order to make this evaluation we need a set of suitable non-Hamiltonian graphs. As mentioned in Section 1.2.1, HCP is NP-complete even when restricted to cubic graphs, and cubic graphs can be enumerated efficiently, making them a natural candidate set for testing these models. Selecting small enough instances (e.g. no more than 20 vertices) enables us to undertake exhaustive searches for Hamiltonian cycles, so the true Hamiltonicity can be determined for comparison with the results.

There are 556 471 cubic graphs with between 4 and 20 vertices, a vast majority (roughly 97%) of which are Hamiltonian while only 16 425 (roughly 3%) are non-Hamiltonian. The four models we compare, MCF_{HCP} , $MCF_{+\text{HCP}}$, SST_{HCP} and the Base Model, are necessarily feasible for Hamiltonian graphs, so we only consider feasibility of the models for non-Hamiltonian graphs. Ideally, all non-Hamiltonian graphs would induce infeasibility. However, as shown in Table 2.5, the models are feasible for approximately one tenth of these instances. MCF_{HCP} , $MCF_{+\text{HCP}}$ and SST_{HCP} have feasible LPs for the same set of 1720 graphs, while the Base Model performed marginally better on the 18-vertex and 20-vertex graphs, with an additional 98 graphs inducing infeasibility. The Base Model is thus strictly better than MCF, MCF+ and SST on this set of instances in the sense that the graphs inducing infeasibility

in the Base Model are a proper superset of the graphs inducing infeasibility in any of the other three models.

Table 2.5: The number of infeasible LPs for MCF_{HCP} , $\text{MCF}^+_{\text{HCP}}$, SST_{HCP} and the Base Model on non-Hamiltonian cubic graphs up to order 20. The final column gives the number of additional instances solved by the Base Model relative to the other models.

Vertices	NH	MCF	MCF+	SST	Base M.	Add.
10	2	1	1	1	1	
12	5	4	4	4	4	
14	35	30	30	30	30	
16	231	192	192	192	192	
18	1666	1477	1477	1477	1487	10
20	14 498	13 001	13 001	13 001	13 089	88
Total	16 425	14 705	14 705	14 705	14 803	98

We remark that the vast majority of graphs tested that induce infeasibility in the four models are bridge graphs. Indeed, the Base Model was proved in [28] to be infeasible for all bridge graphs. Later, in Theorem 2.23, we will prove that the other three models are infeasible for all non-tough graphs which, in particular, include all bridge graphs. Hence, we will exclude bridge graphs from all future experiments described in this thesis. To that end, we now define *NHNB20* to be the set of all 2099 non-Hamiltonian non-bridge cubic graphs containing up to 20 vertices. A list of all instances of *NHNB20* is given in Appendix A.1. Table 2.6 shows the results of the four models considered when restricted to this problem set. Figure 2.7 displays the smallest instance of *NHNB20* that induces infeasibility in each of these models. The problem set *NHNB20* will be given particular focus in Chapters 3 and 4.

Although these results indicate that the Base Model is stronger than the other three models, in most cases the graphs that induced feasible LPs for those other models also induced feasible LPs for the Base Model. This raises the question: To what extent do these models vary in their feasible regions, or, as visualised in Figure 2.1, how close are they to a polytope corresponding to the convex hull of Hamiltonian cycles? Given the results here, we may

Table 2.6: The number of infeasible LPs for MCF_{HCP} , $\text{MCF}^+_{\text{HCP}}$, SST_{HCP} and the Base Model on NHNB20. The final column gives the number of additional instances solved by the Base Model relative to the other models.

Vertices	NHNB	MCF	MCF+	SST	Base M.	Add.
10	1	0	0	0	0	
12	1	0	0	0	0	
14	6	1	1	1	1	
16	33	6	6	6	6	
18	231	42	42	42	52	10
20	1827	330	330	330	418	88
Total	2099	379	379	379	477	98

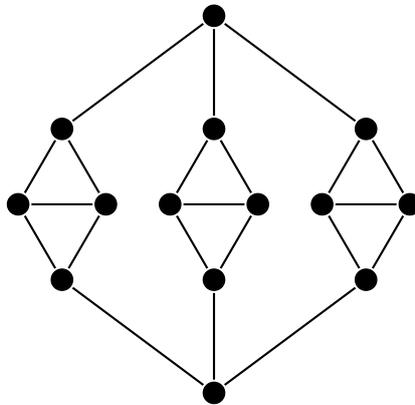


Figure 2.7: The smallest instance of NHNB20, G_{14}^{120} , that induces infeasibility in MCF_{HCP} , $\text{MCF}^+_{\text{HCP}}$, SST_{HCP} and the Base Model.

expect the Base Model to have a tighter feasible region, but are there any instances for which the Base Model is outperformed by the other models, and how may the differences amongst them be quantified? To investigate these questions further, we next consider the TSP versions of these models.

2.2.3 Adapting the Base Model to solve TSP

Although the Base Model was designed with the goal of detecting non-Hamiltonicity, with the addition of an appropriate objective function the Base Model may also be used to find lower bounds for general TSP instances. Constraints specific to sparse graphs will be considered later in Chapter 4, but for now note that the Base Model as defined does not require the graph to

be sparse, so the Base Model can be used for any graph (including complete graphs).

Whereas the definitions of MCF, MCF+ and SST naturally included suitable objective functions for TSP, the Base Model was not originally intended as a model for solving TSP and hence an objective function was not included. We show how an appropriate objective function may be written and then simplified using the constraints of the Base Model.

Consider the Base Model and fix some vertex k as the starting point of a tour. Let \mathbf{x} represent the vector of variables $x_{r,ia}^k$. We will argue that the objective function below, which is to be minimised, is a valid expression to express the cost of a tour according to the definition of TSP:

$$\begin{aligned} f(\mathbf{x}) &= \sum_{i=1}^n \sum_{j \in N(i)} \sum_{r=0}^{n-1} c_{ij} x_{r,ij}^k \\ &= \sum_{i=1}^n \sum_{j \in N(i)} c_{ij} \left(\sum_{r=0}^{n-1} x_{r,ij}^k \right). \end{aligned} \quad (2.67)$$

Note that $\sum_{r=0}^{n-1} x_{r,ij}^k$ in (2.67) may be interpreted as the probability of starting at vertex k and using the arc $i \rightarrow j$ at some step during the tour. With binary variables, this will be 1 only where an arc $i \rightarrow j$ is used; so the total sum will be just the sum of costs c_{ij} for each of the used edges only. By (2.36) from the Base Model, the choice of vertex k will not influence the sum here. In particular, we can use this fact, without loss of generality, to fix $k = i$ for each respective summand, and thus obtain an expression that no longer depends on the choice of k ;

$$f(\mathbf{x}) = \sum_{i=1}^n \sum_{j \in N(i)} c_{ij} \left(\sum_{r=0}^{n-1} x_{r,ij}^i \right). \quad (2.68)$$

To further simplify the objective function, we introduce the following lemma.

Lemma 2.9. *Let $G = (V, E)$ be a graph. For any $i \in V$ and $a \in N(i)$, the linear constraints of the Base Model imply*

$$x_{r,ia}^i = 0, \quad \forall r = 1, 2, \dots, n-1.$$

Proof. Setting $k = i$ in (2.38), we obtain

$$\sum_{r=0}^{n-1} \sum_{a \in N(i)} x_{r,ia}^i = 1, \quad \forall i.$$

The outer sum may be split into two parts, so

$$\sum_{a \in N(i)} x_{0,ia}^i + \sum_{r=1}^{n-1} \sum_{a \in N(i)} x_{r,ia}^i = 1, \quad \forall i. \quad (2.69)$$

Next, by setting $r = 0$ in (2.39), we obtain

$$\sum_{k=1}^n \sum_{a \in N(i)} x_{0,ia}^k = 1, \quad \forall i.$$

Combining this with (2.40), all the terms on the LHS are zero when $k \neq i$; therefore,

$$\sum_{a \in N(i)} x_{0,ia}^i = 1, \quad \forall i. \quad (2.70)$$

Substituting (2.70) into (2.69), we arrive at

$$1 + \sum_{r=1}^{n-1} \sum_{a \in N(i)} x_{r,ia}^i = 1, \quad \forall i.$$

Therefore,

$$\sum_{r=1}^{n-1} \sum_{a \in N(i)} x_{r,ia}^i = 0, \quad \forall i,$$

and finally, by non-negativity of the variables in (2.41), it follows that each summand is exactly zero. \square

We may interpret Lemma 2.9 as ensuring that if a tour starts at some vertex i , that vertex i may only be departed at the first step ($r = 0$); not at any later step. Applying the lemma, we can remove the zero terms from the

right side of (2.68) to obtain

$$f(\mathbf{x}) = \sum_{i=1}^n \sum_{j \in N(i)} c_{ij} x_{0,ij}^i. \quad (2.71)$$

Accordingly, in the context of solving any TSP instance, we henceforth consider the Base Model to include (2.71) as an objective function to be minimised.

2.2.4 Generating TSP instances based on cubic graphs

Having established the correctness of the TSP objective function for the Base Model, it is necessary to select a set of TSP instances for testing. While there are sets of TSP instances available in literature, for example in TSPLIB [63], these were found to have too many vertices against which to reasonably test a model with time complexity $\mathcal{O}(n^4)$. Recall that the Base Model has time complexity $\mathcal{O}(n^3)$ for sparse graphs. Given this, it was decided that a new set of TSP instances should be constructed for testing, with the following goals in mind:

- Constructed instances should have relatively few vertices.
- An exact optimal tour for each instance should be known.
- Instances should be relatively difficult as far as the Base Model is concerned, to allow as much room as possible for improving the solutions, a direction we consider in Chapter 4.
- Given the previously discussed benefits of cubic graphs, it is desirable for the constructed instances to have some relation to cubic graphs, both Hamiltonian and non-Hamiltonian non-bridge.

In light of these goals, we now introduce Algorithm 2.1 for generating sets of asymmetric TSP instances. Following the algorithm, we make a number

of comments about choosing appropriate inputs and parameters, and how this influences the tractability of finding exact optimal tours in Step 3 of the algorithm. This is followed by a discussion of a particular set of TSP instances generated and the results on those instances.

Algorithm 2.1 Generate asymmetric TSP instances from cubic graphs

Input: G_1, \dots, G_N are cubic graphs

r is the number of candidates to generate from each graph

q is the maximum number of output graphs ($q \leq rN$)

m is the maximum cost to assign to edges from the graphs

l is the cost to assign to non-edges from the graphs

LPMODEL is a linear program for solving ATSP

Output: T_1, \dots, T_M are ATSP instances ($M \leq q$)

O_1, \dots, O_M are optimal tours for each ATSP instance

- 1 For each graph G_i , produce r candidate instances by assigning, for each candidate, uniformly random integer costs between 0 and m to every arc.
 - 2 For each candidate, complete the graph by adding edges between all pairs of non-adjacent vertices, and assign a bi-directional cost of l to each of these new edges.
 - 3 Calculate the optimal tour for each candidate.
 - 4 Execute LPMODEL for each candidate and discard any where the obtained lower bound is equal to the optimal tour cost.
 - 5 If the number of remaining candidates exceeds q , set M equal to q . Otherwise, set M equal to the number of remaining candidates.
 - 6 Select the M candidates with the largest gaps as a percentage of their optimal tour costs, and return these candidates T_1, T_2, \dots and their respective optimal tours O_1, O_2, \dots .
-

Since one of the goals was to generate difficult instances as far as the Base Model is concerned, it was decided that the algorithm should generate many candidate instances randomly, and only return those having sizeable gaps. Recall from Definition 1.28 that the gap is defined to be the difference between the LP lower bound and the exact optimal tour length. Determining the gap therefore requires the exact optimal tour length to be known, an NP-hard problem in general. Indeed, a naïve enumeration of all tours would take a prohibitively long time even for small graphs. However, by restricting the input graphs to be *traceable* graphs (those containing a Hamiltonian path) of order n and setting $l = mn$, we can find the optimal tour much more

efficiently by Lemma 2.10 below. In this way, only the Hamiltonian cycles or paths from the original graph G need be considered, which can be done orders of magnitude more quickly than considering all tours in the complete instance.

Lemma 2.10. *Let $G = (V, E)$ be a traceable graph with n vertices, and let m and l be positive integers. Suppose that a complete ATSP instance of order n were constructed such that the arcs corresponding to those in G have costs chosen from $\{0, \dots, m\}$, and the remaining arcs have cost l . If $l \geq mn$, then:*

- (i) *If G is Hamiltonian, any optimal tour is guaranteed to lie on the arcs corresponding to a Hamiltonian cycle of G .*
- (ii) *If G is non-Hamiltonian, any optimal tour is guaranteed to lie on arcs corresponding to a Hamiltonian path of G with one additional arc from the complement of E .*

Proof. Consider the case that G is Hamiltonian. For any Hamiltonian cycle from the original graph, it is clear that the cost of the tour corresponding to this HC can be at most mn (when all n arcs in the tour have maximal cost m). Using even a single arc from the complement of E will increase the tour cost to be at least as large as this; $l \geq mn$, plus the remaining cost of the tour. Therefore, at least one of the Hamiltonian cycles of G corresponds to the optimal tour.

Alternatively, consider the case that G is non-Hamiltonian. By the traceability of G , there is at least one Hamiltonian path. The cost of using the corresponding $n - 1$ arcs of this path can be at most $m(n - 1)$. To close the path it is necessary to go directly from the last vertex in the path to the first. This additional arc cannot be in E , since that would imply that G is Hamiltonian, so the cost of using this arc is l . The maximum cost for such a cycle is thus $m(n - 1) + l$. If, instead, two or more arcs from the complement of E were used, the cost would be at least $2l$, which is strictly greater than

$m(n - 1) + l$. Therefore, at least one of the Hamiltonian paths is optimal when closed. \square

Using Algorithm 2.1, a particular set of TSP instances was generated from cubic graphs with 16 vertices. There are 4060 cubic graphs with 16 vertices comprising 3841 Hamiltonian graphs and 219 non-Hamiltonian graphs. The 219 non-Hamiltonian graphs can be further classified into 186 bridge graphs and 33 non-Hamiltonian non-bridge (NHNB) graphs. All cubic graphs on 16 vertices are traceable except for one bridge graph, however, we do not consider any bridge graphs here as the models considered already perform very well on them (see Section 2.2.2). For Hamiltonian and NHNB instances from this set then, Lemma 2.10 may be used.

The cost parameters chosen were $m = 100$ and $l = mn = 1600$, and LPMODEL was set to be the Base Model. To ensure balance in the generated problem set, it was decided to separately collect 200 instances based on Hamiltonian graphs, and 200 instances based on NHNB graphs. For both the Hamiltonian and NHNB subsets then, q was set to 200. The parameter r was set to 2 for Hamiltonian graphs (for 7682 candidates) and set to 10 for NHNB graphs (for 330 candidates.) Histograms showing the gaps from the Base Model for the 8012 candidates are shown in Figure 2.8.

Combining both sets, the 400 ATSP instances returned are included in Appendix B and will be referred to as problem set *ATSP16A*. Although the problems generated by this method are complete graphs, it is trivial to remove the extra edges (all having cost of 1600) and to consider the related problem set of cubic ATSP problems, which will be referred to as *ATSP16AC*; this latter set will become useful when considering linear constraints that only hold for cubic or other sparse graphs.

The new problem sets *ATSP16A* and *ATSP16AC* provide a way of quantitatively measuring the relative efficacy of the LP models under consideration,

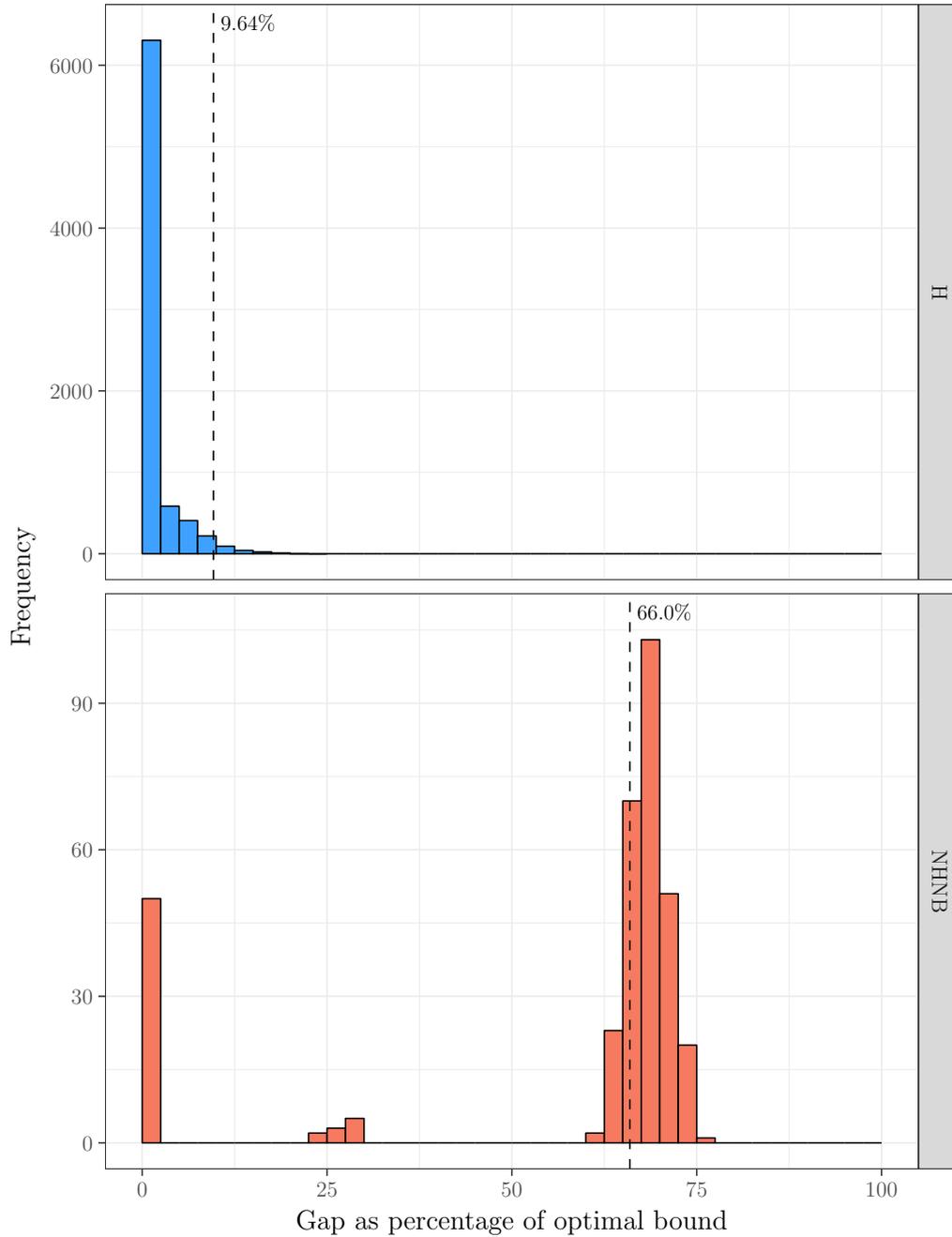


Figure 2.8: Histogram showing gaps obtained with the Base Model as a percentage of the optimal tour cost for 8012 candidate ATSP instances generated by Algorithm 2.1. The gaps are grouped by whether the input graph was Hamiltonian or non-Hamiltonian non-bridge, of which in total there were 7682 and 330 candidates respectively. The vertical dashed lines represent the cutoffs, to the right of which the 200 instances with the largest percentage gaps were retained for the two input types.

and are sensitive enough that small improvements to the models can be detected if found. The key measure is the gap for each instance in the problem set; the difference between the lower bound found by the linear program and the optimal tour cost.

We remark that in the case of the 200 non-Hamiltonian cubic instances in ATSP16AC, there is no optimal tour, and a sufficiently tight linear model might in theory be infeasible for some or all of these instances. In the following section, and again in Chapter 4, we consider results of linear models on these instances, but for convenience of terminology we continue to refer to the *gaps* for these instances, using a special case definition of the term:

Definition 2.11 (Gaps for non-Hamiltonian instances of ATSP16AC). For any non-Hamiltonian instance of ATSP16AC, we define the *gap* to be the optimal tour cost of the corresponding complete instance in ATSP16A minus the lower bound found for the linear program. If the linear program is infeasible, we say the gap is not defined.

This definition is practical, since, for all linear models considered, the non-Hamiltonian instances of ATSP16AC have feasible solutions with similar lower bounds to that of the corresponding ATSP16A instances. In theory, if a linear model were infeasible for a non-Hamiltonian instance of ATSP16AC, we would report those instances separately, but this does not occur for any model considered in this thesis. Note that the definition of gaps for non-Hamiltonian instances of ATSP16AC could also be used as the definition of the gap for the Hamiltonian instances, since the optimal tours of the corresponding instances of ATSP16A are necessarily the same.

2.2.5 Results of LP models on TSP instances

Using the TSP instances constructed in Section 2.2.4, we can now examine more finely the relative performance of MCF, MCF+, SST, and the Base

Model. Rather than simply a binary result of feasible or infeasible as in Section 2.2.2, we obtain a gap which may theoretically be any non-negative rational number. The lower the gap, the better the model performs on that instance, and any difference or improvement in the gap can be measured quantitatively.

Aggregated results for the four models are presented in Table 2.9 for the instances in set ATSP16A and in Table 2.10 for ATSP16AC. Recall that the former are complete graphs, while the latter are the corresponding instances having only the edges of the cubic graph from which they are derived. Note that none of the four models were able to find the optimal tour for any of the instances.

Table 2.9: Aggregated results of MCF, MCF+, SST and the Base Model on the 200 NHNB-derived and 200 Hamiltonian-derived instances of ATSP16A.

Model	NHNB-derived		Ham.-derived	
	Sum of gaps	Mean	Sum of gaps	Mean
MCF	295 768.0	1478.8	22 693.1	114.8
MCF+	294 799.8	1474.0	22 368.9	111.8
SST	293 721.7	1468.6	20 705.3	103.5
Base Model	289 064.2	1445.3	16 864.2	84.3

Table 2.10: Aggregated results of MCF, MCF+, SST and the Base Model on the 200 NHNB-derived and 200 Hamiltonian-derived instances of ATSP16AC.

Model	NHNB-derived		Ham.-derived	
	Sum of gaps	Mean	Sum of gaps	Mean
MCF	295 768.0	1478.8	22 963.1	114.8
MCF+	294 799.8	1474.0	22 368.9	111.8
SST	293 721.7	1468.6	20 705.3	103.5
Base Model	288 979.2	1444.9	16 864.2	84.3

As can be seen from Tables 2.9 and 2.10, the Base Model outperforms MCF, MCF+ and SST in the average case. Recall that the instances of ATSP16A and ATSP16AC were specifically chosen over others because the

Base Model was the *least effective* on them; despite this, the Base Model dominated MCF+, and hence MCF, for every instance tested. This provides strong empirical evidence that the Base Model may strictly contain MCF+, a conjecture we present in Section 2.2.6.

For comparison with SST, Figure 2.11 shows a plot of the gaps for the Base Model on these instances against the gaps for SST, the latter being necessarily tighter than MCF+ and MCF in turn, as discussed previously. This plot shows that the Base Model outperforms SST in almost all cases, but that there are four instances of ATSP16A and the corresponding four instances of ATSP16AC for which the gap obtained by SST was less than that obtained by the Base Model. These four instances have the IDs 92, 105, 259 and 338; the edge lists and costs for which may be found in Appendix B. In these instances, the difference in gaps between the two models was small; no more than 1.5%. In contrast, the Base Model provided a tighter bound in all remaining 396 instances of both sets. Although the Base Model is stronger on average, there must be information about Hamiltonian cycles expressed in SST that is not captured by the Base Model. This presents an opportunity to improve the Base Model by adding constraints similar to those of SST, an extension we consider in Chapter 4.

2.2.6 A conjecture on the strength of the Base Model

The results shown in Sections 2.2.2 and 2.2.5 lead naturally to the following conjecture.

Conjecture 2.12. *The Base Model is stronger than MCF+.*

Specifically, by *stronger* we mean that for any given instance of HCP or TSP, the set of feasible solutions to the Base Model when projected to the x_{ij} variables of MCF+, is a subset of the set of feasible solutions to MCF+ when projected to the same variables. To make this projection, we note the natural

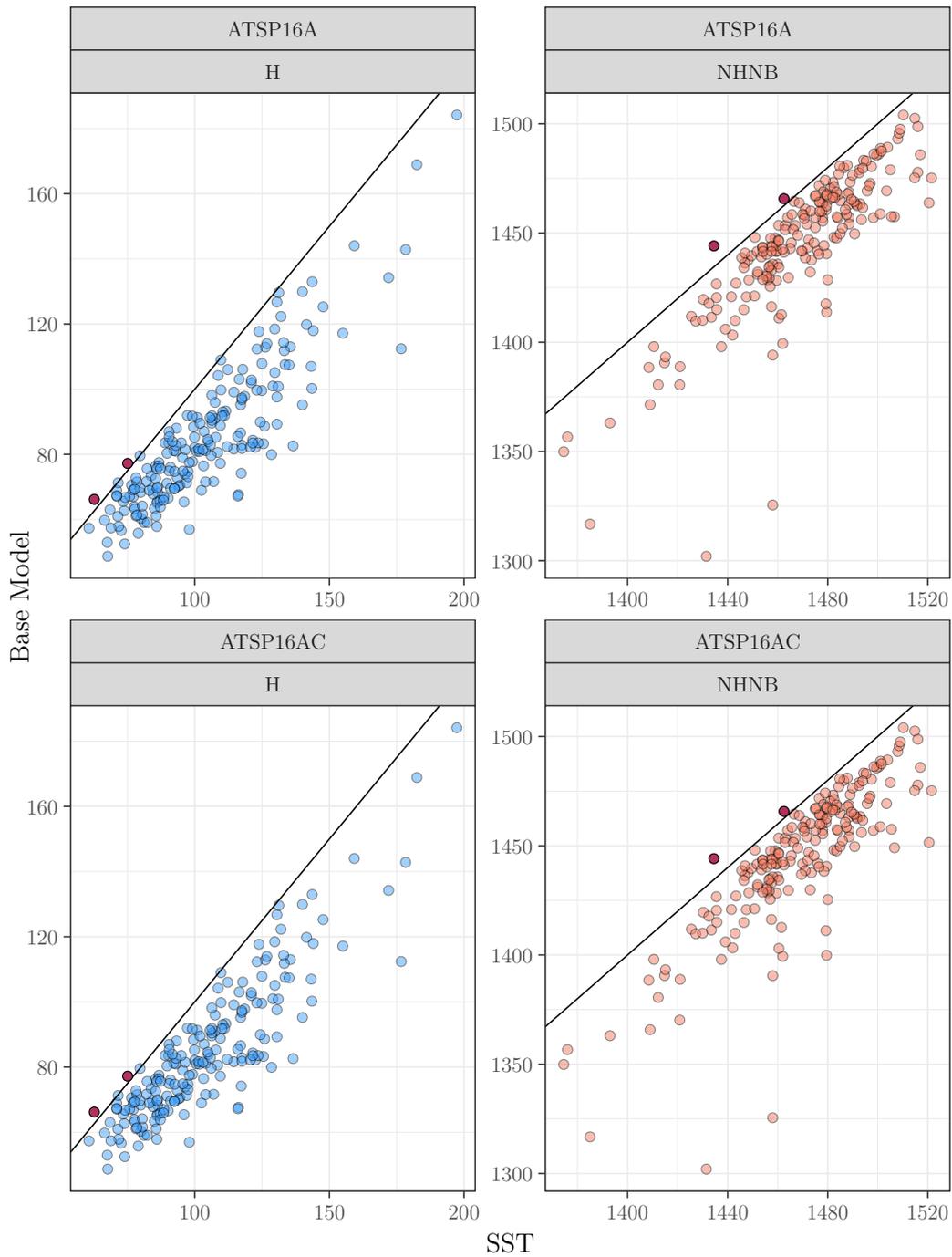


Figure 2.11: Gaps for the Base Model plotted against gaps for SST, for the Hamiltonian-derived and NHHB-derived instances of ATSP16A and ATSP16AC. The solid line $y = x$ corresponds to the gaps being the same for both models. The four instances from each of ATSP16A and ATSP16AC for which SST outperforms the Base Model are shown as solid red points.

equivalence of the Base Model variables $x_{0,ij}^i$ and the MCF+ variables x_{ij} in their respective objective functions (2.71) and (2.42).

We remark that Conjecture 2.12 implies that the Base Model is in turn stronger than MCF, and MCF is in turn equivalent to DFJ. Therefore, one approach to proving the conjecture would be to establish that:

- (i) The Base Model implies constraints equivalent to those of DFJ and hence those of MCF.
- (ii) Assuming (i), the Base Model also implies constraints equivalent to (2.20) – (2.22), the constraints of MCF+ without analogues in MCF.

We now give a partial proof of (i). First, we express the constraints of DFJ in terms of the variables of the Base Model. By the observation above, the DFJ variables x_{ij} are equivalent to the Base Model variables $x_{0,ij}^i$. Therefore, constraints (2.1) – (2.3), and the relaxation of (2.4), may be written as

$$\sum_{a \in N(i)} x_{0,ia}^i = 1 \quad \forall i = 1, \dots, n \quad (2.72)$$

$$\sum_{a \in N(i)} x_{0,ai}^a = 1 \quad \forall i = 1, \dots, n \quad (2.73)$$

$$\sum_{i \in S} \sum_{a \in N(i) \setminus S} (x_{0,ia}^i + x_{0,ai}^a) \geq 2 \quad \forall S \subset V, 0 < |S| < n \quad (2.74)$$

$$0 \leq x_{0,ia}^i \leq 1 \quad \forall i = 1, \dots, n; a \in N(i). \quad (2.75)$$

Lemma 2.13. *The constraints of the Base Model imply constraints (2.72), (2.73) and (2.75).*

Proof. Observe that (2.72) follows immediately from (2.38) if we set $k = i$ and apply Lemma 2.9. Next, (2.75) follows immediately from (2.41) and (2.72). Hence we now focus on (2.73).

Consider any vertices i and k . Taking (2.34) and fixing $r = 1$, we obtain

$$\sum_{a \in N(i)} x_{1,ia}^k = \sum_{a \in N(i)} x_{0,ai}^k. \quad (2.76)$$

From (2.40), it is clear that the RHS of (2.76) reduces to $x_{0,ki}^k$ if k is adjacent to i , and 0 otherwise. Therefore,

$$\sum_{a \in N(i)} x_{1,ia}^k = \begin{cases} x_{0,ki}^k & \text{if } k \in N(i), \\ 0 & \text{otherwise.} \end{cases} \quad (2.77)$$

Next, consider (2.39) for $r = 1$:

$$\sum_{k=1}^n \sum_{a \in N(i)} x_{1,ia}^k = 1. \quad (2.78)$$

Substituting (2.77) into (2.78), we obtain the desired equality;

$$\sum_{k \in N(i)} x_{0,ki}^k = 1. \quad \square$$

We now consider the remaining constraint (2.74). We will show that (2.74) is implied by

$$\sum_{i \in S} \sum_{a \in N(i) \setminus S} x_{0,ia}^i \geq 1 \quad \forall S \subset V, 0 < |S| < n. \quad (2.79)$$

Lemma 2.14. *Constraint (2.74) is satisfied if the constraints (2.72), (2.73) and (2.79) are satisfied.*

Proof. Summing over (2.72) we obtain

$$\sum_{i \in S} \sum_{a \in N(i)} x_{0,ia}^i = |S|. \quad (2.80)$$

We can then separate the summed terms of the LHS of (2.80):

$$\sum_{i \in S} \sum_{a \in N(i)} x_{0,ia}^i = \sum_{i \in S} \sum_{a \in N(i) \setminus S} x_{0,ia}^i + \sum_{i \in S} \sum_{a \in N(i) \cap S} x_{0,ia}^i. \quad (2.81)$$

Substituting (2.79) and (2.80) into (2.81), we obtain

$$\sum_{i \in S} \sum_{a \in N(i) \cap S} x_{0,ia}^i \leq |S| - 1.$$

Similarly, summing over (2.73) we obtain

$$|S| = \sum_{i \in S} \sum_{a \in N(i)} x_{0,ai}^a = \sum_{i \in S} \sum_{a \in N(i) \setminus S} x_{0,ai}^a + \sum_{i \in S} \sum_{a \in N(i) \cap S} x_{0,ai}^a. \quad (2.82)$$

It may be seen that

$$\sum_{i \in S} \sum_{a \in N(i) \cap S} x_{0,ai}^a = \sum_{i \in S} \sum_{a \in N(i) \cap S} x_{0,ia}^i \leq |S| - 1. \quad (2.83)$$

Hence, substituting (2.83) into (2.82), we obtain

$$\sum_{i \in S} \sum_{a \in N(i) \setminus S} x_{0,ai}^a \geq 1,$$

which along with (2.79) implies (2.74). \square

The upcoming theorem will require the following result, shown in [28].

Lemma 2.15. *The constraints of the Base Model imply that $x_{n-1,ia}^k = 0$ for all $a \neq k$, and $x_{r,ik}^k = 0$ for all $r \neq n - 1$.*

For the sake of neatness, in the proof of the following theorem we will permit sums over variables corresponding to arcs that may not exist in the graph. In such a case, we treat these variables as identically zero.

Theorem 2.16. *The constraints of the Base Model imply (2.74) for all subsets $S \subset V$ such that $|S| \in \{1, 2, 3, n - 3, n - 2, n - 1\}$.*

Proof. First, we argue that if (2.74) is satisfied for all S such that $|S| = k$, it is also satisfied for all S such that $|S| = n - k$. Suppose that (2.74) is satisfied for all $|S| = k$. That is, for any S such that $|S| = k$, we have

$$\sum_{i \in S} \sum_{a \notin S} (x_{0,ia}^i + x_{0,ai}^a) \geq 2. \quad (2.84)$$

If we consider the complement of S , then the LHS of (2.74) is

$$\sum_{i \notin S} \sum_{a \in S} (x_{0,ia}^i + x_{0,ai}^a). \quad (2.85)$$

It is clear that (2.85) contains the identical terms as the LHS of (2.84). Since any S such that $|S| = n - k$ can be obtained by taking the complement of a set of size k , we conclude that (2.74) is satisfied for any S such that $|S| = n - k$ as well.

Recall from Lemma 2.14 that (2.74) is satisfied if (2.72), (2.73) and (2.79) are satisfied. By Lemma 2.13, the Base Model implies (2.72) and (2.73). We now show that (2.79) is satisfied for $k = 1, 2, 3$. Without loss of generality, we will assume that $S = \{1, \dots, k\}$; that is, S contains the first k vertices of the graph. It is clear that for other choices of S the graph can be relabelled so that the remaining arguments are applicable.

For $k = 1$, the result follows immediately from (2.72). Next, for $k = 2$, we seek to prove the following:

$$\sum_{a>2} x_{0,1a}^1 + \sum_{a>2} x_{0,2a}^2 \geq 1. \quad (2.86)$$

The LHS of (2.86) can be rewritten using (2.72) for the first sum, and (2.36), (2.40), and Lemma 2.9 for second sum as follows:

$$1 - x_{0,12}^1 + \sum_{r=1}^{n-1} \sum_{a>2} x_{r,2a}^1. \quad (2.87)$$

Note that by Lemma 2.15, we have

$$\sum_{a>2} x_{n-1,2a}^1 = 0. \quad (2.88)$$

Also, using (2.34) and (2.40), we have

$$\sum_{a>2} x_{1,2a}^1 = x_{0,12}^1. \quad (2.89)$$

Substituting (2.88) and (2.89) into (2.87), we see the LHS of (2.86) becomes

$$\sum_{a>2} x_{0,1a}^1 + \sum_{a>2} x_{0,2a}^2 = 1 + \sum_{r=2}^{n-2} \sum_{a>2} x_{r,2a}^1. \quad (2.90)$$

Hence, from the non-negativity of the $x_{r,ia}^k$ variables, (2.86) is satisfied.

Finally, for $k = 3$, we seek to prove the following:

$$\sum_{i \leq 3} \sum_{a > 3} x_{0,ia}^i \geq 1. \quad (2.91)$$

We can rewrite the LHS of (2.91) as

$$\sum_{i \leq 2} \sum_{a > 2} x_{0,ia}^i - \sum_{i \leq 2} x_{0,i3}^i + \sum_{a > 3} x_{0,3a}^3. \quad (2.92)$$

Then, substituting (2.90) into (2.92), and separating the cases when $r = 2$ and $r = n - 2$, we obtain

$$1 + \sum_{r=3}^{n-3} \sum_{a > 2} x_{r,2a}^1 + \sum_{a > 2} x_{2,2a}^1 + \sum_{a > 2} x_{n-2,2a}^1 - \sum_{i \leq 2} x_{0,i3}^i + \sum_{a > 3} x_{0,3a}^3. \quad (2.93)$$

Then, by (2.34) and (2.35), we can rewrite (2.93) as

$$1 + \sum_{r=3}^{n-3} \sum_{a > 2} x_{r,2a}^1 + \sum_{a > 2} x_{1,a2}^1 + \sum_{a > 2} x_{1,a1}^2 - \sum_{i \leq 2} x_{0,i3}^i + \sum_{a > 3} x_{0,3a}^3. \quad (2.94)$$

Now, consider the rightmost sum in (2.94). It follows from (2.37) where we set $r = 0$ and $s = 1$, along with (2.40), that each term of the form $x_{0,3a}^3$ can be expressed as

$$x_{0,3a}^3 = \sum_{k=1}^n x_{1,3a}^k,$$

and thus

$$\begin{aligned} \sum_{a > 3} x_{0,3a}^3 &= \sum_{k=1}^n \sum_{a > 3} x_{1,3a}^k \\ &= \sum_{a > 3} x_{1,3a}^1 + \sum_{a > 3} x_{1,3a}^2 + \sum_{k > 3} \sum_{a > 3} x_{1,3a}^k. \end{aligned} \quad (2.95)$$

Then, by (2.34), (2.40), and Lemma 2.15, we can rewrite (2.95) as

$$\sum_{a > 3} x_{0,3a}^3 = x_{0,13}^1 - x_{1,32}^1 + x_{0,23}^2 - x_{1,31}^2 + \sum_{k > 3} \sum_{a > 3} x_{1,3a}^k. \quad (2.96)$$

Finally, substituting (2.96) into (2.94), we see that the LHS of (2.91) becomes

$$\sum_{i \leq 3} \sum_{a > 3} x_{0,ia}^i = 1 + \sum_{r=3}^{n-3} \sum_{a > 2} x_{r,2a}^1 + \sum_{a > 3} x_{1,a2}^1 + \sum_{a > 3} x_{1,a1}^2 + \sum_{k > 3} \sum_{a > 3} x_{1,3a}^k.$$

Hence, from the non-negativity of the $x_{r,ia}^k$ variables, (2.91) is satisfied. \square

We expect that arguments similar to the above could be used to prove that the Base Model implies (2.74) for the remaining cardinalities of $S \subset V$.

2.3 Classifications of difficult cubic graphs

A natural question to ask about the non-Hamiltonian graphs identified and those not identified by these models is whether they may be distinguished by a particular classification. For example, what characteristics distinguish, or tend to distinguish the 14 803 non-Hamiltonian graphs identified as such by infeasibility of the Base Model, from the 1622 graphs that were not? In particular, we consider the classification of cubic graphs by connectivity, and by toughness, with regard to identifying non-Hamiltonicity. We prove that non-tough graphs necessarily induce infeasibility in the DFJ model and models with equivalent constraints. We conjecture based on empirical evidence and the previous Conjecture 2.12 that the same result holds for the Base Model.

2.3.1 Vertex and edge connectivity

Two fundamental properties of any graph are its *vertex connectivity* and *edge connectivity*. The *vertex connectivity*, or simply *connectivity*, of a graph G is defined as the maximum value of k for which G is k -connected. Similarly, the *edge connectivity* of G is defined as the maximum value of k for which G is k -edge-connected.

Note that the vertex connectivity can be at most 3 for any cubic graph. This is due to the fact that for any cubic graph $G = (V, E)$, other than the complete graph K_4 , it is possible to disconnect G by removing the three vertices adjacent to any vertex $v \in V$. For the remaining case of K_4 , which is 3-connected, the definition of k -connected precludes K_4 from being 4-connected, so K_4 has a connectivity of 3. Furthermore, for any cubic

graph, the vertex connectivity and edge connectivity are always equal by Lemma 2.17 below. We also note that the connectivity of a cubic graph can be found in polynomial time; at worst, all subsets of 3 vertices must be considered for removal, but there are only $\mathcal{O}(n^3)$ such subsets. Examples of the smallest cubic graphs with vertex connectivities 1, 2 and 3 are shown in Figure 2.12.

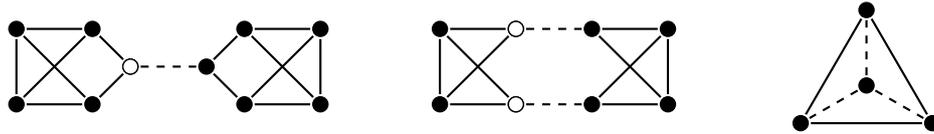


Figure 2.12: The smallest cubic graphs having connectivity 1 (left), 2 (centre) and 3 (right). Examples of vertex cuts are shown with hollow vertices, and examples of edge cuts are shown with dashed edges. The graph on the right side, K_4 , does not have a 3 vertex cut set, but is 3-connected as it cannot be 4-connected by definition.

The following lemma is a well-known result.

Lemma 2.17. *Let G be a connected cubic graph with connectivity $\kappa(G)$ and edge connectivity $\lambda(G)$. Then $\kappa(G) = \lambda(G)$.*

All connected graphs of a given order n may be considered to lie on a scale of varying connectivities. At one extreme are graphs with vertex connectivity 1, being necessarily non-Hamiltonian. At the other extreme are the complete graphs K_n , necessarily Hamiltonian and having vertex connectivity $(n - 1)$. One might then predict that the ratio of Hamiltonian graphs to non-Hamiltonian graphs increases with higher connectivity. For empirical evidence to support this prediction, consider all connected graphs with 10 vertices. There are 11 716 571 such graphs up to isomorphism, summarised by Hamiltonicity and vertex connectivity in Table 2.13. These results were collected using the database from the Encyclopedia of Finite Graphs [41]. Note that having vertex connectivity of at least $n/2$, or 5 in the case of these 10-vertex graphs, is a sufficient condition for Hamiltonicity by a well-known theorem of Dirac [21] which states that any graph with minimum degree $n/2$

Table 2.13: Hamiltonicity of connected 10-vertex graphs up to isomorphism by vertex connectivity.

Vertex connectivity	Non-Ham.	Ham.	% Ham.
1	1 973 029	0	0
2	424 177	4 205 286	90.84
3	14 177	3 888 167	99.64
4	70	1 109 035	99.99
5	0	99 419	100
6	0	3124	100
7	0	81	100
8	0	5	100
9	0	1	100

is Hamiltonian. This follows since any graph with a vertex connectivity of $n/2$ must have a minimum degree of $n/2$.

Restricting our attention to cubic graphs, and considering all such graphs up to order 20, Table 2.14 displays a strong correlation between connectivity and Hamiltonicity. Indeed, 87.2% of the non-Hamiltonian cubic graphs have connectivity 1, followed by 6.8% having connectivity 2 and the remaining 6.0% having connectivity 3. This is the case, despite graphs with connectivity 2, and especially connectivity 3, being far more common than graphs of lesser connectivity. Treating connectivity as an indicator of the likelihood of a graph being non-Hamiltonian, approximately 1 in 100 of the connectivity 2 graphs were non-Hamiltonian, while only 1 in 435 of the connectivity 3 graphs were non-Hamiltonian. Furthermore, as shown Table 2.15, the differences in proportions appear to increase with order.

Excluding the trivial case of bridge graphs, the measure of connectivity on its own has very poor sensitivity and specificity for classifying cubic graphs as Hamiltonian or non-Hamiltonian. A contingency table, effectively a summary of the data in Table 2.14, is shown in Table 2.16. In a probabilistic sense, it seems that non-Hamiltonian graphs with connectivity 3 are rarer, and hence more difficult to detect as such than for graphs with con-

Table 2.14: The number of (a) non-Hamiltonian, and (b) Hamiltonian cubic graphs up to order 20 by connectivity and number of vertices.

(a) Non-Hamiltonian					(b) Hamiltonian				
n	Connectivity			Total	n	Connectivity			Total
	1	2	3			1	2	3	
4	0	0	0	0	4	0	0	1	1
6	0	0	0	0	6	0	0	2	2
8	0	0	0	0	8	0	1	4	5
10	1	0	1	2	10	0	4	13	17
12	4	0	1	5	12	0	23	57	80
14	29	2	4	35	14	0	137	337	474
16	186	15	18	219	16	0	1031	2810	3841
18	1435	117	114	1666	18	0	9281	30354	39635
20	12671	979	848	14498	20	0	100689	395302	495991
Total	14326	1113	986	16425	Total	0	111166	428880	540046

Table 2.15: The percentage of cubic graphs up to order 20 that are Hamiltonian by connectivity and number of vertices.

n	Connectivity			
	1	2	3	All
4			100	100
6			100	100
8		100	100	100
10	0	100	92.86	89.47
12	0	100	98.28	94.12
14	0	98.56	98.83	93.12
16	0	98.57	99.36	94.61
18	0	98.76	99.63	95.97
20	0	99.04	99.79	97.16
All	0	99.01	99.77	97.05

Table 2.16: Contingency table for cubic graphs up to order 20 by Hamiltonicity and connectivity.

Connectivity	Hamiltonian	Non-Hamiltonian	Total
1	0	14 326	14 326
2	111 166	1113	112 279
3	428 880	986	429 886
Total	540 046	16 425	556 471

Table 2.17: Contingency table for non-Hamiltonian cubic graphs up to order 20 by Base Model feasibility and connectivity.

Connectivity	Feasible	Infeasible	Total
1	0	14 326	14 326
2	636	477	1113
3	986	0	986
Total	1622	14 803	16 425

nectivity 2. We also consider how connectivity relates to accurate detection of non-Hamiltonian graphs by the Base Model. The results shown in Table 2.17 clearly demonstrate that non-Hamiltonian graphs with connectivity 3, though less common, are much more difficult to identify using the Base Model. Indeed, none of the 968 graphs with connectivity 3 were detected as non-Hamiltonian, in contrast to 477 out of 1113, or 40%, of the non-Hamiltonian graphs with connectivity 2, and 100% of the non-Hamiltonian graphs with connectivity 1.

2.3.2 Graph toughness

A related concept to connectivity is that of *toughness*. Graph toughness was introduced by Chvátal in 1973 and described as “[measuring] in a simple way how tightly various pieces of a graph hold together” [15]. While connectivity measures the number of vertices or edges that must be removed just to disconnect a graph, toughness measures the most economical ratio of vertices removed to the resulting number of connected components.

Definition 2.18 (*t*-tough graph). A graph is said to be *t*-tough if, for every integer $k \geq 2$, the removal of fewer than tk vertices always results in fewer than k connected components.

Definition 2.19 (Graph toughness). The *toughness* $\tau(G)$ of a graph G is the maximum value t for which G is *t*-tough. If G is a complete graph then it is necessarily *t*-tough for every value of t , thus in this case we say $\tau(G) = \infty$.

The minimum toughness of a cubic graph is $1/3$, when a single vertex may be removed to give 3 connected components. The maximum toughness of a cubic graph, excluding K_4 which has infinite toughness by definition, is $3/2$, when exactly three vertices must be removed to disconnect the graph into two connected components. Toughness and Hamiltonicity are known to be related. In particular, any graph with a toughness less than 1 is known to be non-Hamiltonian [15], and it remains an open problem as to whether there is a t_0 such that all t_0 -tough graphs are necessarily Hamiltonian [12]. Certainly in the case of $3/2$ -tough graphs, the maximum for non-complete cubic graphs, there are both Hamiltonian and non-Hamiltonian graphs. We note that 1-toughness being a necessary condition for Hamiltonicity makes it a special case, so 1-tough graphs are simply called *tough* while graphs with toughness less than 1 are called *non-tough*. An obvious example of a non-tough graph is a graph with vertex connectivity 1; the graph can be broken into two connected components by removing one vertex, and so it must have toughness no larger than $1/2$.

Figure 2.18 shows a number of minimal examples of tough and non-tough cubic graphs; the smallest cubic graphs with toughnesses $1/3$, $1/2$, 1, and $3/2$, as well as the smallest non-Hamiltonian graph with (maximal) toughness $3/2$. To find the smallest non-Hamiltonian cubic graph with toughness $3/2$, Theorem 2.21 due to Jackson and Katerinis [44] was utilised. Since the 10-vertex Petersen graph is the uniquely smallest 3-connected non-Hamiltonian cubic graph, its inflation (replacing all the vertices with triangles, under

which Hamiltonicity is invariant) must therefore be the uniquely smallest $3/2$ -tough non-Hamiltonian cubic graph.

Definition 2.20 (Graph inflation [15]). Let $G = (V, E)$ be a cubic graph. The *inflation* of G is the graph G^* obtained by first replacing each vertex of G with a copy of K_3 . Then, for each vertex $v \in V$ in the original graph G , consider its three incident edges. For each of these edges, let there be a corresponding edge in G^* , such that these three corresponding edges are each incident to a different vertex of the copy of K_3 that corresponds to v . The resulting graph is cubic and has $3|V|$ vertices.

Theorem 2.21 (Characterisation of $3/2$ -tough cubic graphs [44]). *Let G be a cubic graph. Then G is $3/2$ -tough if and only if $G = K_4$, $G = K_2 \times K_3$, or G is the inflation of a 3-connected-cubic graph.*

Unlike connectivity which can be determined for cubic graphs in polynomial time, the decision problem of determining whether a graph is (1-)tough is NP-hard [4], even when only cubic graphs are considered [5]. Consequently, the best known algorithms for determining graph toughness take exponential time, and this prevents toughness from being a useful diagnostic criterion in determining Hamiltonicity.

Table 2.19 shows the distribution of toughness for cubic graphs up to order 20. The most common toughness for this collection of graphs was 1 (30% of the total), followed closely by graphs with toughness $9/8$ (28% of the total). Toughness was calculated by removing every possible subset of k vertices, from $k = 1$ to $|V| - 2$, and counting the number of resulting connected components, finding the lowest possible value of $t = \frac{k}{\text{components}}$ whenever there are at least two connected components. The maximum possible number of connected components after removing k vertices is $|V| - k$, so the processing may stop once the current bound for t is less than $\frac{k}{|V| - k}$ for all remaining values of k . Note that counting the number of connected components at each

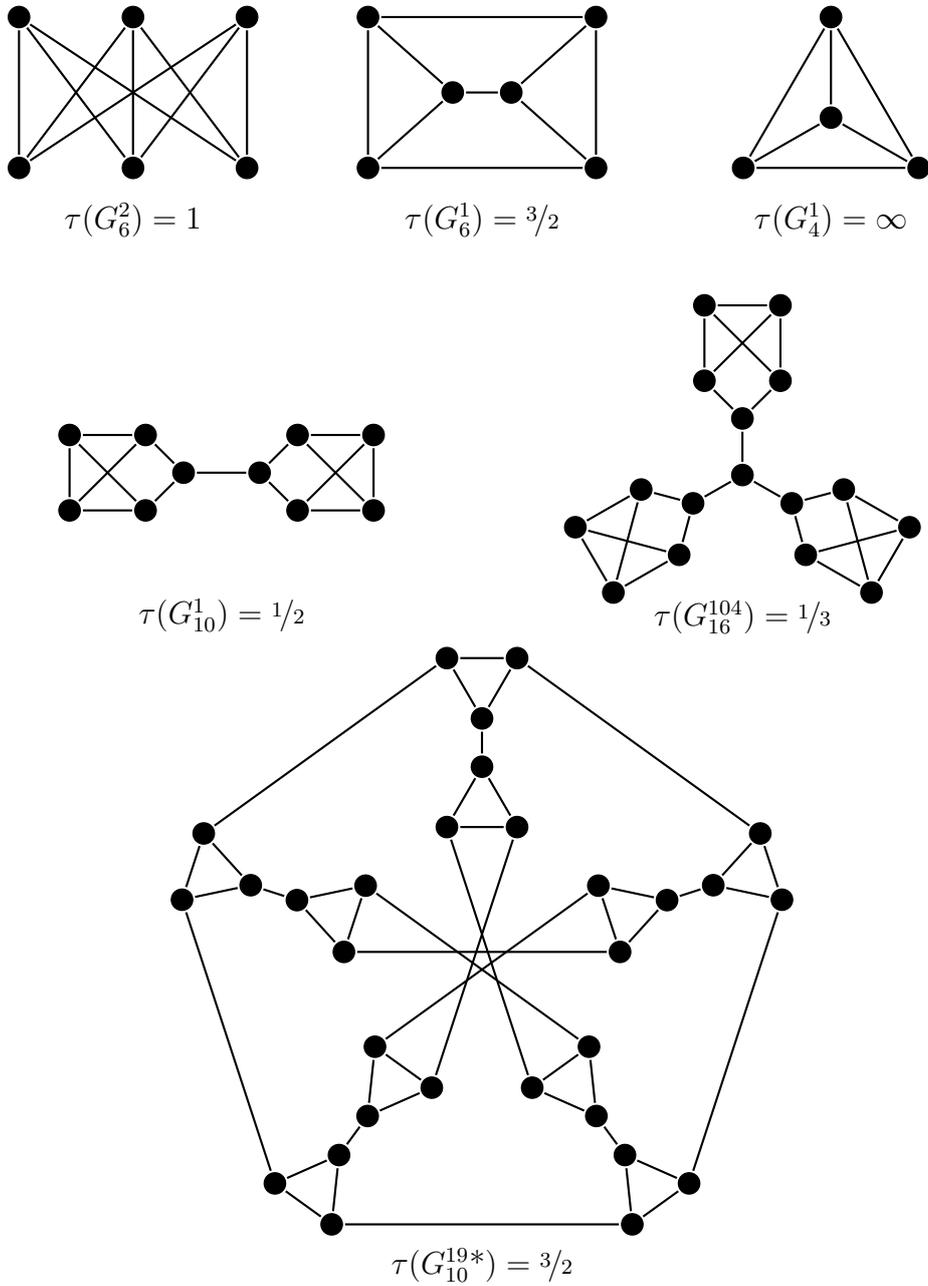


Figure 2.18: Selected examples of tough and non-tough cubic graphs. The top row, from left to right, shows the uniquely smallest cubic graphs with toughness 1, with toughness $3/2$, and with toughness ∞ . The middle row, from left to right, shows the uniquely smallest cubic graph with toughness $1/2$ and with toughness $1/3$. The bottom graph shows the smallest non-Hamiltonian graph with toughness $3/2$, the inflated Petersen graph (see Figure 1.3 for the uninflated graph).

Table 2.19: Hamiltonian and non-Hamiltonian cubic graphs up to order 20 by toughness.

Toughness	Non-Hamiltonian	Hamiltonian
$1/3$	34	0
$1/2$	14 292	0
$2/3$	230	0
$3/4$	41	0
$4/5$	16	0
$5/6$	6	0
1	1077	164 630
$10/9$	0	48 924
$9/8$	147	157 809
$8/7$	179	77 089
$7/6$	134	31 642
$6/5$	146	18 741
$5/4$	95	38 094
$9/7$	24	2972
$4/3$	3	131
$7/5$	0	6
$10/7$	1	3
$3/2$	0	4
∞	0	1

step may be done more easily if every step only removes or restores a single vertex from the graph; this can be done without repeating any subset by using a monotonic Gray code [65]. We remark that there is an interesting coincidence here with respect to HCP; Gray codes are themselves Hamiltonian cycles on the vertices of a hypercube.

In Table 2.20 we consider all non-Hamiltonian cubic graphs containing up to order 20, partitioned by their toughness. In each case, we give the number of graphs with feasible and infeasible LPs in the Base Model. As the table shows, all tested non-tough graphs, which are necessarily non-Hamiltonian, induce infeasibility. Interestingly, it is also the case that every graph tested with a toughness exceeding 1 has a feasible Base Model LP.

Conducting the same experiment with MCF_{HCP} , $MCF+_{HCP}$ and SST_{HCP} , we found that all the tested non-tough cubic graphs induce infeasibility in these models just as in the Base Model. These experiments suggest that toughness is a necessary condition for feasibility of the four models. We will

Table 2.20: Base Model feasibility for non-Hamiltonian cubic graphs up to order 20 by toughness.

Toughness	Infeasible	Feasible
$1/3$	34	0
$1/2$	14 292	0
$2/3$	230	0
$3/4$	41	0
$4/5$	16	0
$5/6$	6	0
1	184	893
$9/8$	0	147
$8/7$	0	179
$7/6$	0	134
$6/5$	0	146
$5/4$	0	95
$9/7$	0	24
$4/3$	0	3
$10/7$	0	1

show, by Theorem 2.23 below, that this is indeed the case for any model which includes constraints equivalent to or stronger than the constraints of DFJ. This result therefore applies to MCF_{HCP} , $\text{MCF}_{+\text{HCP}}$ and SST_{HCP} , since the weakest of them, MCF_{HCP} , is equivalent to DFJ. For the Base Model, however, it is unknown whether constraints equivalent to those of DFJ are implied, so we make the following conjecture.

Conjecture 2.22. *Non-toughness is a sufficient condition for infeasibility of the Base Model.*

Recall that in Section 2.2.6 we presented a partial proof that the Base Model implies constraints equivalent to those of DFJ. If the remaining components of that proof were established, Conjecture 2.22 would follow immediately from Theorem 2.23.

Theorem 2.23. *If $G = (V, E)$ is a non-tough graph, then the LP from the DFJ model is infeasible.*

Proof. Since G is non-tough, by definition it is possible to remove fewer than k vertices and be left with k connected components, for some integer

$k > 1$. Denote by V_0 the set of removed vertices, and let V_t denote the set of vertices in the t -th connected component that remains when V_0 is removed for $t = 1, \dots, k$. Then V_0, \dots, V_k is a partitioning of the vertices of the graph, such that $|V_0| < k$, and every edge $uv \in E$ where $u \in V_t$ and $v \in V_s$ satisfies $t = s$, $t = 0$, or $s = 0$.

Now, recall the subtour elimination constraints (2.3) of the DFJ model,

$$\sum_{i \in S} \sum_{j \notin S} (x_{ij} + x_{ji}) \geq 2 \quad \forall S \subset V, 0 < |S| < n.$$

The constraints of DFJ are posed for complete graphs. Rather than modify the constraints to remove x_{ij} variables which do not correspond to arcs in G , we may instead assume, without loss of generality, that $x_{ij} = x_{ji} = 0$ if $ij \notin E$. Next, if we take $S = V_t$ for $t = 1, \dots, k$, and sum each corresponding inequality (2.3), we obtain

$$\sum_{t=1}^k \sum_{i \in V_t} \sum_{j \notin V_t} (x_{ij} + x_{ji}) = \sum_{i \notin V_0} \sum_{j \in V_0} (x_{ij} + x_{ji}) \geq 2k. \quad (2.97)$$

However, from (2.1) and (2.2) we have the following:

$$\sum_{i \notin V_0} (x_{ij} + x_{ji}) \leq 2,$$

and since $|V_0| < k$, this implies

$$\sum_{j \in V_0} \sum_{i \notin V_0} (x_{ij} + x_{ji}) < 2k. \quad (2.98)$$

Clearly, (2.97) and (2.98) cannot both be true, and so a contradiction is obtained. Hence, (2.97) cannot be satisfied and the LP from the DFJ model is infeasible for G . \square

As noted earlier, determining if a graph is tough is an NP-hard problem, but here we can identify almost all of the considered tough graphs by feasibility of an LP model. If any of the models were to be feasible *only* for tough graphs, then it would imply that $P = NP$. Hence, it is interest-

ing to consider the tough graphs with infeasible LPs, which must necessarily be non-Hamiltonian. From Table 2.20, it appears that these instances are relatively rare, and perhaps, only occur for graphs with toughness precisely equal to 1. Ironically, the poorer performance of a model such as MCF_{HCP} relative to the Base Model is an advantage in this context, as fewer tough graphs induce infeasibility. If these graphs could be characterised and efficiently identified, then that would provide a polynomial-time algorithm for recognising tough graphs. Figure 2.21 shows the uniquely smallest example of a tough cubic graph that induces infeasibility in the Base Model. In fact, the 16-vertex graph shown induces infeasibility in all four of MCF_{HCP} , $\text{MCF}^+_{\text{HCP}}$, SST_{HCP} and the Base Model. Note the similarity between the graph in Figure 2.21 and the graph in Figure 2.7, which also induced infeasibility in these four models. Attempting to characterise all such graphs is a ripe topic for future research.

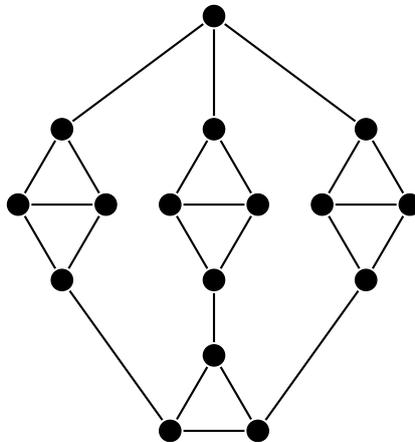


Figure 2.21: The smallest tough cubic graph that induces infeasibility in each of MCF, MCF+, SST and the Base Model. The graph, G_{16}^{547} , has a toughness of exactly 1.

2.4 Concluding remarks on the Base Model

Although the Base Model appears to be strictly stronger than MCF+, and stronger than SST in the average case, the benefits gained in terms of HCP

are minimal. Indeed, only an additional 98 (4.7%) of the 2099 instances of NHNB20 are identified by the Base Model compared to MCF+ and SST. It is therefore desirable to attempt to improve upon the Base Model, particularly in the context of determining non-Hamiltonicity. Such improvements logically fall into two categories. Either we can attempt to modify the graphs to make them more suitable for the Base Model, without altering their Hamiltonicity, or we can attempt to improve the Base Model directly.

To this end, it is natural to consider whether the 1622 instances of NHNB20 with feasible Base Model LPs described in Section 2.2.2 tend to have any identifiable properties that we can exploit to improve the Base Model. One such property that we have identified is the presence of symmetries, with 1437 (88.6%) of the instances having a non-trivial automorphism group. Another property is the presence of certain structures within the graph; for example, cubic graphs often contain at least one triangle.

In Chapter 3 we therefore consider a number of graph reductions, which permit us to remove edges or vertices from a graph without changing the Hamiltonicity. As will be shown in that chapter, this is particularly effective on graphs with non-trivial automorphism groups. We also consider graph reductions based on the presence of structures such as triangles. After reducing the graphs for which this is possible, it will be shown that many of them can then be identified as non-Hamiltonian immediately, while others induce infeasibility in the Base Model after being reduced. This provides us with an effective alternative approach for the instances where the Base Model does not detect non-Hamiltonicity. Then, to further assist in the identification of non-Hamiltonian graphs, in Chapter 4 we consider extensions to the Base Model that allow us to identify many of the remaining instances.

Chapter 3

Hamiltonicity-preserving graph reductions

In this chapter a method is presented that can, in many cases, reduce the size of instances of the Hamiltonian cycle problem (HCP) and thus reduce the computational complexity of identifying their Hamiltonicity. The method works by attempting to identify edges or vertices in the graph that can be removed in a way that preserves Hamiltonicity. These edges and vertices are identified through examination of the graph's structure and symmetries. Results of applying the method to cubic graphs are presented, along with the performance of the Base Model on the resulting reduced graphs.

As introduced in Section 1.1, HCP is an NP-complete problem, and to date there is no known method that can determine if an arbitrary graph is Hamiltonian in polynomial time. In the case of cubic graphs with n vertices, the best known exact algorithms¹ have time complexity $\mathcal{O}(1.276^n)$ by Epstein [23], $\mathcal{O}(1.251^n)$ by Iwama and Nakashima [43], and recently $\mathcal{O}(1.2312^n)$ by Xiao and Nagamochi [75]. In light of this, any reduction in the size of the instance will reduce the time required to solve it by an exponential factor.

¹These algorithms are designed for the travelling salesman problem but any instance of HCP may be easily expressed as an instance of TSP.

For example, if it were possible to reduce the number of vertices in a cubic graph by k vertices for a given instance in polynomial time, while ensuring the solution to the problem were the same, then the required time could be reduced by factor of at least 1.2312^k with current techniques.

To formalise the concept of reducing the size of a graph while maintaining the same HCP solution, we introduce the concepts of a *Hamiltonicity-preserving graph reduction* and a *graph reduction algorithm* below, before establishing their existence and introducing several such graph reductions.

Definition 3.1 (Graph reduction). Let $\psi : \mathcal{G} \rightarrow \mathcal{G}'$ be a function whose domain and codomain are sets of graphs. We say that ψ is a *graph reduction*, or simply *reduction*, if for every $G = (V, E) \in \mathcal{G}$, $\psi(G) = G' = (V', E')$ meets the conditions $|V'| \leq |V|$ and $|E'| \leq |E|$. Provided that at least one of these inequalities is strict, the reduction is called *proper* and the graph G' is called the *reduced graph* of G under ψ .

Definition 3.2 (Hamiltonicity-preserving graph reduction). A graph reduction $\psi : \mathcal{G} \mapsto \mathcal{G}'$ is said to be *Hamiltonicity-preserving* provided that G' is Hamiltonian if and only if G is Hamiltonian, for any choice of G in the domain of ψ . Equivalently, we say that such a ψ *preserves Hamiltonicity*. Such a reduction is additionally said to be *recoverable* if, given ψ and any Hamiltonian cycle in G' , it is possible to find a Hamiltonian cycle in G in polynomial time (in the number of vertices).

Note that by Definition 3.2, any Hamiltonicity-preserving graph reduction acting on a non-Hamiltonian graph is necessarily recoverable, as there can be no Hamiltonian cycles in the reduced graph.

Definition 3.3 (Graph reduction algorithm). A *graph reduction algorithm* is any method to search for a suitable reduction ψ for a given graph $G = (V, E)$. If the reduction ψ found by the method is such that $\psi(G) = (V', E')$ satisfies $|V'| < |V|$ or $|E'| < |E|$, then G is said to be *reducible* under the algorithm;

otherwise, G is said to be *irreducible* under the algorithm. The algorithm itself is said to *preserve Hamiltonicity* if, given any graph G , the returned reduction ψ preserves Hamiltonicity.

Definition 3.4 (Trivially Hamiltonian and non-Hamiltonian graphs). Let G be a connected graph. We say that G is *trivially Hamiltonian* if G is isomorphic to K_3 . Similarly, we say that G is *trivially non-Hamiltonian* if G is isomorphic to K_2 . If, instead, G has more than two vertices and is not isomorphic to either of K_2 or K_3 , then we say that G is *non-trivial*.

Figure 3.1 shows the trivially Hamiltonian and trivially non-Hamiltonian graphs as defined in Definition 3.4. Note that in this definition we implicitly leave aside the question of whether graphs with just one or zero vertices are Hamiltonian.

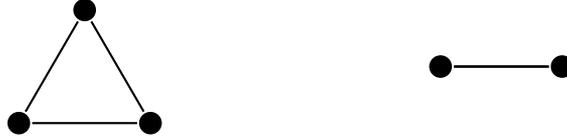


Figure 3.1: Trivially Hamiltonian graph K_3 (left) and trivially non-Hamiltonian graph K_2 (right) that are irreducible (while maintaining connectedness).

Lemma 3.5. *Let $G = (V, E)$ be a non-trivial graph. There exists a proper Hamiltonicity-preserving graph reduction ψ whose domain contains G .*

Proof. Suppose G is non-Hamiltonian. Any edge may be removed and the resulting graph will remain non-Hamiltonian. The reduction ψ can be defined to remove any edge in E and (non-)Hamiltonicity is preserved.

Alternatively, suppose G is Hamiltonian. Let $v_1, \dots, v_n \in V$ trace out a Hamiltonian cycle in G . Since G is non-trivial, it is not isomorphic to K_3 , implying $n \geq 4$. Define ψ that removes v_n and its incident edges from G while adding an edge v_1v_{n-1} if it is not present. It is clear that v_1, \dots, v_{n-1} will be a Hamiltonian cycle in $\psi(G)$, thus ψ preserves Hamiltonicity. \square

Lemma 3.5 guarantees the existence of proper graph reductions for any non-trivial graph. However, unless $P = NP$, there cannot exist a polynomial-time algorithm that, given any non-trivial graph, is guaranteed to find a proper reduction. If there were such an algorithm, it could be used to solve HCP for any graph in polynomial time by repeated application (no more times than the number of edges and vertices) until the graph became trivially (non-)Hamiltonian, thus solving HCP in polynomial time. Therefore, in practice we restrict our focus to developing a polynomial-time graph reduction algorithm, with the expectation that many graphs will be irreducible under the algorithm.

Rather than trying to design a single graph reduction to be as general as possible, we will instead introduce many specialised graph reductions and a method to find compositions of such reductions. We now show that key properties of the individual reductions extend to the composition of those reductions.

Lemma 3.6. *If the function $\psi = \psi_k \circ \dots \circ \psi_2 \circ \psi_1$ is the composition of k Hamiltonicity-preserving graph reductions, then ψ also preserves Hamiltonicity. Additionally, if ψ_1, \dots, ψ_k are proper and recoverable graph reductions, then ψ is also proper and recoverable.*

Proof. Firstly, if $k = 1$ then the result is trivial. Assume then that the proposition holds for the composition of $k - 1$ reductions; the proof will proceed by induction: Let G be a graph in the domain of ψ and let $\psi' = \psi_{k-1} \circ \dots \circ \psi_1$. Given that ψ_k is Hamiltonicity-preserving, $\psi_k(\psi'(G)) = \psi(G)$ has the same Hamiltonicity as $\psi'(G)$, which by the induction assumption has the same Hamiltonicity as G . Thus ψ preserves Hamiltonicity.

Similarly, if ψ_1, \dots, ψ_k are proper and recoverable graph reductions, then given any Hamiltonian cycle in $\psi_k(\psi'(G))$, we can recover a Hamiltonian cycle in $\psi'(G)$ in polynomial time. By the induction assumption, given this

Hamiltonian cycle in $\psi'(G)$, it is then possible to find a Hamiltonian cycle in G in the sum of $k - 1$ separate polynomial times. As ψ_1, \dots, ψ_k are proper reductions, k cannot exceed the combined number of edges and vertices in G , $\mathcal{O}(n^2)$. Therefore, the total time elapsed remains polynomial in the number of vertices and ψ is recoverable. Further, since each of ψ_1, \dots, ψ_k is proper, it immediately follows that ψ is also proper. \square

In the first stage of any reduction algorithm, it may be beneficial to check sufficient or necessary conditions for Hamiltonicity or non-Hamiltonicity, at least when these conditions can be checked in polynomial time. For example, a necessary condition for a graph G to be Hamiltonian is that it must be 2-connected. Another example is Ore's Theorem [59] shown below, which gives a sufficient condition for Hamiltonicity; equivalently, the contrapositive provides a necessary condition for non-Hamiltonicity. There are other sufficient or necessary conditions that may be checked (see [72, 33, 26]) but in our algorithm we will just check for 2-connectivity and the conditions of Ore's Theorem.

Theorem 3.7 (Ore's Theorem [59]). *Let $G = (V, E)$ be a graph with $|V| \geq 3$ vertices. The graph G is Hamiltonian if*

$$\deg(u) + \deg(v) \geq |V| \quad \forall u, v \in V \text{ where } u \neq v \text{ and } uv \notin E.$$

If the Hamiltonicity of a graph is determined by checking sufficient or necessary conditions, we may apply the appropriate graph reduction ψ_H or ψ_{NH} , defined as follows. These are defined for use later in Section 3.5.

Definition 3.8 (ψ_H graph reduction). We define the constant function ψ_H to return the trivially Hamiltonian graph K_3 , namely

$$\psi_H(G) = K_3.$$

Domain of ψ_H : The set of all Hamiltonian graphs.

Definition 3.9 (ψ_{NH} graph reduction). We define the constant function ψ_{NH} which returns the trivially non-Hamiltonian graph K_2 , namely

$$\psi_{\text{NH}}(G) = K_2.$$

Domain of ψ_{NH} : The set of all non-Hamiltonian graphs.

By the definitions of ψ_{H} and ψ_{NH} , it is clear that both reductions preserve Hamiltonicity. Also, ψ_{NH} is recoverable by definition, since the reduced graph contains no Hamiltonian cycles. Unfortunately, ψ_{H} is not necessarily recoverable. That is, knowing the obvious Hamiltonian cycle in the reduced graph K_3 does not help us find a Hamiltonian cycle in the original graph. However, in practice we only apply ψ_{H} to graphs that meet the conditions of Ore's Theorem. As noted in [61], the argument used by Ore to prove the theorem effectively constitutes a polynomial-time algorithm to find Hamiltonian cycles in graphs meeting the conditions. Therefore, if we restrict the domain of ψ_{H} to graphs satisfying Ore's Theorem, which we have in the upcoming algorithm, then ψ_{H} is recoverable.

In contrast to testing a sufficient condition for Hamiltonicity, it will be shown that there are also occasions where the structure of a graph makes a particular Hamiltonian cycle evident. To handle such cases where a Hamiltonian cycle is serendipitously identified during our search for applicable reductions, we introduce ψ_{hcycle} , defined below.

We remark that due to the number of graph reductions introduced in this chapter, descriptive subscripts are used for graph reductions to avoid confusion. This and later graph reductions are parametrised families of functions with parameters listed in square brackets.

Definition 3.10 ($\psi_{\text{hcycle}}[v_1, \dots, v_n]$ graph reduction). Given a graph $G = (V, E)$ and vertices v_1, \dots, v_n that trace out a Hamiltonian cycle in G , we define $\psi_{\text{hcycle}}[v_1, \dots, v_n]$ to remove any edge in E other than those in the

cycle, namely

$$\psi_{\text{hcycle}}[v_1, \dots, v_n](G) = (V, \{v_1v_2, \dots, v_{n-1}v_n, v_nv_1\}).$$

Domain of $\psi_{\text{hcycle}}[v_1, \dots, v_n]$: The set of graphs $G = (V, E)$ satisfying

- (i) $V = \{v_1, \dots, v_n\}$
- (ii) $v_1v_2, \dots, v_{n-1}v_n, v_nv_1 \in E$.

Since ψ_{hcycle} is only defined for Hamiltonian graphs and outputs a cycle graph, it is clear that it preserves Hamiltonicity. Given the Hamiltonian cycle in the reduced graph it may be seen that all the same edges must be present in the original graph and hence ψ_{hcycle} is also recoverable.

3.1 Graph reductions based on subgraphs

When it is not possible to reduce a graph based on checking a necessary or sufficient condition, we then begin to look at structures within the graph that could lead to other reductions. For example, one common structure in graphs is the triangle, which is a well-known example of a subgraph that can be replaced with a single vertex in many instances [73]. In particular, triangles may be contracted to a single vertex without altering the Hamiltonicity of the graph under the conditions described in Proposition 3.12 below, which utilises the following well-known lemma.

Lemma 3.11. *Let $G = (V, E)$ be a graph and let $\{V_1, V_2\}$ be a partition of V . Let E_{12} be the set $\{uv \in E \mid u \in V_1 \text{ and } v \in V_2\}$; that is, the subset of edges with an endpoint in each part. The total number of edges in E_{12} used in any given Hamiltonian cycle of G must be a positive even integer.*

For an illustration of the operation described in the following proposition, refer to Figure 3.2.

Proposition 3.12. *Let $G = (V, E)$ be a graph with $|V| \geq 5$ having three degree-3 vertices $u, v, w \in V$ such that the subgraph induced by $\{u, v, w\}$ is a triangle. Let $G' = (V', E')$ be an altered copy of G wherein the vertices v and w have been contracted into vertex u ; that is, v and w have been removed from the set of vertices, and edges from u to all the other originally adjacent vertices of v and w have been added where not already present. Then G' will be Hamiltonian if and only if G is Hamiltonian.*

Proof. Note that the vertices $\{u, v, w\}$ are connected to $V \setminus \{u, v, w\}$, the remainder of the vertices in G , via exactly three edges. Let these three edges be denoted by ua, vb and wc for the edges respectively incident to u, v and w . Note that the other endpoints a, b and c are not necessarily distinct ($1 \leq |\{a, b, c\}| \leq 3$).

Suppose that G' is Hamiltonian. Let C' be any Hamiltonian cycle in G' . Then C' must use exactly two edges incident to u , that is, two edges from $\{au, bu, cu\}$. Without loss of generality, suppose that edges au and bu are used in C' . Then C' can be viewed as a path P from a to b that avoids vertex u and visits all other vertices, plus au and bu . It is clear that P also exists in G , visiting all vertices other than u, v and w . Thus, a Hamiltonian cycle in G can be formed by $C = P \cup \{ua, uv, vw, vb\}$. An equivalent argument can be made for C' containing au and cu , or bu and cu . Hence, if G' is Hamiltonian, G must be as well.

Now, suppose that G is Hamiltonian. By Lemma 3.11, any Hamiltonian cycle C in G must use exactly two edges of $\{ua, vb, wc\}$, and hence C in G visits all three vertices of the triangle consecutively before traversing the rest of the graph. Without loss of generality, suppose C starts at u , then goes to w , then v . Then C can be defined as $\{uw, wv, vb, ua\} \cup P$, with P defined as earlier. Then a Hamiltonian cycle C' exists in G' , defined as $P \cup \{au, bu\}$. Hence, G' is Hamiltonian if and only if G is Hamiltonian. \square

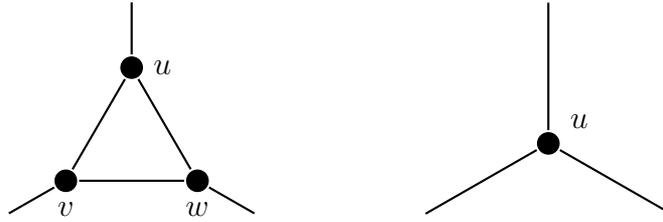


Figure 3.2: A triangle u, v, w of degree-3 vertices in a graph before (left) and after (right) contracting vertices v and w into vertex u . In the resulting graph, u has between 1 and 3 incident edges; one for each distinct neighbour of u, v and w in the original graph (shown here with 3).

Given our particular interest in solving HCP for cubic graphs, it is notable that a majority of cubic graphs contain at least one triangle. Precisely, it has been established [74] that the probability of a random labelled cubic graph containing no 3-cycles asymptotically approaches $e^{-4/3}$ as $|V| \rightarrow \infty$. Therefore, the probability that a random labelled cubic graph contains at least one triangle (3-cycle) approaches $1 - e^{-4/3} \approx 73.6\%$. For every such cubic graph apart from K_4 , the number of vertices can then be reduced by at least 2 while maintaining Hamiltonicity, as shown in Proposition 3.12. Furthermore, it is straightforward to find triangles in polynomial time (for example, by checking if any pair of adjacent vertices has a common neighbour).

In practice, it is useful to distinguish two cases involving triangles of degree-3 vertices: (i) Triangles where each vertex in the triangle has a distinct neighbour outside the triangle; and (ii) triangles where two vertices in the triangle share a common degree-3 neighbour outside the triangle. The latter situation corresponds to a subgraph which is sometimes called a diamond (see Figure 3.3, left.) To handle these two cases we now introduce the graph reductions ψ_{triangle} and ψ_{diamond} .

Definition 3.13 ($\psi_{\text{triangle}}[u, v, w]$ graph reduction). Given a graph $G = (V, E)$ and vertices $u, v, w \in V$ forming a triangle in G , we define the graph reduction $\psi_{\text{triangle}}[u, v, w]$ to contract v and w into the remaining vertex u as

shown in Figure 3.2. That is,

$$\begin{aligned}\psi_{\text{triangle}}[u, v, w](G) &= G' = (V', E'), \\ \text{where } V' &= V \setminus \{v, w\}, \\ E' &= \{ab \in E \mid a, b \notin \{v, w\}\} \\ &\quad \cup \{ub \mid b \in N(v) \cup N(w)\}.\end{aligned}$$

Domain of $\psi_{\text{triangle}}[u, v, w]$: The set of all graphs $G = (V, E)$ where the three vertices $u, v, w \in V$ satisfy

- (i) $\deg(u), \deg(v), \deg(w) = 3$
- (ii) $uv, uw, vw \in E$
- (iii) $|N(u) \cup N(v) \cup N(w)| = 6$.

Definition 3.14 ($\psi_{\text{diamond}}[u, v, w, x]$ graph reduction). Given a graph $G = (V, E)$, we define the function $\psi_{\text{diamond}}[u, v, w, x]$ to contract v, w and x , three vertices of a diamond into the remaining vertex u as shown in Figure 3.3. That is,

$$\begin{aligned}\psi_{\text{diamond}}[u, v, w, x](G) &= G' = (V', E') \\ \text{where } V' &= V \setminus \{v, w, x\} \\ E' &= \{ab \in E \mid a, b \notin \{v, w, x\}\} \\ &\quad \cup \{ub \mid b \in N(x) \setminus \{v, w\}\}.\end{aligned}$$

Domain of $\psi_{\text{diamond}}[u, v, w, x]$: The set of graphs $G = (V, E)$ where the four distinct vertices $u, v, w, x \in V$ satisfy

- (i) $\deg(u), \deg(v), \deg(w), \deg(x) = 3$
- (ii) $uv, uw, vw, vx, wx \in E$
- (iii) $|N(u) \cap N(x)| = 2$.

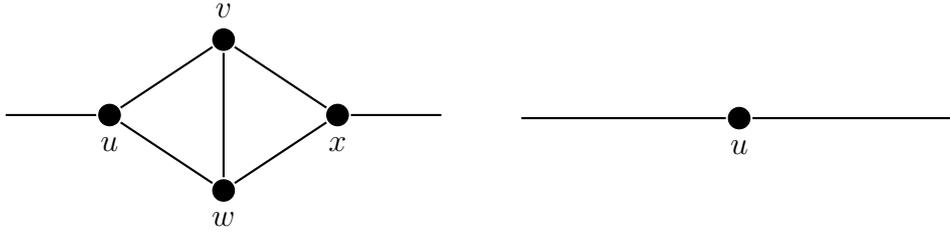


Figure 3.3: A diamond in a graph before (left) and after (right) its reduction with $\psi_{\text{diamond}}[u, v, w, x]$.

Lemma 3.15. *The reductions $\psi_{\text{triangle}}[u, v, w]$ and $\psi_{\text{diamond}}[u, v, w, x]$ preserve Hamiltonicity and are recoverable.*

Proof. First consider ψ_{triangle} . It follows as a direct consequence of Proposition 3.12 that ψ_{triangle} preserves Hamiltonicity, and given any Hamiltonian cycle in the reduced graph the argument made in Proposition 3.12 may be used to recover a Hamiltonian cycle in the original graph.

Next consider ψ_{diamond} . It is clear that $\psi_{\text{diamond}}[u, v, w, x]$ is equivalent to contracting the triangle uvw by applying Proposition 3.12 and then combining u and x into one vertex by contracting the edge between them. Since u and x have degree 2, it is clear that this preserves Hamiltonicity, and the Hamiltonian cycle in the original graph can be recovered accordingly. \square

3.2 Graph reductions based on Hamiltonian and non-Hamiltonian edges

In this section we consider two useful graph reductions that are applicable in certain situations. In particular, if we know that an edge must be used in all Hamiltonian cycles, or if we know that an edge cannot be used in any Hamiltonian cycle, then under certain additional conditions graph reductions are possible. We begin by defining the concepts of *redundant edges*, *Hamiltonian edges*, *non-Hamiltonian edges*, and *forced edges*.

Definition 3.16 (Redundant edge). An edge uv of a graph $G = (V, E)$ is said to be *redundant* if removing the edge does not affect the Hamiltonicity; that is, G is Hamiltonian if and only if $G' = (V, E \setminus \{uv\})$ is Hamiltonian.

An edge that is not redundant must therefore be one whose removal changes the graph from being Hamiltonian to being non-Hamiltonian, since a non-Hamiltonian graph cannot be made Hamiltonian through the removal of an edge. In general, a redundant edge may be used in some but not all of the Hamiltonian cycles of a graph.

It is useful to also have terms for edges used in *all* of the Hamiltonian cycles, and edges used in *none* of the Hamiltonian cycles of a graph.

Definition 3.17 (Hamiltonian and non-Hamiltonian edges). An edge that is used in every Hamiltonian cycle of a graph will be called a *Hamiltonian edge*. On the other extreme, an edge not used in any Hamiltonian cycle of a graph will be called a *non-Hamiltonian edge*.

To avoid ambiguity, we remark that in the case of a non-Hamiltonian graph, where every edge is used in all (zero) yet also none of the Hamiltonian cycles, we will say that every edge of a non-Hamiltonian graph is both Hamiltonian and non-Hamiltonian. This flexibility of notation is necessary as the Hamiltonicity of a graph under consideration will typically not be known in advance. Note that in earlier literature, Hamiltonian edges and non-Hamiltonian edges are sometimes called *a-edges* and *b-edges* respectively [39]. Note also that, by definition, non-Hamiltonian edges are necessarily redundant.

In general, determining whether any given edge is redundant, Hamiltonian, non-Hamiltonian, or in none of these categories, is as difficult as solving HCP. However, there are some special cases where we can efficiently (in polynomial time) identify Hamiltonian edges or non-Hamiltonian edges from the structure of a graph. In practice then, it is useful to distinguish be-

tween the set of all Hamiltonian edges of a graph, which may not be known *a priori*, and the subset of Hamiltonian edges that have been deduced as such by some efficient calculation. Henceforth, the latter will be referred to as *forced edges*,² defined as follows.

Definition 3.18 (Forced edges). Given a graph $G = (V, E)$, a subset of the edges $F \subseteq E$ is said to be *forced* if every edge of F is known to be a Hamiltonian edge. For convenience, we additionally define $F(v) \subseteq V$ to be the subset of vertices that are adjacent to $v \in V$ using an edge in F .

Observe that if $|F(v)| > 2$ for any vertex $v \in V$, then G is necessarily non-Hamiltonian. This condition will be checked as part of the upcoming graph reduction algorithm.

One efficient test for Hamiltonian edges, which will be used in the upcoming graph reduction algorithm to identify a set of forced edges F , is given in Lemma 3.19 as follows.

Lemma 3.19. *Let $G = (V, E)$ be a graph, let $e \in E$ be an edge in G , and let $G' = (V, E \setminus \{e\})$ be the graph obtained by removing the edge e . A sufficient condition for e to be a Hamiltonian edge is that G' is not 2-connected.*

Proof. All Hamiltonian graphs are known to be 2-connected. Since G' is not 2-connected, there cannot be a Hamiltonian cycle using the edges of G' . Therefore, if G has a Hamiltonian cycle it must necessarily pass through the edge e . Alternatively, if G is not Hamiltonian, then e is a Hamiltonian edge by definition. \square

The following result follows immediately from Definition 3.18.

Lemma 3.20. *Let $G = (V, E)$ be a graph, let $v \in V$ be a vertex, and let $F \subseteq E$ be a set of forced edges. If $|F(v)| = 2$ and $\deg(v) \geq 3$, v has incident non-Hamiltonian edges going to each vertex of the set $N(v) \setminus F(v)$.*

²We note that some authors have used the term forced edges as a synonym for Hamiltonian edges. However, in this thesis we make a distinction between the two terms in order to provide an algorithm that can be executed in polynomial time.

By Lemma 3.20, we define below a Hamiltonicity-preserving graph reduction $\psi_{\text{forced}}[u, v_1, \dots, v_m]$. After using this reduction, it is common for there to be a path of three or more forced edges in the graph. This can in turn be handled by another Hamiltonicity-preserving graph reduction $\psi_{\text{path}}[v_1, \dots, v_m]$ in the upcoming Definition 3.22.

Definition 3.21 ($\psi_{\text{forced}}[u, v_1, \dots, v_m]$ graph reduction). Given a graph $G = (V, E)$, we define the function $\psi_{\text{forced}}[u, v_1, \dots, v_m]$ to remove from the graph the non-Hamiltonian edges uv_1, \dots, uv_m , that is

$$\psi_{\text{forced}}[u, v_1, \dots, v_m](G) = (V, E \setminus \{uv_1, \dots, uv_m\}).$$

An example is shown in Figure 3.4.

Domain of $\psi_{\text{forced}}[u, v_1, \dots, v_m]$: The set of graphs $G = (V, E)$ having vertices $u, v_1, \dots, v_m \in V$ such that the edges $uv_1, \dots, uv_m \in E$ are all known to be non-Hamiltonian edges (for example by Lemma 3.20.)

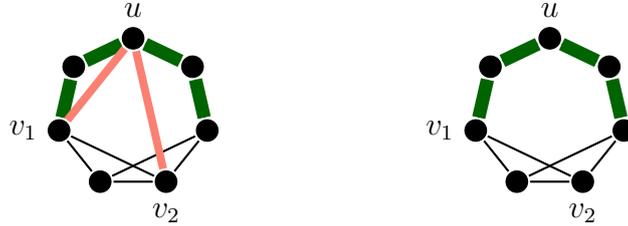


Figure 3.4: A graph with known Hamiltonian edges (green) and known non-Hamiltonian edges (red), before (left) and after (right) its reduction with $\psi_{\text{forced}}[u, v_1, v_2]$.

Definition 3.22 ($\psi_{\text{path}}[v_1, \dots, v_m]$ graph reduction). Given a graph $G = (V, E)$, we define the function $\psi_{\text{path}}[v_1, \dots, v_m]$ for $m \geq 3$ to contract the vertices v_2, \dots, v_{m-1} into the vertex v_1 , that is

$$\psi_{\text{path}}[v_1, \dots, v_m](G) = G' = (V', E')$$

$$\text{where } V' = V \setminus \{v_2, \dots, v_{m-1}\},$$

$$E' = \{ab \in E \mid a, b \notin \{v_2, \dots, v_{m-1}\}\} \cup \{v_1 v_m\}.$$

An example is shown in Figure 3.5.

Domain of $\psi_{\text{path}}[v_1, \dots, v_m]$: The set of graphs $G = (V, E)$ satisfying

- (i) $v_1, \dots, v_m \in V$
- (ii) $v_i \neq v_j$ when $i \neq j$ and $i, j = 1, \dots, m$
- (iii) $3 \leq m \leq |V| - 1$
- (iv) $\deg(v_i) = 2$ for $i = 1, \dots, m - 1$
- (v) $v_1v_2, v_2v_3, \dots, v_{m-1}v_m \in E$.

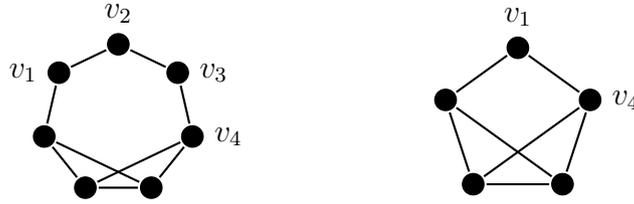


Figure 3.5: A graph with a path of degree-2 vertices, before (left) and after (right) its reduction with $\psi_{\text{path}}[v_1, v_2, v_3, v_4]$.

Lemma 3.23. *The reductions $\psi_{\text{forced}}[u, v_1, \dots, v_m]$ and $\psi_{\text{path}}[v_1, \dots, v_m]$ preserve Hamiltonicity and are recoverable.*

Proof. Consider first ψ_{forced} . It follows from Definition 3.21 that this reduction does not remove any edges that could be in a Hamiltonian cycle. Hence, any Hamiltonian cycle in the reduced graph must also exist in the original graph. Therefore, ψ_{forced} preserves Hamiltonicity and is recoverable.

Next consider ψ_{path} . Suppose there is a Hamiltonian cycle C' in the reduced graph. Since v_1 has degree 2, C' must contain v_1v_m , plus a path P from v_m to v_1 . Then a Hamiltonian cycle can be recovered in the original graph consisting of P and the edges $v_1v_2, \dots, v_{m-1}v_m$. Using an equivalent argument, it can be seen that if there is a Hamiltonian cycle C in the original graph, there is a corresponding Hamiltonian cycle in the reduced graph. Hence, ψ_{path} preserves Hamiltonicity and is recoverable. \square

3.3 Edge orbits and their classification

Another way to identify applicable graph reductions is to examine the symmetries of a graph. In the presence of certain symmetries, it is possible to take a subset of the edges of a graph and efficiently demonstrate that one or more of those edges is redundant and hence can be removed while preserving Hamiltonicity. These edge subsets are constructed from the symmetries of the graph by the action of the graph's automorphism group, defined below.

In this section we introduce the necessary background, with examples, before providing a novel classification of edge orbits. This classification will be used to identify redundant edges in the following section. The interested reader is referred to Godsil and Royle [32] for a more in-depth treatment of automorphism groups and related theory from a graph theoretic perspective.

Definition 3.24 (Graph automorphism). Given a graph $G = (V, E)$, a bijection φ from V to itself is called an *automorphism* of G if, for any pair of vertices $u, v \in V$, $\varphi(u)\varphi(v) \in E$ if and only if $uv \in E$.

Definition 3.25 (Automorphism group). Let $\Gamma = \text{Aut}(G)$ denote the set of all automorphisms of a graph G . These automorphisms form a group under the operation of composition, where the identity element is the identity map on V [40]. Any automorphisms other than the identity map, if they exist, are called *non-trivial automorphisms*. The cardinality of an automorphism group is called its *order*.

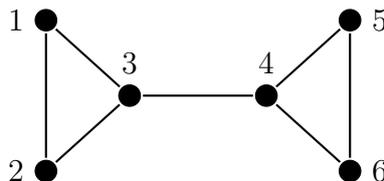


Figure 3.6: A 6-vertex graph with automorphism group of order 8.

Example 3.26. Consider the graph in Figure 3.6 and its automorphism group of order 8, $\Gamma = \{\varphi_1, \varphi_2, \dots, \varphi_8\}$ below, where each bijection on the

vertices $\{1, 2, \dots, 6\}$ is represented as a product of disjoint cycles:

$$\begin{aligned} \varphi_1 &= () & \varphi_5 &= (12)(56) \\ \varphi_2 &= (12) & \varphi_6 &= (1526)(34) \\ \varphi_3 &= (56) & \varphi_7 &= (1625)(34) \\ \varphi_4 &= (15)(26)(34) & \varphi_8 &= (16)(25)(34). \end{aligned}$$

Each non-trivial automorphism represents a symmetry of the graph. For example, φ_2 represents a reflection of the vertices 1 and 2, if we picture the other four vertices lying in a different plane. The automorphism φ_4 represents a horizontal reflection of Figure 3.6. As another example, φ_8 represents a rotation through the centre of the figure of the graph by 180 degrees. Note that $\{\varphi_2, \varphi_4\}$ is a set of generators for the whole group, meaning that any element of the group can be written as some composition of those two elements:

$$\begin{aligned} \varphi_1 &= \varphi_2^2 & \varphi_5 &= (\varphi_2 \circ \varphi_4)^2 \\ \varphi_2 &= \varphi_2 & \varphi_6 &= \varphi_2 \circ \varphi_4 \\ \varphi_3 &= \varphi_4 \circ \varphi_2 \circ \varphi_4 & \varphi_7 &= \varphi_4 \circ \varphi_2 \\ \varphi_4 &= \varphi_4 & \varphi_8 &= \varphi_2 \circ \varphi_4 \circ \varphi_2. \end{aligned}$$

It may be shown that this particular group is equivalent to the dihedral group of order 8, which is the symmetry group of a square [35].

Definition 3.27 (Asymmetric graphs). A graph is said to be *asymmetric* if it has no non-trivial automorphisms. Table 3.7 shows the number of asymmetric and non-asymmetric cubic graphs for up to 20 vertices.

See Figure 3.8 for an example of an asymmetric graph with 12 vertices; the Frucht graph, described in [29].

Definition 3.28 (Vertex and edge orbits). Given a graph $G = (V, E)$ and its automorphism group $\Gamma = \text{Aut}(G)$, the *vertex orbit* of a vertex $v \in V$,

Table 3.7: Number of asymmetric and non-asymmetric cubic graphs by order up to 20 vertices.

Vertices	Asymmetric	Non-asymmetric
4	0	1
6	0	2
8	0	5
10	0	19
12	5	80
14	103	406
16	1547	2513
18	22 124	19 177
20	327 580	182 909
Total	351 359	205 112

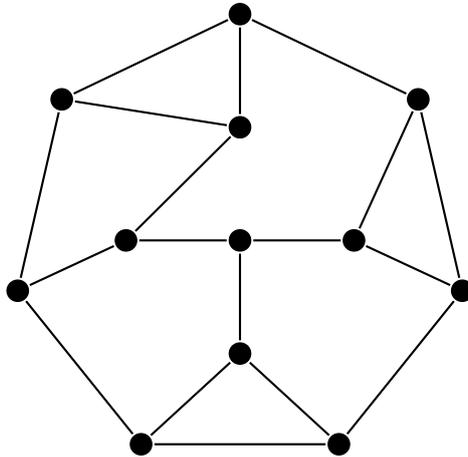


Figure 3.8: The Frucht graph, one of the five minimal asymmetric cubic graphs.

denoted by $\Gamma(v)$, is defined as the set

$$\Gamma(v) = \{\varphi(v) \mid \varphi \in \Gamma\}.$$

Similarly, given an edge $uv \in E$, we define the *edge orbit* of uv , denoted by $\Gamma(uv)$, as the set

$$\Gamma(uv) = \{\varphi(u)\varphi(v) \mid \varphi \in \Gamma\}.$$

We now define the notations $\Gamma(V)$ and $\Gamma(E)$, which by Lemma 3.30 below are partitions of the vertices and edges of a graph, respectively. Note the distinction between $\Gamma(V)$ and $\Gamma(v)$, the latter being the orbit of a particular vertex v as defined above; similarly for $\Gamma(E)$ and $\Gamma(uv)$.

Definition 3.29 (Vertex and edge partitions). Let $G = (V, E)$ be a graph, and let Γ be the automorphism group of G . The partition of the vertices V by Γ is defined as

$$\Gamma(V) = \{\Gamma(v) \mid v \in V\},$$

and the partition of the edges E by Γ is defined as

$$\Gamma(E) = \{\Gamma(uv) \mid uv \in E\}.$$

The following result is well-known and follows from the definitions of vertex and edge orbits.

Lemma 3.30. *Let Γ be the automorphism group of a graph $G = (V, E)$. The sets $\Gamma(V)$ and $\Gamma(E)$ are partitions of V and E , respectively.*

Example 3.26 (Continued). Continuing the previous example of graph automorphisms, we now consider the vertex and edge orbits of the graph shown previously in Figure 3.6. Recalling that

$$\begin{aligned} \Gamma = \{(), (12), (56), (15)(26)(34), (12)(56), \\ (1526)(34), (1625)(34), (16)(25)(34)\}, \end{aligned}$$

it is now straightforward to calculate the vertex orbits

$$\begin{aligned} \Gamma(1) = \Gamma(2) = \Gamma(5) = \Gamma(6) &= \{1, 2, 5, 6\} \\ \Gamma(3) = \Gamma(4) &= \{3, 4\}, \end{aligned}$$

and to calculate the edge orbits

$$\begin{aligned} \Gamma(12) = \Gamma(56) &= \{12, 56\} \\ \Gamma(13) = \Gamma(23) = \Gamma(45) = \Gamma(46) &= \{13, 23, 45, 46\} \\ \Gamma(34) &= \{34\}. \end{aligned}$$

Furthermore, this example clearly shows the partitioning of the six vertices

and seven edges, so that

$$\Gamma(V) = \{\{1, 2, 5, 6\}, \{3, 4\}\}$$

$$\Gamma(E) = \{\{12, 56\}, \{13, 23, 45, 46\}, \{34\}\}.$$

These vertex and edge orbits induced by Γ are shown with colours in Figure 3.9.

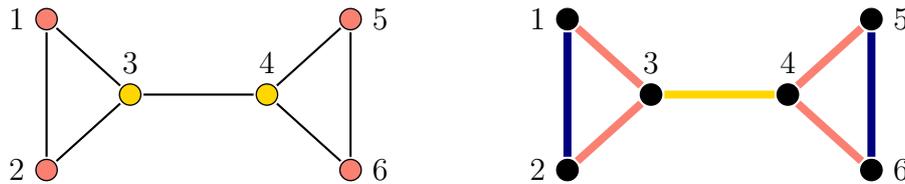


Figure 3.9: The graph shown previously in Figure 3.6 but with its orbits shown in different colours. On the left, vertices are filled with either red or yellow according to their vertex orbit. On the right, edges are highlighted with blue, red or yellow according to their edge orbit.

Of the partitions $\Gamma(V)$ and $\Gamma(E)$, it is particularly the edge partition $\Gamma(E)$ of a graph that we have found to be useful for identifying graph reductions. The motivating principle here is that graphs typically contain edges not required for forming a particular Hamiltonian cycle, and the goal is to remove some of these edges. That is, given a graph G and a Hamiltonian cycle C in G , then all the edges not used in C are redundant with respect to determining the Hamiltonicity G . Alternatively, if G does not contain a Hamiltonian cycle, then all of the edges can be removed and the graph will remain non-Hamiltonian. Unfortunately, without *a priori* knowledge of a Hamiltonian cycle (or their absence), deciding if a particular edge is redundant would, in general, require solving two instances of the NP-complete decision problem; deciding if the graph is Hamiltonian, and then deciding if the graph is Hamiltonian after the removal of the edge in question. However, in the case of graphs with certain edge orbits, some of these redundant edges can be efficiently identified by finding incompatible edge sets, as will be shown in the following section, Section 3.4.

For the purposes of finding edge orbits containing redundant edges, it is convenient to have a classification of edge orbits. Such a classification is developed in Theorem 3.36 through the use of the Propositions 3.33 and 3.34 and Lemma 3.35. Although a classification with more categories may be possible, this classification provides enough granularity for our purposes while still allowing us to classify orbits efficiently.

Prior to introducing our classification of edge orbits, we first provide a definition of *semiregular graphs*:

Definition 3.31. (Semiregular bipartite graph) Let $G = (U \cup V, E)$ be a bipartite graph with bipartition $\{U, V\}$. The graph G is said to be *semiregular* if every vertex in U has the same degree, and every vertex in V has the same degree. Further, if the degrees of vertices in U and V are given by a and b respectively, we may specifically say that G is (a, b) -semiregular or equivalently (b, a) -semiregular. Note that if $a = b$ then G is also a -regular.

Given any graph $G = (V, E)$, its automorphism group Γ , and any edge $e \in E$, Propositions 3.33 and 3.34 and Lemma 3.35 are concerned with the subgraph H induced by the edges of $\Gamma(e)$. Propositions 3.33 and 3.34 require the following definition.

Definition 3.32 (Line graph). Let $G = (V, E)$ be a graph. The *line graph* of G , denoted by $L(G)$, is defined as the graph

$$L(G) = (E, E'),$$

where

$$E' = \{(uv, wx) \in E^2 \mid |\{u, v, w, x\}| = 3\}.$$

That is, each vertex of $L(G)$ corresponds to an edge of G , and two vertices of $L(G)$ are adjacent precisely when their two corresponding edges in G are incident to a common vertex.

Figure 3.10 shows an example of a graph and its line graph.

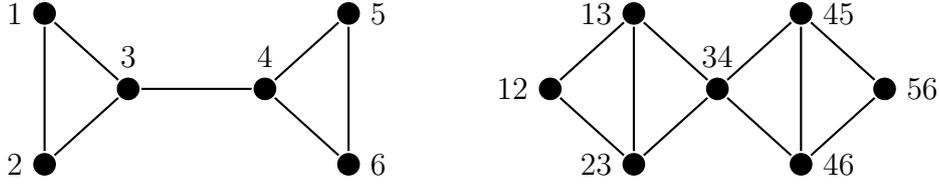


Figure 3.10: A graph (left) and its line graph (right). Vertices of the line graph are labelled with their corresponding edges in the original graph.

Proposition 3.33. *If H is the subgraph induced by an edge orbit $\Gamma(e)$, then the line graph of H is regular.*

Proof. First we consider the case that $|\Gamma(e)| = 1$, that is, the orbit contains just a single edge. In this case the line graph $L(H)$ is a singleton graph and is 0-regular.

Otherwise, $|\Gamma(e)| > 1$ so there are multiple edges in the orbit and we may consider taking any two distinct vertices $l_1, l_2 \in L(H)$. To complete the proof it must be shown that $\deg(l_1) = \deg(l_2)$.

Let vertex l_1 in the line graph correspond to an edge $u_1v_1 \in \Gamma(e)$, and similarly let vertex l_2 in the line graph correspond to an edge $u_2v_2 \in \Gamma(e)$. Note that the edges u_1v_1 and u_2v_2 may share at most one endpoint, so there are at least three distinct vertices amongst u_1, u_2, v_1, v_2 . Since u_1v_1 and u_2v_2 are both in $\Gamma(e)$, by definition there exists an automorphism $\varphi \in \Gamma$ such that $\varphi(u_1v_1) = u_2v_2$. Without loss of generality, assume the indices are set so that $\varphi(u_1) = u_2$ and $\varphi(v_1) = v_2$.

The degree of l_1 in the line graph can be expressed as the cardinality of a particular subset of vertices neighbouring u_1 and v_1 in H as follows.

$$\deg(l_1) = |\{w \in V \setminus \{u_1, v_1\} \mid wu_1 \in \Gamma(e) \text{ or } wv_1 \in \Gamma(e)\}|.$$

By definition of edge orbits and the automorphism φ , a condition such as $wu_1 \in \Gamma(e)$ holds if and only if $\varphi(w)\varphi(u_1) \in \Gamma(e)$. Therefore,

$$\begin{aligned} \deg(l_1) &= |\{w \in V \setminus \{u_1, v_1\} \mid \varphi(w)\varphi(u_1) \in \Gamma(e) \text{ or } \varphi(w)\varphi(v_1) \in \Gamma(e)\}| \\ &= |\{w \in V \setminus \{u_1, v_1\} \mid \varphi(w)u_2 \in \Gamma(e) \text{ or } \varphi(w)v_2 \in \Gamma(e)\}|. \end{aligned}$$

Applying the automorphism φ to both sides of the condition $w \in V \setminus \{u_1, v_1\}$, and letting $x = \varphi(w)$, we obtain

$$\begin{aligned} \deg(l_1) &= |\{\varphi(w) \in V \setminus \{\varphi(u_1), \varphi(v_1)\} \mid \varphi(w)u_2 \in \Gamma(e) \text{ or } \varphi(w)v_2 \in \Gamma(e)\}| \\ &= |\{x \in V \setminus \{u_2, v_2\} \mid xu_2 \in \Gamma(e) \text{ or } xv_2 \in \Gamma(e)\}| \\ &= \deg(l_2). \end{aligned} \quad \square$$

The following result is inspired by a similar result in [32], Lemma 1.7.5, which is stated in terms of line graphs rather than edge orbits. The proof below is more detailed, with [32] leaving steps to the reader as an exercise.

Proposition 3.34. *If H is the subgraph induced by an edge orbit $\Gamma(e)$ and H_1 is a connected component of H , then either H_1 is non-bipartite and regular, or H_1 is bipartite and semiregular.*

Proof. First we deal with the trivial case that H_1 contains only one edge; H_1 is then bipartite and $(1, 1)$ -semiregular. Otherwise, H_1 contains at least two edges. Since H_1 is a connected component of H , it follows that $L(H_1)$ must be a connected component of $L(H)$. By Proposition 3.33, the line graph $L(H)$ is regular, therefore $L(H_1)$ is also regular with the same degree; let this degree be k .

Let uv and vw be any two adjacent edges in H_1 . Calculating the degrees of u , v and w with respect to H_1 , the k -regularity of $L(H_1)$ guarantees that

$$\deg(u) + \deg(v) = k + 2, \text{ and}$$

$$\deg(v) + \deg(w) = k + 2.$$

Equating the left hand sides yields

$$\deg(u) = \deg(w).$$

Since the only condition on vertices u and w is that they have a path of length 2 between them (via v in this case), we may conclude that *all* pairs of vertices in H_1 with a path of length 2 between them necessarily have the same degree.

Let A be the set containing u and all vertices with paths of even length from u . Similarly, let B be the set containing v and all vertices with paths of even length from v . Applying the argument above, all vertices in A have the same degree, and all vertices in B have the same degree; let these degrees be a and b respectively. Since every vertex in H_1 has a path of even length to either u or v , or to both, $A \cup B$ contains all the vertices of H_1 . Finally, there are just two cases to consider: If H_1 contains a cycle of odd length, then $A = B$ and thus H_1 will be non-bipartite and a -regular. Otherwise, if H_1 contains no cycles of odd length, then $A \cap B = \emptyset$, and H_1 must be bipartite and (a, b) -semiregular. \square

Lemma 3.35. *If the subgraph H induced by an edge orbit $\Gamma(e)$ has more than one connected component, every such component of H is isomorphic to the other components.*

Proof. Let H_1 and H_2 be two connected components of H , let u_1v_1 be an edge of H_1 , and let u_2v_2 be an edge of H_2 . By the definition of $\Gamma(e)$, there must be an automorphism $\varphi \in \Gamma$ such that $\varphi(u_1)\varphi(v_1) = u_2v_2$. Note that φ must also map any neighbouring edges of u_1v_1 , if any, to neighbouring edges of u_2v_2 . This argument can be repeated inductively on those neighbouring edges, et cetera, until the entire connected component H_1 is mapped to H_2 by φ . Similarly, it can be shown that the entire connected component H_2 is mapped to H_1 by φ^{-1} . Since a one-to-one mapping exists between H_1 and

H_2 , they are by definition isomorphic, and as H_1 and H_2 could be any two components of H , this proves that all the components are isomorphic. \square

For Theorem 3.36 below, we use the notation kG , where $k \in \mathbb{N}$ and G is a graph, to denote the disjoint union of k copies of G . The notations X_r and $X_{r,s}$, further described in the theorem, are used to denote generic regular graphs with minimum degree 3, and semiregular bipartite graphs with minimum degree 2, respectively.

Theorem 3.36. *Given a graph $G = (V, E)$ and any edge $e \in E$, the edge orbit $\Gamma(e)$ may be classified into one of the following six mutually exclusive types that can be identified by the number of connected components k in the subgraph H induced by $\Gamma(e)$ and the structure of those components.*

(kK_2) Each component of H is a complete graph with two vertices.

(kP_2) Each component of H is a path graph with two edges.

(kS_r) Each component of H is a star graph with r edges, where $r \geq 3$.

(kC_n) Each component of H is a cycle graph with n vertices, where $n \geq 3$.

(kX_r) Each component of H is isomorphic to the same r -regular non-bipartite cyclic graph X_r , where $r \geq 3$.

($kX_{r,s}$) Each component of H is isomorphic to the same (r, s) -semiregular bipartite cyclic graph $X_{r,s}$, where $r \geq s \geq 2$ and $r \geq 3$.

Proof. Firstly, observe that each of the six cases are mutually exclusive. Next, by Lemma 3.35 we know that all the connected components of H are isomorphic to one another so we only need to consider one connected component H_1 of H . We will show that H_1 is in one of the six forms listed in the theorem. The primary tool to distinguish amongst forms is Proposition 3.33; each edge in H_1 has the same number of neighbouring edges. Thus, we take any edge e from H_1 and let l be the degree of $L(H_1)$.

By Proposition 3.34 we know that H_1 is either regular or semiregular. In the former case let a and b both equal the degree of H_1 . In the latter case let a and b be such that $a \geq b$ and H_1 is (a, b) -semiregular. The following easily-verified equation will be used several times in the remainder of the proof:

$$a + b = l + 2. \quad (3.1)$$

For the purposes of this proof it is useful to separate the cases based on whether H_1 is cyclic or acyclic. First we consider all the possible cases when H_1 is acyclic: If $l = 0$, then H_1 contains only one edge and the orbit is of type kK_2 . If $l = 1$, then H_1 must be a 2-path and the orbit must be of type kP_2 . Otherwise, if $l \geq 2$, then we will show that H_1 is a star graph S_{l+1} . Since we assume H_1 is acyclic, it must contain vertices of degree 1. Therefore, $b = 1$ and by (3.1), $a = l + 1 \geq 3$. It is clear that the star graph S_a is the only $(1, a)$ -semiregular connected graph, thus H_1 is isomorphic to S_a and the orbit is of type kS_a .

In turn, we consider all the possible cases when H_1 is a cyclic graph. If H_1 contains a cycle, it necessarily follows that $l \geq 2$ since each edge on a cycle has at least two adjacent edges; this also implies that $a \geq b \geq 2$. The first case to consider here is when $l = 2$; in this case the lower bounds on a and b , together with (3.1), imply that $a = b = 2$. Since H_1 is connected this leaves a cycle graph as the only possibility and thus the orbit is of type kC_n with n being the number of edges in H_1 . Lastly, we consider the case when $l \geq 3$; here, the lower bound on b and ordering of a and b , together with (3.1), imply that $a \geq 3$. There are two sub-cases, depending on the bipartiteness of H_1 : If H_1 is non-bipartite, then by Proposition 3.34 H_1 must be regular with $a = b = \frac{l+2}{2}$, so the orbit is of type kX_a . Otherwise, H_1 must be bipartite and (a, b) -semiregular, so the orbit is of type $kX_{a,b}$.

Table 3.12: Percentage of edges in each type of orbit, as classified by Theorem 3.36, for non-symmetric cubic graphs by order up to 20 vertices.

Vertices	Graphs	kK_2	kP_2	kS_r	kC_n	kX_r	$kX_{r,s}$
4	1	0	0	0	0	100	0
6	2	16.67	0	0	33.33	50.00	0
8	5	25.00	13.33	0	31.67	20.00	10.00
10	19	38.60	19.65	3.16	29.12	5.26	4.21
12	80	49.58	27.64	1.67	20.28	0	0.83
14	406	58.95	29.04	0.74	10.60	0.25	0.42
16	2513	65.91	26.87	0.24	6.84	0.04	0.10
18	19 177	71.43	24.21	0.04	4.28	5×10^{-3}	0.03
20	182 909	76.08	21.18	0.01	2.72	1×10^{-3}	7×10^{-3}
≤ 20	205 112	75.55	21.51	0.02	2.91	3×10^{-3}	0.01

Since we have enumerated all possible cases, H must belong to one of the six listed types, concluding the proof. \square

An example graph containing five of these six orbit types may be seen in Figure 3.11. Interestingly, the graph displayed is the only instance of NHNB20 to feature at least five different classes of orbit. The only type of orbit not shown in Figure 3.11 is the regular X_r type, which for cubic graphs can only appear in edge-transitive graphs, for example the Petersen graph in Figure 1.3.

Table 3.12 shows the prevalence of edges in non-symmetric cubic graphs up to order 20 constituting each of these types of orbits.

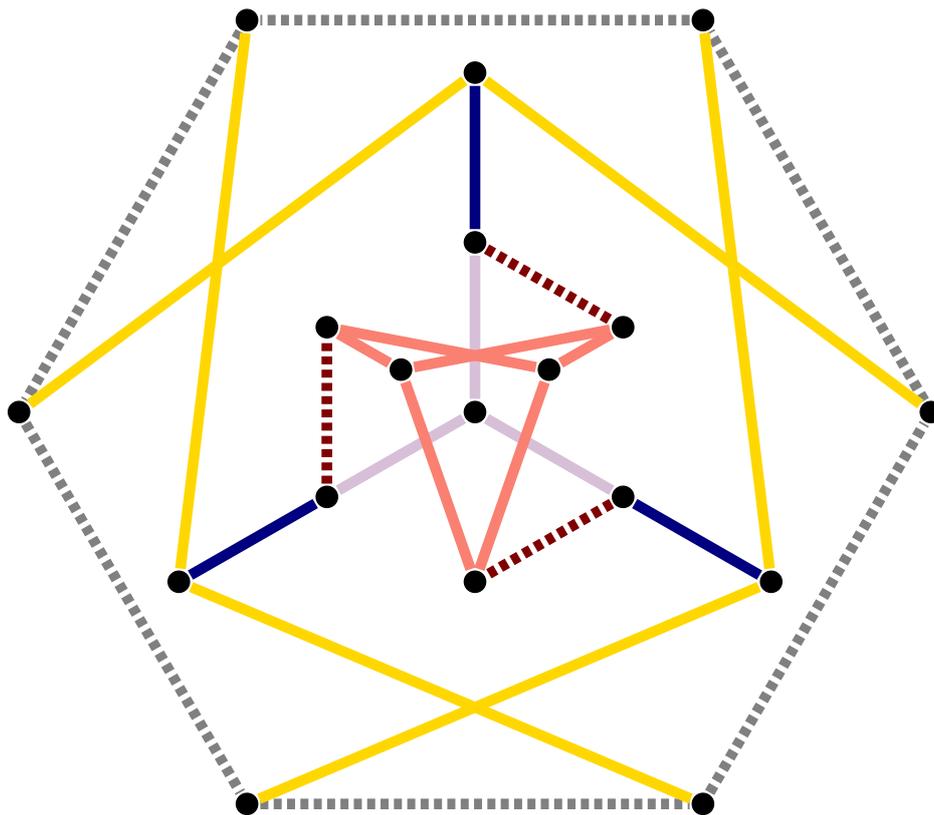


Figure 3.11: An 18-vertex non-Hamiltonian cubic graph G_{18}^{34034} with six edge orbits highlighted to demonstrate five different types of orbit as classified by Theorem 3.36: The outer cycle orbit $1C_6$ in dashed grey, a triple 2-path orbit $3P_2$ in yellow, a triple edge orbit $3K_2$ in blue, a star orbit $1S_3$ in lilac, a second triple edge orbit $3K_2$ in dashed maroon, and lastly a bipartite $(3, 2)$ -semiregular orbit $X_{3,2}$ in red.

3.4 Graph reductions based on edge orbits

We now turn our attention to considering how edge orbits may aid in the identification of graph reductions, and hence introduce several new Hamiltonicity-preserving graph reductions. We begin by defining the concept of an *incompatible edge set*.

Definition 3.37 (Incompatible edge set). We define a non-empty subset D of the edges E in a graph to be *incompatible* if it is not possible to use all the edges of D in the same Hamiltonian cycle.

In general, determining whether an arbitrary subset of edges is incompatible requires knowledge of all the Hamiltonian cycles of the graph, so in practice we just consider some common structures that are guaranteed to be incompatible. A list of these common structures is given in Theorem 3.38, although this list is not intended to be exhaustive. Examples of sets of edges satisfying the conditions listed in Theorem 3.38 are shown in Figure 3.13.

Theorem 3.38. *Let $G = (V, E)$ be a graph and let $D \subseteq E$ be a non-empty subset of the edges. Then D is incompatible if any of the following three conditions hold:*

- (i) $|D| \geq 3$ and every edge in D is incident to the same vertex $v \in V$.
- (ii) $|D| < |V|$ and the subgraph of G induced by D is a cycle graph.
- (iii) $|D|$ is odd and D is an edge cut set such that there exists a connected component G_1 of $(V, E \setminus D)$ in which every edge of D has exactly one endpoint.

Proof. If G does not contain a Hamiltonian cycle, then by definition any (non-empty) subset of the edges is incompatible. It then remains only to prove the sufficiency of these conditions for Hamiltonian graphs. The proof

will proceed by contradiction; that is, assume G contains a Hamiltonian cycle using every edge of D and let $C \supseteq D$ be the edges of this cycle.

If D meets condition (i), this would imply a Hamiltonian cycle using three or more edges incident to v , which is a contradiction as a Hamiltonian cycle must enter and exit each vertex exactly once. If D meets condition (ii) then D traces out a short cycle (visiting fewer than $|V|$ vertices), and since a cycle graph cannot be a subgraph of a larger cycle graph, $D \not\subseteq C$; a contradiction.

Finally, assume D meets condition (iii). Since D is the edge cut set that separates G_1 from the remainder of the graph, we have a partition of the vertices into two sets with only edges in D having one endpoint in each set. Then, by Lemma 3.11 the number of edges of D used in C must be even. But this contradicts the assumption that every edge in D , of which there is an odd number, is used. \square

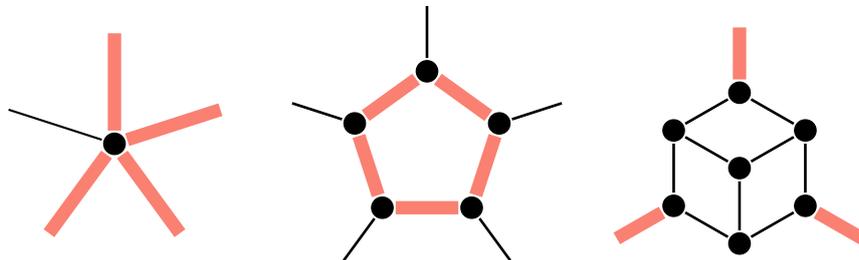


Figure 3.13: Examples of incompatible edge sets as given by Theorem 3.38. The highlighted edges belong to incompatible edge sets. On the left is a subset of edges with more than two edges incident to the same vertex. In the centre is a short cycle. On the right is an edge cut with an odd number of edges separating a connected component from the rest of the graph.

Lemma 3.39. *Suppose that $D \subseteq E$ is an incompatible edge set of the graph $G = (V, E)$. Then at least one of the edges in D is redundant.*

Proof. By definition, it is not possible to use all the edges in D in the same Hamiltonian cycle. Therefore, either D is a set containing a single non-Hamiltonian edge (in which case it is necessarily redundant), or D contains

more than one edge. In the latter case, without loss of generality, suppose that $u_1v_1 \in D$ and $u_2v_2 \in D$ are not both used in the same Hamiltonian cycle. If there is a Hamiltonian cycle that uses u_1v_1 , then u_2v_2 may therefore be removed without changing the Hamiltonicity. Alternatively, if there is not a Hamiltonian cycle that uses u_1v_1 , then u_1v_1 may be removed without changing the Hamiltonicity. Therefore, at least one of the edges u_1v_1 and u_2v_2 is redundant. \square

By Lemma 3.39, any incompatible edge set D is guaranteed to contain a redundant edge. The question then arises; which edges of D are redundant? As mentioned earlier, in general this question is not necessarily any easier to answer than the original decision problem (HCP). Neither is it easy to decide whether a given subset of edges is incompatible. Therefore, we restrict our attention to only certain incompatible edge sets; in particular, those formed by the edge partition $\Gamma(E)$, and only those which can be easily proved to be incompatible. The key to this process is given in the following theorem.

Theorem 3.40. *Given a graph $G = (V, E)$, its automorphism group Γ , and an edge orbit $\Gamma(uv) \in \Gamma(E)$, then one of the following conditions must hold:*

- (i) *Every edge of $\Gamma(uv)$ is redundant.*
- (ii) *Every edge of $\Gamma(uv)$ is a Hamiltonian edge.*
- (iii) *In the case that G is non-Hamiltonian, both (i) and (ii).*

Proof. If G is not Hamiltonian, then by definition every edge in $E \supseteq \Gamma(uv)$ is a Hamiltonian edge, and is also redundant. Thus for the remainder of the proof we only need to consider graphs G that are Hamiltonian.

Suppose that none of the edges of $\Gamma(uv)$ are redundant. Then by definition, each of the edges is Hamiltonian.

Alternatively, suppose that at least one of the edges of $\Gamma(uv)$ is redundant. Without loss of generality, let $e \in \Gamma(uv)$ be redundant. That is, there exists

a Hamiltonian cycle C in G that does not contain e . Consider any other edge $f \in \Gamma(uv)$. By the definition of the automorphism group Γ , there exists an automorphism φ such that $\varphi(e) = f$. Then there exists a Hamiltonian cycle C' using the edges $\{\varphi(c) \mid c \in C\}$. Since $e \notin C$, then it follows that $f \notin C'$. Therefore, f is also redundant in G . Since this argument may be made for any other edge in $\Gamma(uv)$, every edge in $\Gamma(uv)$ is redundant. \square

Definition 3.41 ($\psi_{\text{star}}[u, v_1, \dots, v_m]$ graph reduction). Given a graph $G = (V, E)$, we define the function $\psi_{\text{star}}[u, v_1, \dots, v_m]$ for $m \geq 3$ to remove one redundant edge uv_m from G out of a collection of redundant edges uv_1, \dots, uv_m incident to the same vertex u . There may be other edges incident to vertex u which are not known to be redundant.

$$\psi_{\text{star}}[u, v_1, \dots, v_m](G) = (V, E \setminus \{uv_m\}).$$

An example is shown in Figure 3.14.

Domain of $\psi_{\text{star}}[u, v_1, \dots, v_m]$: The set of graphs $G = (V, E)$ having vertices $u, v_1, \dots, v_m \in V$, $m \geq 3$, where the edges $uv_1, \dots, uv_m \in E$ are all known to be redundant.

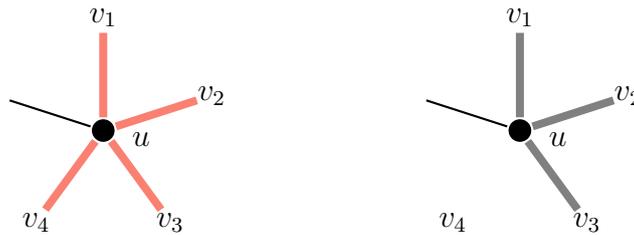


Figure 3.14: A graph with known redundant edges uv_1, uv_2, uv_3, uv_4 , before (left) and after (right) its reduction with $\psi_{\text{star}}[u, v_1, v_2, v_3, v_4]$. If the four edges uv_1, uv_2, uv_3, uv_4 are in the same orbit (shown in red), their redundancy is guaranteed by Theorems 3.38 and 3.40.

While ψ_{star} may be used with any incompatible edge set whose edges are incident to a common vertex, there is a special case in which may one use a stronger reduction, defined as follows.

Definition 3.42 ($\psi_{\text{pinwheel}}[u, v_1, \dots, v_m]$ graph reduction). Given a graph $G = (V, E)$, we define the function $\psi_{\text{pinwheel}}[u, v_1, \dots, v_m]$ for $m \geq 2$ to remove all but one edge uv_1 from G out of a collection of redundant edges uv_1, \dots, uv_m in the same edge orbit where: (i) v_1, \dots, v_m are adjacent to the vertex u , and (ii) one Hamiltonian edge uw is also incident to u .

$$\psi_{\text{pinwheel}}[u, v_1, \dots, v_m](G) = (V, E \setminus \{uv_2, \dots, uv_m\}).$$

An example is shown in Figure 3.15.

Domain of $\psi_{\text{pinwheel}}[u, v_1, \dots, v_m]$: The set of graphs $G = (V, E)$ with $u, v_1, \dots, v_m \in V$, $m \geq 2$, and edges $uv_1, \dots, uv_m \in E$ that are all known to be redundant and where $\Gamma(uv_1) = \Gamma(uv_2) = \dots = \Gamma(uv_m)$. Further, there must exist another vertex $w \notin \{v_1, \dots, v_m\}$ in G such that uw is known to be Hamiltonian.

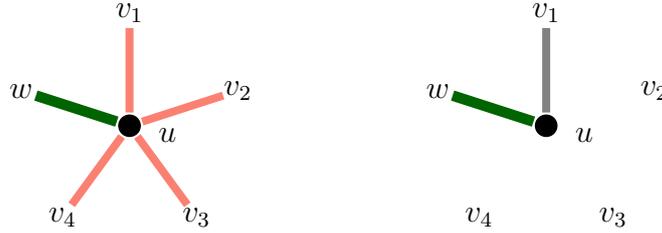


Figure 3.15: A graph with known Hamiltonian edge uw (green) and known redundant edges uv_1, uv_2, uv_3, uv_4 , before (left) and after (right) its reduction with $\psi_{\text{pinwheel}}[u, v_1, v_2, v_3, v_4]$. If the four edges uv_1, uv_2, uv_3, uv_4 are in the same orbit (shown in red), their redundancy is guaranteed by Theorems 3.38 and 3.40.

We now define another two reductions ψ_{cycle} and ψ_{cut} , as follows.

Definition 3.43 ($\psi_{\text{cycle}}[v_1, \dots, v_m]$ graph reduction). Given a graph $G = (V, E)$, we define the function $\psi_{\text{cycle}}[v_1, \dots, v_m]$ to remove a redundant edge $v_m v_1$ from a short cycle of edges $(v_1 v_2, v_2 v_3, \dots, v_m v_1)$ in G .

$$\psi_{\text{cycle}}[v_1, \dots, v_m](G) = (V, E \setminus \{v_m v_1\}).$$

An example is shown in Figure 3.16.

Domain of $\psi_{\text{cycle}}[v_1, \dots, v_m]$: The set of graphs $G = (V, E)$ with vertices $v_1, \dots, v_m \in V$, $3 \leq m < |V|$, and with edges forming a short cycle $v_1v_2, v_2v_3, \dots, v_mv_1 \in E$ where v_mv_1 is known to be redundant.

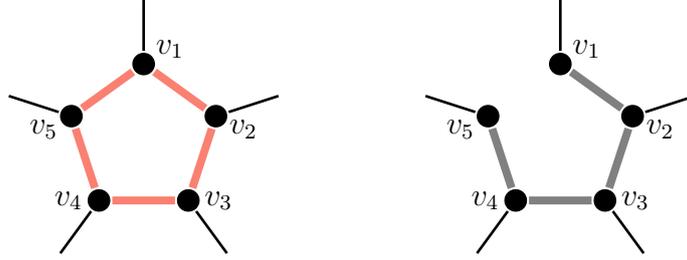


Figure 3.16: A graph with known redundant edges $v_1v_2, v_2v_3, \dots, v_5v_1$ in a short cycle, before (left) and after (right) its reduction with $\psi_{\text{cycle}}[v_1, v_2, v_3, v_4, v_5]$. If the edges are in the same orbit (shown in red), their redundancy is guaranteed by Theorems 3.38 and 3.40.

Definition 3.44 ($\psi_{\text{cut}}[u_1, v_1, u_2, v_2, \dots, u_m, v_m]$ graph reduction). Given a graph $G = (V, E)$, we define $\psi_{\text{cut}}[u_1, v_1, u_2, v_2, \dots, u_m, v_m]$ to remove a redundant edge u_mv_m from an edge cut set $\{u_1v_1, \dots, u_mv_m\} \subset E$ with odd cardinality.

$$\psi_{\text{cut}}[u_1, v_1, u_2, v_2, \dots, u_m, v_m](G) = (V, E \setminus \{u_mv_m\}).$$

An example is shown in Figure 3.17.

Domain of $\psi_{\text{cut}}[u_1, v_1, u_2, v_2, \dots, u_m, v_m]$: The set of graphs $G = (V, E)$ with distinct vertices $u_1, \dots, u_m, v_1, \dots, v_m \in V$ and edges u_1v_1, \dots, u_mv_m such that m is odd and $\{u_1v_1, \dots, u_mv_m\}$ is a *minimal* cut set; that is, removing all the edges in the set disconnects the graph but adding any one of them back decreases the number of (connected) components. Note that this is an incompatible edge set by Theorem 3.38.

Lemma 3.45. *The reductions ψ_{star} , ψ_{pinwheel} , ψ_{cycle} and ψ_{cut} preserve Hamiltonicity and are recoverable.*

Proof. In the cases of ψ_{star} , ψ_{cycle} and ψ_{cut} , only a single redundant edge is removed, and so it is clear that these reductions preserve Hamiltonicity.

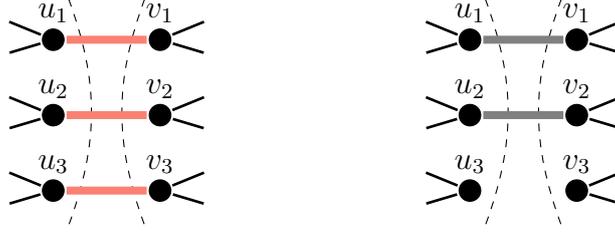


Figure 3.17: A graph with known redundant edges u_1v_1 , u_2v_2 and u_3v_3 forming a minimal cut set, before (left) and after (right) its reduction with $\psi_{\text{cut}}[u_1, v_1, u_2, v_2, u_3, v_3]$. If the edges are in the same orbit (shown in red), their redundancy is guaranteed by Theorems 3.38 and 3.40.

Furthermore, any Hamiltonian cycle in the reduced graph must necessarily be present in the original graph, so recoverability follows immediately.

In the case of ψ_{pinwheel} , recovery is similarly trivial, so all that remains is to prove that Hamiltonicity is preserved. From the definition of ψ_{pinwheel} , the reduction removes edges uv_2, \dots, uv_m , each of which is redundant and lies in the edge orbit $\Gamma(uv_1)$, from a graph G containing a Hamiltonian edge uw . Note that any Hamiltonian cycle in G must therefore contain uw , and hence contain at most one of the edges uv_1, \dots, uv_m . If none of the edges uv_1, \dots, uv_m are used in a Hamiltonian cycle of G , then the removal of any of these edges cannot alter the Hamiltonicity of G and thus Hamiltonicity is preserved. Alternatively, let C be a Hamiltonian cycle in G using one of the edges $e \in \{uv_1, \dots, uv_m\}$. Then, since $\Gamma(uv_1) = \dots = \Gamma(uv_m)$, there is an automorphism φ such that $\varphi(e) = uv_1$. Hence, there is a Hamiltonian cycle that contains uv_1 , and so the removal of uv_2, \dots, uv_m does not alter the Hamiltonicity. Therefore, in all cases, Hamiltonicity is preserved. \square

3.5 Graph reduction algorithm

Having introduced eleven Hamiltonicity-preserving graph reductions and also characterised the situations in which they may be applied, it is now possible to describe a graph reduction algorithm that searches for applicable reduc-

tions or applicable compositions of these reductions. Before presenting the algorithm, it is useful to consider what should be done when multiple reductions are applicable to a given graph simultaneously; that is, should there be a preferred order to search for reductions?

Firstly it is clear that the reductions ψ_H and ψ_{NH} which reduce the graph to the maximum extent possible (to a trivially Hamiltonian or non-Hamiltonian graph) should have the highest priority if they are determined to be applicable. Next, it may be argued that the reductions ψ_{triangle} and ψ_{diamond} , being based on particular subgraphs, may reasonably be applied prior to reductions based on edge orbits: Since non-trivial edge orbits are only present when there is some kind of symmetry in the graph, any subgraphs whose modification would affect the edge orbits would necessarily share in the same symmetries. Therefore, as long as all such subgraphs are modified in the same way (e.g. by ψ_{triangle} or ψ_{diamond}), the symmetries upon which the orbits are based will remain. In fact, by contracting subgraphs that are not involved in symmetries, new symmetries may appear.

Table 3.18 shows empirical results on cubic graphs with at least one triangle, between 6 and 20 vertices in order. After performing all applicable ψ_{triangle} and ψ_{diamond} reductions, the order of the automorphism group increased by a factor of 2.91 on average and the number of asymmetric graphs reduced by 25.7%. By a similar argument, any reductions made to or at forced edges (such as ψ_{forced} and ψ_{path}) will not affect symmetries elsewhere in the graph as long as all such structures are modified in the same way.

Based on this reasoning, the upcoming algorithm first searches for conditions allowing the reductions ψ_H and ψ_{NH} , then for reductions based on forced edges (ψ_{forced} and ψ_{path}), then for reductions based on subgraphs (ψ_{triangle} and ψ_{diamond}) before finally searching for reductions based on edge orbits. For these reductions based on edge orbits, the only reduction that should have a clear priority over the others is ψ_{cycle} , which we will use when an

Table 3.18: Automorphism group size of cubic graphs of order between 6 and 20 with at least one triangle, before and after performing all applicable ψ_{triangle} and ψ_{diamond} reductions. The mean factor increase in the order of the automorphism group for the graphs modified is also given, as well as the number of asymmetric graphs ($|\Gamma| = 1$) before and after.

Vertices	Graphs	Mean $ \Gamma $			Asymmetric	
		Before	After	Factor	Before	After
6	1	12.00	24.00	$\times 2.00$	0	0
8	3	10.67	33.33	$\times 4.08$	0	0
10	13	9.23	31.08	$\times 5.71$	0	0
12	63	7.83	24.89	$\times 7.36$	5	0
14	399	5.31	18.30	$\times 7.49$	89	4
16	3268	3.88	12.42	$\times 6.15$	1253	317
18	33 496	2.70	7.58	$\times 4.29$	17 372	9016
20	412 943	2.05	4.47	$\times 2.76$	253 557	193 017
All	450 186	2.11	4.77	$\times 2.91$	272 276	202 354

edge orbit $C_{|V|}$ is present, because that leads to a graph that is simple to establish as Hamiltonian. For the other reductions based on edge orbits (ψ_{star} , ψ_{pinwheel} , ψ_{cycle} , and ψ_{cut}) it is less obvious how the priorities should be ranked, or even if the ordering makes any significant difference. To investigate this, a target set of graphs was chosen and all applicable reductions at each step of the process were compared to determine an appropriate order in which to search for these reductions.

The target graphs chosen to evaluate the edge orbit reduction order were the 45 982 cubic graphs up to order 18. Each graph was first reduced only with ψ_{H} , ψ_{NH} , ψ_{forced} , ψ_{path} , ψ_{triangle} , and ψ_{diamond} , following the first stage of the algorithm later presented in Algorithm 3.1. Next, the orbits were examined to see which graph reductions based on edge orbits would be applicable. If ψ_{hcycle} was applicable, or otherwise if only one edge orbit reduction was applicable, then it would be applied to the graph and the process would restart from the beginning on the new graph. However, when two or more edge orbit reductions (other than ψ_{hcycle}) were applicable, each of them would be

attempted one at a time before restarting the reduction search, recursively determining which choice could potentially lead to a graph with the fewest edges. Unfortunately, always trying all possible orderings of reductions makes the algorithm run in exponential time, so a specific order must be fixed.

The differences in the number of resulting edges, even if zero, were then recorded for each pair of available reductions at every step. In total, there were 615 115 pairwise comparisons in processing 6041 (13%) of the starting graphs, summaries of which are shown in Tables 3.19 to 3.21. Note that the application of ψ_{cycle} was split into two separate cases; one where there is a short cycle orbit kC_n , and the other where there is a kK_2 or kP_2 orbit that forms a short cycle when combined with forced edges. These two cases were compared separately as they occur in fundamentally different circumstances despite using the same reduction function; Table 3.20 shows the former as ψ_{cycle} and the latter as $\psi_{\text{cycle (forced)}}$.

From Table 3.19 it can be seen that on these graphs where there are multiple ways to order the sequence of reductions, the average best and worst case performance is very close. Specifically, as a percentage of edges removed with the best possible reduction ordering, the worst case ordering still reduces 90% as many edges on average. Table 3.20 shows a matrix of the number of times each pair of reductions was compared, and Table 3.21 shows a matrix of the number of times one reduction outperformed another.

To determine a suitable ranking for the reductions, we consider the proportion of comparisons where each reduction is outperformed by others. For example, ψ_{cut} is never outperformed, so it is reasonable to give it the highest priority amongst the five. If we then eliminate ψ_{cut} from the table of comparisons, that then leaves ψ_{star} as never outperformed by other remaining reductions. Thus we give ψ_{star} the second highest priority. At this point,

excluding the already ranked ψ_{cut} and ψ_{star} , we have:

$$\begin{aligned} \text{Comparisons where } \psi_{\text{pinwheel}} \text{ outperformed} &= \frac{128 + 115}{220233 + 9466} \approx 0.11\%, \\ \text{Comparisons where } \psi_{\text{cycle}} \text{ outperformed} &= \frac{645 + 198}{220233 + 2478} \approx 0.38\%, \\ \text{Comparisons where } \psi_{\text{cycle (forced)}} \text{ outperformed} &= \frac{12}{9466 + 2478} \approx 0.10\%. \end{aligned}$$

Hence, $\psi_{\text{cycle (forced)}}$ has the lowest ratio here, but ψ_{pinwheel} is very close. Just considering the 9466 comparisons between this pair, $\psi_{\text{cycle (forced)}}$ outperforms ψ_{pinwheel} 115 times compared to only 12 times for the converse. Therefore $\psi_{\text{cycle (forced)}}$ is given the third highest priority, and of the remaining two reductions ψ_{pinwheel} is outperformed less often, leaving ψ_{cycle} to be the lowest priority of the five reductions.

Table 3.19: Cubic graphs up to order 18 where multiple graph reductions of the types ψ_{star} , ψ_{pinwheel} , ψ_{cycle} , and ψ_{cut} were simultaneously applicable at the same point. The table shows the mean difference in the number of edges reduced between the best and worst orders to apply the reductions.

Vertices	Graphs	Comparisons	Mean reduction in $ E $		
			Worst	Best	Gap
8	1	1	9	9	0
10	5	179	10.20	12.40	2.20
12	22	1491	11.86	12.91	1.05
14	122	7664	13.97	15.86	1.89
16	751	65 748	16.13	17.91	1.78
18	5140	540 032	17.71	19.62	1.91
≤ 18	6041	615 115	17.41	19.30	1.89

Table 3.20: The number of comparisons made between each pair of reductions. A dash indicates that the given pair were never both applicable at the same point for the graphs tested.

	ψ_{star}	ψ_{pinwheel}	ψ_{cycle}	$\psi_{\text{cycle (forced)}}$	ψ_{cut}
ψ_{star}	238	–	569	75	776
ψ_{pinwheel}	–	372 544	220 233	9466	–
ψ_{cycle}	569	220 233	1394	2478	529
$\psi_{\text{cycle (forced)}}$	75	9466	2478	6802	–
ψ_{cut}	776	–	529	–	11

Table 3.21: The number of comparisons between reductions where one reduction led to a graph with fewer edges than the other reduction. For example, the 450 in the ψ_{star} row and ψ_{cycle} column indicates that ψ_{star} outperformed ψ_{cycle} on 450 occasions. A dash indicates that the given pair were never both applicable at the same point for the graphs tested.

Worse Better	ψ_{star}	ψ_{pinwheel}	ψ_{cycle}	$\psi_{\text{cycle (forced)}}$	ψ_{cut}
ψ_{star}	10	–	450	0	0
ψ_{pinwheel}	–	826	645	12	–
ψ_{cycle}	0	128	119	0	0
$\psi_{\text{cycle (forced)}}$	0	115	198	0	–
ψ_{cut}	11	–	466	–	0

Having determined a suitable ordering in which to search for reductions, Algorithms 3.1 to 3.4 are presented on the following pages. For the sake of readability and modularity, the main algorithm, GRAPHREDUCTION (Algorithm 3.1), makes repeated calls to three separate functions, each of which is a graph reduction algorithm in its own right: FORCEDEDGEREDUCTION (Algorithm 3.2) searches for reductions based on forced edges, SUBGRAPHREDUCTION (Algorithm 3.3) searches for reductions based on particular subgraphs, and EDGEORBITREDUCTION (Algorithm 3.4) searches for reductions based on edge orbits.

Prior to the pseudocode of the algorithms, Figure 3.22 shows a flowchart of the main steps in Algorithm 3.1, and Figure 3.23 shows flowcharts of the main steps in Algorithms 3.2 to 3.4. A GNU Octave / MATLAB implementation may be found in Appendix C. Section 3.6 presents empirical results of Algorithm 3.1 on the set NHNB20, with a discussion of the findings, concluded with three examples of graphs reduced by the algorithm.

Theorem 3.46. *Algorithm 3.1 terminates in polynomial time for graphs of bounded degree.*

Proof. At each iteration of the algorithm, it either terminates, or removes at least one edge. Since the graph is of bounded degree, there is order $\mathcal{O}(n)$

edges, so there are polynomially many iterations. Hence, we focus on the complexity of each iteration.

During each iteration we may need to check for one or more of the following: Connectivity, the criterion of Ore’s theorem, the presence of triangles or diamonds, consecutive degree-2 vertices, cycles containing forced edges, and minimal edge cut sets. Each of these can be checked in polynomial time. During this process, we may also need to find the edge orbits. The edge orbits can be computed in polynomial time since finding a set of generators for the automorphism group is known to be polynomial-time equivalent to the graph isomorphism problem [54] which in turn is of polynomial complexity for graphs of bounded degree [53]. Hence, Algorithm 3.1 will terminate in polynomial time for graphs of bounded degree. \square

In practice, we do not compute the edge orbits by using graph isomorphism directly, instead choosing to use the excellent `nauty` package [55], which we found to terminate very quickly for the graphs we considered. We remark that the restriction of Theorem 3.46 to graphs of bounded degree can be avoided in some sense by converting a non-sparse HCP instance to a sparse instance, and then considering the latter instead. Indeed, any HCP instance can be converted to a cubic instance having the same Hamiltonicity, with only linear growth in the size of the graph [22].

In the upcoming pseudocode, ψ_{identity} denotes the identity function mapping any graph G to itself. Where S is any subset of edges in a graph $G = (V, E)$, we use $N_S(u)$ to denote the set of vertices adjacent to $u \in V$ using only edges in S ; more precisely, $N_S(u) = \{v \in V \mid uv \in S\}$. Further, if $S \subseteq E$ then let G_S denote the subgraph induced by the edges in S . Similarly, if $U \subseteq V$ then let G_U denote the subgraph induced by the vertices in U . Comments in the pseudocode are preceded by \triangleright . Each graph reduction algorithm returns a graph reduction rather than the reduced graph itself.

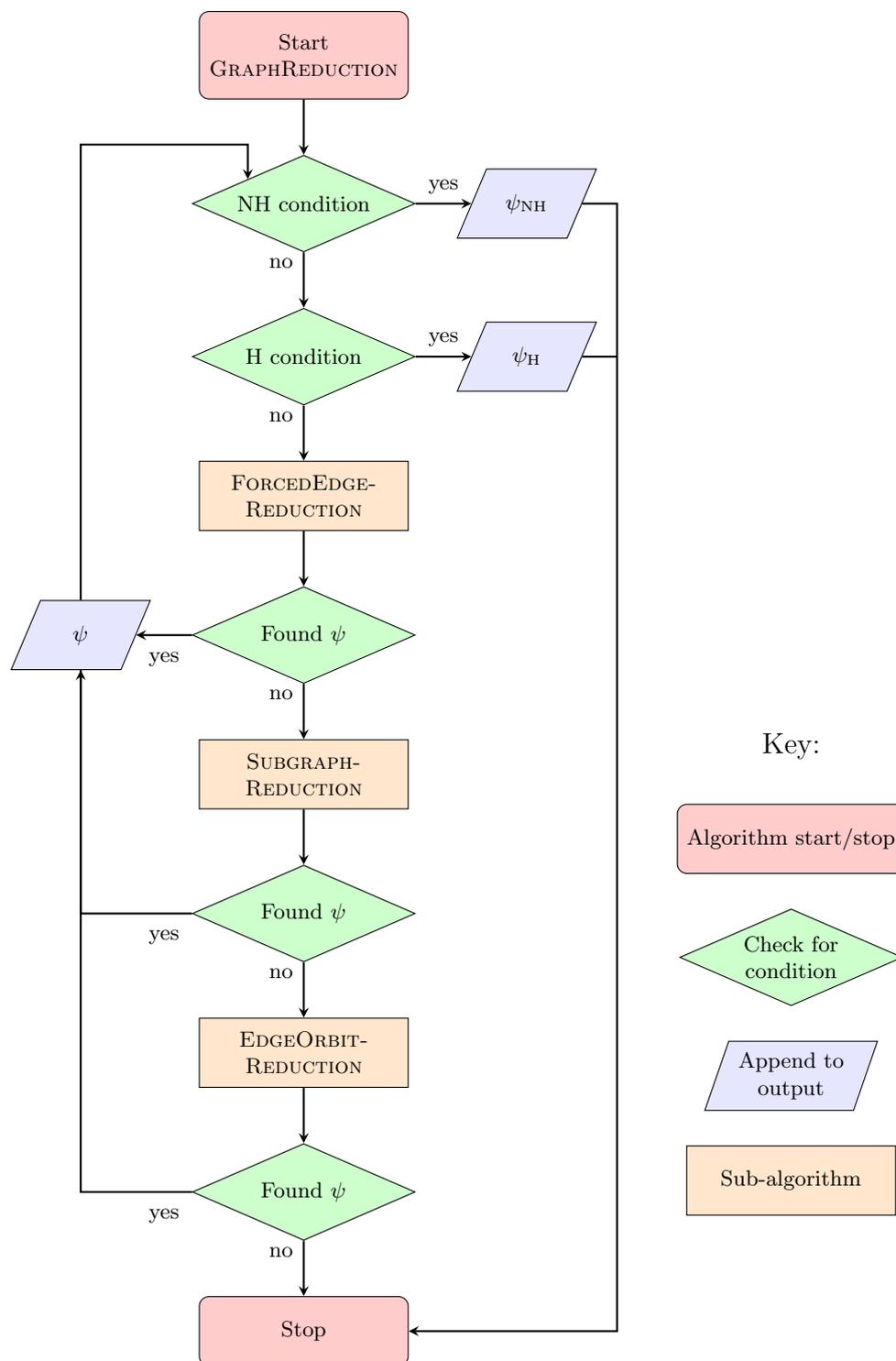


Figure 3.22: Flowchart of Algorithm 3.1.

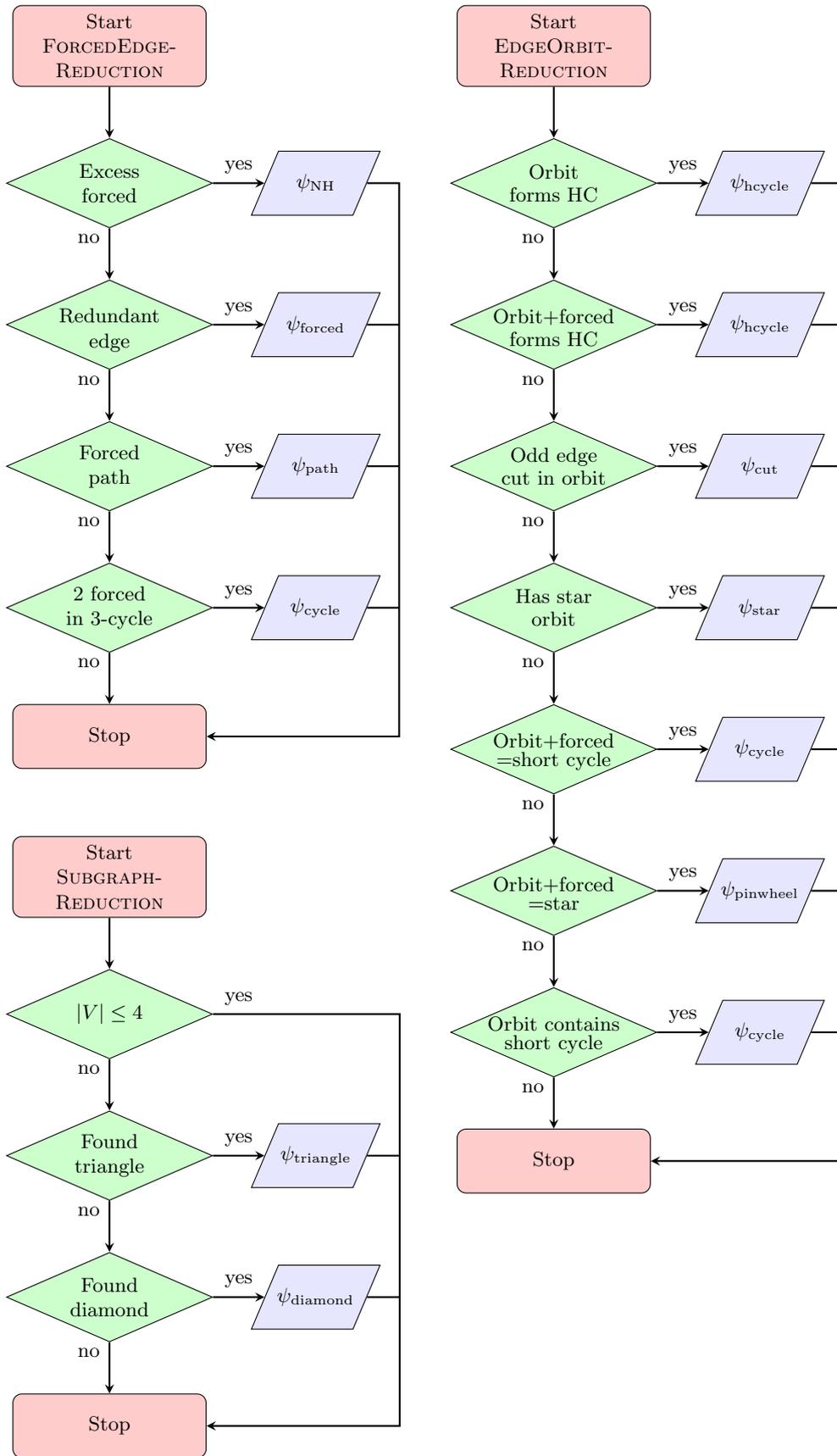


Figure 3.23: Flowchart of Algorithms 3.2 to 3.4. Refer to Figure 3.22 for key.

Algorithm 3.1 Find a Hamiltonicity-preserving graph reduction

Input: $G = (V, E)$ is a graph**Output:** A Hamiltonicity-preserving graph reduction

```

1  function GRAPHREDUCTION( $G$ )
2       $\psi \leftarrow \psi_{\text{identity}}$ 
3      loop
4          if  $\psi = \psi_{\text{NH}} \circ \dots$  then
5              return  $\psi$ 
6          if  $G$  is not 2-connected then
7               $\psi \leftarrow \psi_{\text{NH}} \circ \psi$ 
8              return  $\psi$ 
9          if  $|E| = \frac{1}{2}|V|(|V| - 1)$  then
10              $\psi \leftarrow \psi_{\text{H}} \circ \psi$  ▷  $G$  is a complete graph  $K_n$ ,  $n \geq 3$ 
11             return  $\psi$ 
12         if  $\min_{u,v \in V; uv \notin E; u \neq v} (\deg(u) + \deg(v)) \geq |V|$  then
13              $\psi \leftarrow \psi_{\text{H}} \circ \psi$  ▷ Hamiltonian by Ore's Theorem (3.7)
14             return  $\psi$ 
15          $\psi_{\text{next}} \leftarrow \text{FORCEDEDGEREDUCTION}(G)$ 
16         if  $\psi_{\text{next}} \neq \psi_{\text{identity}}$  then
17              $\psi \leftarrow \psi_{\text{next}} \circ \psi$ 
18              $G \leftarrow \psi_{\text{next}}(G)$ 
19             restart loop
20          $\psi_{\text{next}} \leftarrow \text{SUBGRAPHREDUCTION}(G)$ 
21         if  $\psi_{\text{next}} \neq \psi_{\text{identity}}$  then
22              $\psi \leftarrow \psi_{\text{next}} \circ \psi$ 
23              $G \leftarrow \psi_{\text{next}}(G)$ 
24             restart loop
25          $\psi_{\text{next}} \leftarrow \text{EDGEORBITREDUCTION}(G)$ 
26         if  $\psi_{\text{next}} \neq \psi_{\text{identity}}$  then
27              $\psi \leftarrow \psi_{\text{next}} \circ \psi$ 
28              $G \leftarrow \psi_{\text{next}}(G)$ 
29             restart loop
30     return  $\psi$  ▷ No further reductions found

```

Algorithm 3.2 Find a graph reduction based on forced edges

Input: $G = (V, E)$ is a graph**Output:** A Hamiltonicity-preserving graph reduction

```

1 function FORCEDEDGEREDUCTION( $G$ )
2    $F \leftarrow$  the forced edge set  $\{uv \in E \mid G_{E \setminus \{uv\}}$  is not 2-connected $\}$ 
3   if  $\max_{u \in V} |F(u)| > 2$  then
4     return  $\psi_{\text{NH}}$   $\triangleright$  Too many forced edges at a vertex
5   if  $\exists u \in V$  such that  $|F(u)| = 2$  and  $\deg(u) > 2$  then
6      $v_1, v_2, \dots \leftarrow$  the elements of  $N(u) \setminus F(u)$ 
7     return  $\psi_{\text{forced}}[u, v_1, v_2, \dots]$ 
8    $U \leftarrow \{v \in V \mid \deg(v) = 2\}$ 
9   for each connected component  $P = (P_V, P_E) \subseteq G_U$  do
10    if  $|P_V| > 1$  then
11      if  $|V| = 3$  then
12        return  $\psi_{\text{identity}}$   $\triangleright G$  already reduced to  $K_3$ 
13         $u_1, u_2, \dots \leftarrow$  a sequence of vertices tracing out  $P$ 
14        if  $|P_V| > |V| - 2$  then
15          truncate  $u_1, u_2, \dots$  to the first  $|V| - 2$  items
16           $v \leftarrow$  the vertex in  $V \setminus P_V$  adjacent to the last vertex in  $u_1, u_2, \dots$ 
17          return  $\psi_{\text{path}}[u_1, u_2, \dots, v]$ 
18        else
19           $u \leftarrow$  the one element of  $P_V$ 
20           $v, w \leftarrow$  the two elements of  $N(u)$ 
21          if  $vw \in E$  then
22            return  $\psi_{\text{cycle}}[v, u, w]$   $\triangleright vw$  is a redundant edge
23    return  $\psi_{\text{identity}}$ 

```

Algorithm 3.3 Find a graph reduction based on subgraphs

Input: $G = (V, E)$ is a graph**Output:** A Hamiltonicity-preserving graph reduction

```

1 function SUBGRAPHREDUCTION( $G$ )
2   if  $|V| \leq 4$  then
3     return  $\psi_{\text{identity}}$   $\triangleright$  No subgraph reductions applicable
4   for each vertex set  $\{u, v, w\}$  inducing a triangle in  $G$  do
5     if  $\deg(u), \deg(v), \deg(w) = 3$  and  $|N(u) \cup N(v) \cup N(w)| = 6$  then
6       return  $\psi_{\text{triangle}}[u, v, w]$ 
7   for each vertex set  $\{u, v, w, x\}$  inducing a diamond in  $G$  do
8     order the values of  $u, v, w, x$  so that  $uvw$  and  $vwx$  are triangles
9     if  $\deg(u), \deg(v), \deg(w), \deg(x) = 3$  and  $|N(u) \cap N(x)| = 2$  then
10      return  $\psi_{\text{diamond}}[u, v, w, x]$ 
11  return  $\psi_{\text{identity}}$ 

```

Algorithm 3.4 Find a graph reduction based on edge orbits

Input: $G = (V, E)$ is a graph**Output:** A Hamiltonicity-preserving graph reduction

```

1 function EDGEORBITREDUCTION( $G$ )
2   classify type of each orbit  $O \in \Gamma(E)$  according to Theorem 3.36
3    $F \leftarrow$  the forced edge set  $\{uv \in E \mid G_{E \setminus \{uv\}}$  is not 2-connected $\}$ 
    $\triangleright$  An orbit may trace out a complete Hamiltonian cycle
4   if  $\max_{u \in V} \deg(u) \geq 3$  and  $\exists O \in \Gamma(E)$  of type  $1C_{|V|}$  then
5      $v_1, \dots, v_n \leftarrow$  a sequence of vertices tracing out  $G_O$ 
6     return  $\psi_{\text{hcycle}}[v_1, \dots, v_n]$ 
    $\triangleright$  Search for complete cycles using one or more forced edges
7   if  $\exists O \in \Gamma(E)$  of type  $kK_2$  or  $kP_2$ , s.t.  $G_{O \cup F}$  is a  $|V|$ -cycle then
8      $v_1, \dots, v_n \leftarrow$  a sequence of vertices tracing out  $G_{O \cup F}$ 
9     return  $\psi_{\text{hcycle}}[v_1, \dots, v_n]$ 
    $\triangleright$  Search for minimal edge cut sets of odd size
10  for each  $O \in \Gamma(E)$  of type  $kK_2$  or  $kP_2$ , s.t.  $k \neq 2^n \forall n \in \mathbb{Z}$  do
11    if  $G_{E \setminus O}$  has more than one connected component then
12       $uv \leftarrow$  any edge from  $O$ 
13       $W \leftarrow$  the vertices of the component of  $G_{E \setminus O}$  containing  $u$ 
14       $X \leftarrow$  the vertices of the component of  $G_{E \setminus O}$  containing  $v$ 
15       $u_1w_1, \dots, u_a w_a \leftarrow$  the edges in  $O \setminus \{uv\}$  from  $W$  to  $V \setminus W$ 
16       $v_1x_1, \dots, v_b x_b \leftarrow$  the edges in  $O \setminus \{vu\}$  from  $X$  to  $V \setminus X$ 
17      if  $a + 1$  is odd then
18        return  $\psi_{\text{cut}}[u_1, w_1, \dots, u_a, w_a, u, v]$ 
19      else if  $b + 1$  is odd then
20        return  $\psi_{\text{cut}}[v_1, x_1, \dots, v_b, x_b, v, u]$ 
    $\triangleright$  Search for orbits containing star graphs or star subgraphs
21  if  $\exists O \in \Gamma(E)$  of type  $kS_r$ ,  $kX_r$  or  $kX_{r,s}$ , then
22     $u \leftarrow$  any vertex in  $V$  s.t.  $|N_O(u)| \geq 3$   $\triangleright$  Exists by Theorem 3.36
23     $v_1, v_2, \dots \leftarrow$  the elements of  $N_O(u)$ 
24    return  $\psi_{\text{star}}[u, v_1, v_2, \dots]$ 
    $\triangleright$  Search for short cycles using one or more forced edges
25  if  $\exists O \in \Gamma(E)$  of type  $kK_2$  or  $kP_2$ , s.t.  $G_{O \cup F}$  has a cycle  $C$  then
26     $v_1, \dots, v_m \leftarrow$  a sequence of vertices tracing out  $C$  s.t.  $v_m v_1 \in O$ 
27    return  $\psi_{\text{cycle}}[v_1, \dots, v_m]$ 
    $\triangleright$  Search for forced edge and two orbit edges incident to one vertex
28  for each  $u \in V$  s.t.  $|F(u)| = 1$  do
29    if  $\exists O \in \Gamma(E)$  not of type  $kK_2$  s.t.  $|N_O(u) \setminus F(u)| \geq 2$  then
30       $v_1, v_2, \dots \leftarrow$  the elements of  $N_O(u) \setminus F(u)$ 
31      return  $\psi_{\text{pinwheel}}[u, v_1, v_2, \dots]$ 
    $\triangleright$  Search for an orbit containing a short cycle
32  if  $\exists O \in \Gamma(E)$  of type  $kC_n$  s.t.  $n < |V|$  then
33     $v_1, \dots, v_n \leftarrow$  a sequence of vertices tracing out one cycle in  $O$ 
34    return  $\psi_{\text{cycle}}[v_1, \dots, v_n]$ 
35  return  $\psi_{\text{identity}}$ 

```

3.6 Results of reduction algorithm on cubic graphs

This section presents results of applying Algorithm 3.1 to cubic graphs, the efficacy of the Base Model on the resultant reduced graphs, and three step-by-step examples of graphs with reductions.

A summary of the reducible cubic graphs up to order 20 may be seen in Table 3.24. The algorithm is very effective on these graphs, with reductions found for 455 533 (81.9%) of the graphs, and on average resulting in the removal of nearly one third of the vertices and edges. Table 3.25 shows a summary of reductions found on Hamiltonian graphs, and Table 3.26 shows a summary of reductions found on the non-Hamiltonian non-bridge graphs; that is, the set NHNB20. A table is not included for bridge graphs, since Algorithm 3.1 reduces every bridge graph to the trivial non-Hamiltonian graph K_2 after checking connectivity.

Table 3.24: Number of cubic graphs reducible by Algorithm 3.1 by initial order up to 20. For the resulting reduced graphs, the table shows the mean number of vertices and edges, and the mean percentage decrease in the number of edges.

N	Graphs	Red.	%	Mean size of red. graphs		
				V	E	% ↓ E
4	1	1	100	3	3	50.0
6	2	2	100	3	3	66.7
8	5	5	100	3	3	75.0
10	19	18	94.7	3.28	3.39	77.4
12	85	75	88.2	4.71	5.68	68.4
14	509	433	85.1	6.08	7.95	62.1
16	4060	3403	83.8	8.48	11.85	50.6
18	41 301	34 169	82.7	11.15	16.13	40.2
20	510 489	417 427	81.8	13.85	20.38	32.0
All	556 471	455 533	81.9	13.60	19.98	32.9

Since our main goal is to detect non-Hamiltonian graphs, the fact that the algorithm finds reductions for 1980 (94.3%) of the instances of NHNB20,

Table 3.25: Number of Hamiltonian cubic graphs reducible by Algorithm 3.1, and those reducible to the trivially Hamiltonian graph K_3 , by initial order up to 20. For the resulting reduced graphs, the table shows the mean number of vertices and edges, and the mean percentage decrease in the number of edges.

N	Graphs	Red.	%	Red.		Mean size of red. graphs		
				to K_3	%	$ V $	$ E $	% $\downarrow E $
4	1	1	100	1	100	3	3	50.0
6	2	2	100	2	100	3	3	66.7
8	5	5	100	5	100	3	3	75.0
10	17	16	94.1	15	88.2	3.44	3.69	77.4
12	80	70	87.5	53	66.3	4.71	5.68	68.4
14	474	398	84.0	232	48.9	6.08	7.95	62.1
16	3841	3185	82.9	1175	30.6	8.48	11.85	50.6
18	39 635	32 516	82.0	6608	16.7	11.15	16.13	40.2
20	495 991	403 034	81.3	39 553	8.0	13.85	20.38	32.0
All	540 046	439 227	81.3	47 644	8.8	14.01	19.98	30.6

Table 3.26: Number of graphs in NHNB20 that are reducible by Algorithm 3.1, and those reducible to the trivially non-Hamiltonian graph K_2 , by initial order. For the resulting reduced graphs, the table shows the mean number of vertices and edges, and the mean percentage decrease in the number of edges.

N	Graphs	Red.	%	Red.		Mean size of red. graphs		
				to K_2	%	$ V $	$ E $	% $\downarrow E $
10	1	1	100	1	100	2	1	93.3
12	1	1	100	1	100	2	1	94.4
14	6	6	100	6	100	2	1	95.2
16	33	32	97.0	31	93.9	2.44	1.69	93.0
18	231	218	94.4	193	83.5	3.60	3.55	86.9
20	1827	1722	94.3	1305	71.4	5.58	6.73	77.6
All	2099	1980	94.3	1537	73.2	5.30	6.27	78.9

a significant majority, makes it a valuable preprocessing step. To evaluate the extent to which the algorithm assists detection of non-Hamiltonicity, we now compare the feasibility of the Base Model (introduced in Section 2.1.4) before and after reductions on these graphs. Recall that infeasibility of the Base Model is a sufficient condition for non-Hamiltonicity, so an increase in the number of infeasible LPs indicates that detection has improved. A summary of the results are shown in Table 3.27. Note that although the Base Model as originally defined does not detect K_2 as non-Hamiltonian, it is trivial to include a linear constraint such as $|V| \geq 3$, and thus we treat any graph reduced to K_2 as having an infeasible Base Model regardless.

Table 3.27: Base Model feasibility of reducible instances of NHNB20, before and after reduction.

N	Reduced	Base LP infeasible			
		Before	%	After	%
10	1	0	0	1	100
12	1	0	0	1	100
14	6	1	16.7	6	100
16	32	6	18.8	31	96.9
18	218	52	23.9	196	89.9
20	1722	418	24.3	1346	78.2
All	1980	477	24.1	1581	79.8

Nearly three quarters of the reduced NHNB cubic graphs are reduced to K_2 , so these are straightforward to identify as non-Hamiltonian, but the remaining 443 reduced graphs are only reduced partially, as illustrated in Example 3.49 below. Restricting our analysis to these partially reduced graphs, it is natural to consider the question of whether they are more or less likely to be detected as non-Hamiltonian by the LP. That is, do the (partial) graph reductions merely reduce the size of the problem (and hence the computational complexity to solve), or do the reductions fundamentally alter the graph in a way that makes it easier (or harder) to detect as non-Hamiltonian? Table 3.28 shows a contingency table with feasibility of the Base Model and after making the partial reduction.

Table 3.28: Base Model feasibility after reduction versus Base Model feasibility before reduction, for instances of NHNB20 that are partially reduced by Algorithm 3.1.

	Feasible after	Infeasible after	Total
Feasible before	397	41	438
Infeasible before	2	3	5
Total	399	44	443

It is worth noting that although two of the partially reduced graphs of NHNB20 have an infeasible Base Model LP pre-reduction and a feasible LP post-reduction, this situation can be eliminated in practice by executing the Base Model both before and after reduction. Then, if either is infeasible, the graph is necessarily non-Hamiltonian. At the cost of executing several LPs (though never more than the number of edges in the graph), the model could even be checked after each individual reduction, to detect any cases where only an intermediate reduced graph induces infeasibility during the reduction process.

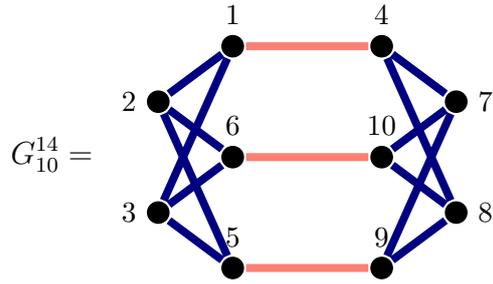
For the 443 graphs of NHNB20 that were partially reduced, there may be opportunities for identifying non-Hamiltonicity in the reduced graphs that did not exist for the original graphs. Indeed, prior to applying the partial reductions, only 5 of these 443 instances were detected as non-Hamiltonian by the Base Model, a proportion of $\frac{5}{443} \approx 1.13\%$. After applying the partial reductions, 44 instances were detected as non-Hamiltonian by the Base Model, a proportion of $\frac{44}{443} \approx 9.9\%$. This difference in proportions is strongly statistically significant, with an exact McNemar's test giving a p -value of 2.2×10^{-10} . That is, even if we can only make a partial reduction to a given graph, we not only decrease the computational complexity of executing a linear program, but likely also increase the chance of detecting non-Hamiltonicity with the Base Model.

It should be noted that many of the 443 partially reduced graphs are isomorphic to one another. In fact, there are only 87 graphs up to iso-

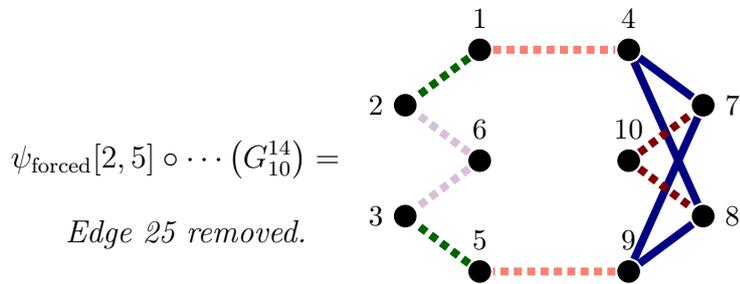
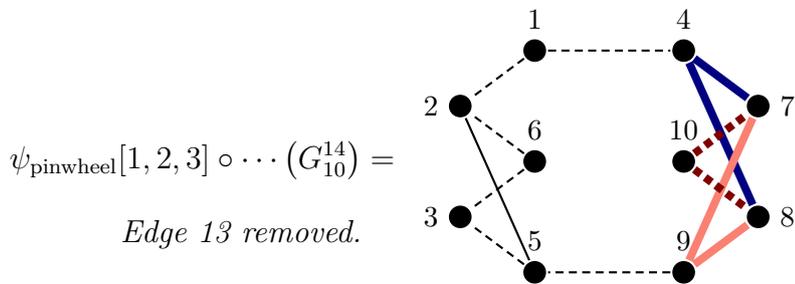
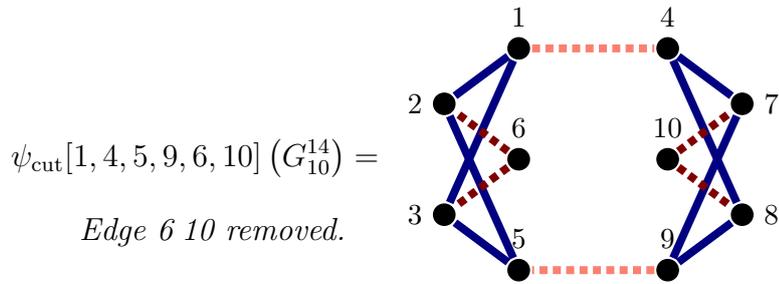
morphism. This means that, in many cases, proving that just one of these partially reduced instances is non-Hamiltonian constitutes a proof of the non-Hamiltonicity of multiple instances of NHNB20. Furthermore, 14 of these 87 instances, corresponding to 215 of the 443 partially reduced instances of NHNB20, were themselves isomorphic to smaller cubic graphs of NHNB20 that were not reducible. Hence, improving the detection for those instances would often lead to a proof of the non-Hamiltonicity of many larger instances as well. We now define the problem set *NHNB20PR* to be this set of 87 non-isomorphic partially reduced graphs. Edge lists of these 87 instances, and the IDs of the 443 instances in NHNB20 to which they correspond, may be found in Appendix A.2. In Chapter 4 we will investigate extensions of the Base Model, and so will have a particular interest in how the extended models perform on instances of NHNB20PR, with the eventual goal of solving even more instances of NHNB20.

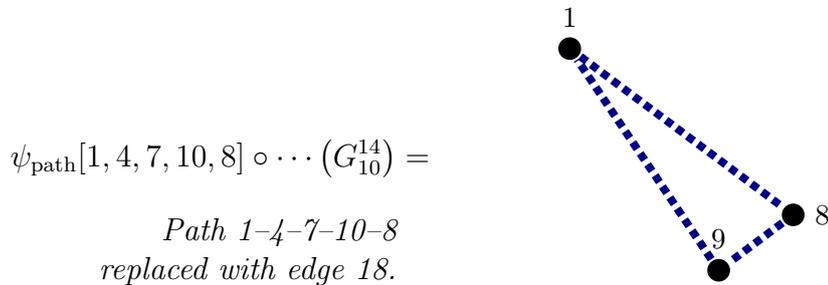
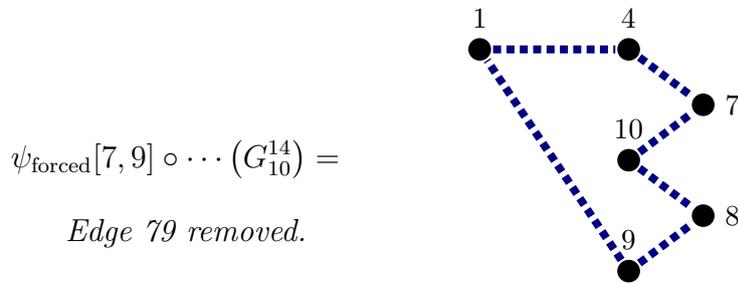
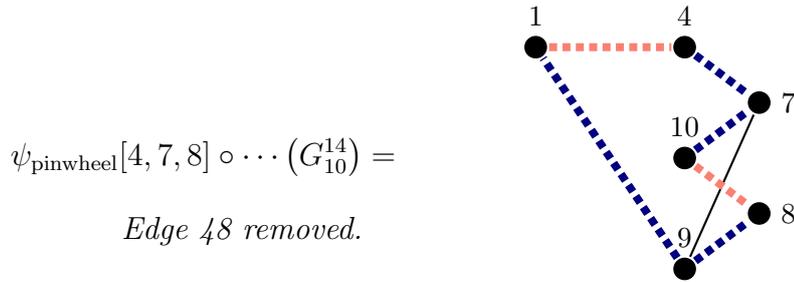
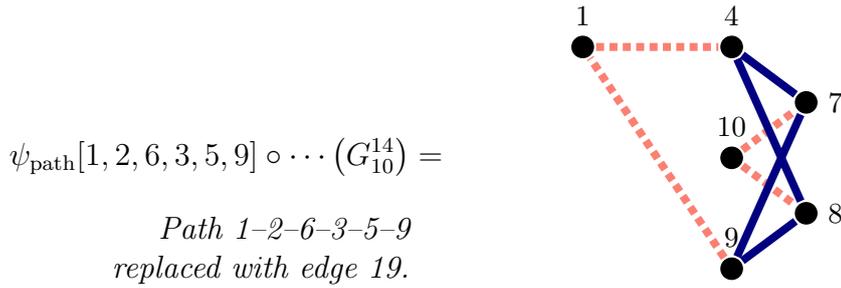
Having demonstrated a significant improvement in the number of non-Hamiltonian graphs detected through polynomial-time methods, we conclude this chapter with three illustrative examples of the reductions found by Algorithm 3.1. Example 3.47 shows a Hamiltonian graph reduced to K_3 along with a recovery of a Hamiltonian cycle; Example 3.48 shows the famous Petersen graph reduced to K_2 ; and Example 3.49 shows a NHNB graph for which only a partial reduction is found. In the examples, edges detected as forced are dashed, and orbits consisting of more than one edge are drawn with thick lines highlighted in different colours, while the remaining orbits are black. The italicised comment below each reduction summarises the change made to the graph since the previous step.

Example 3.47. A triangle-free 10-vertex graph (G_{10}^{14}) reduced to K_3 after applying the reduction found by Algorithm 3.1. The example also demonstrates how a Hamiltonian cycle in the original graph can be recovered from a Hamiltonian cycle in the reduced graph.

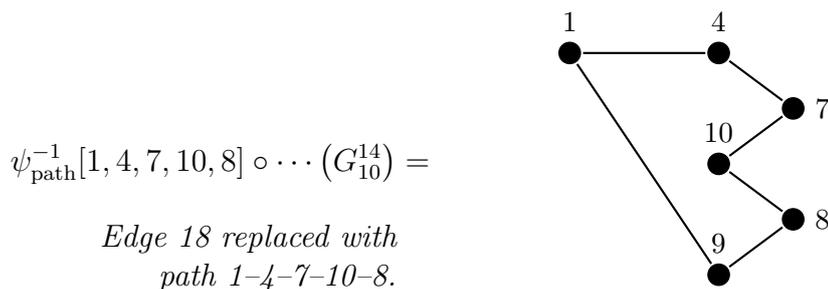


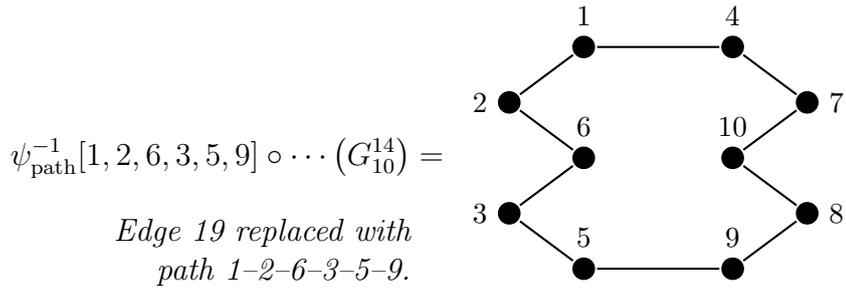
$$\begin{aligned} \text{GRAPHREDUCTION}(G_{10}^{14}) &= \psi_H \circ \psi_{\text{path}}[1, 4, 7, 10, 8] \circ \psi_{\text{forced}}[7, 9] \\ &\quad \circ \psi_{\text{pinwheel}}[4, 7, 8] \circ \psi_{\text{path}}[1, 2, 6, 3, 5, 9] \\ &\quad \circ \psi_{\text{forced}}[2, 5] \circ \psi_{\text{pinwheel}}[1, 2, 3] \\ &\quad \circ \psi_{\text{cut}}[1, 4, 5, 9, 6, 10]. \end{aligned}$$





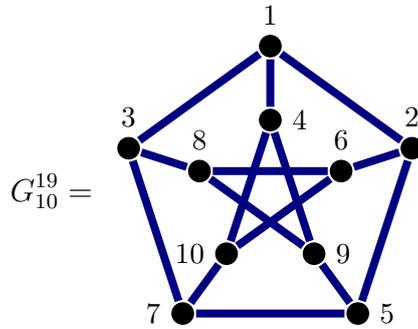
At this point we have a graph isomorphic to K_3 with a Hamiltonian cycle 1-8-9. Applying ψ_H is not strictly necessary. To recover a Hamiltonian cycle in the original graph we take this cycle and apply inverses of just the ψ_{path} reductions:



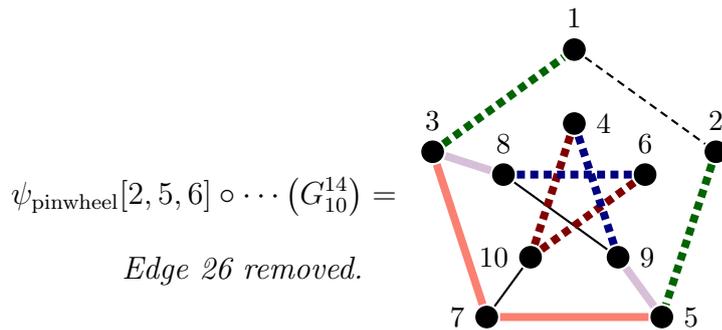
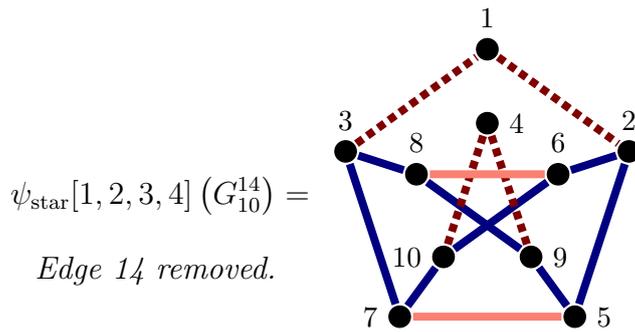


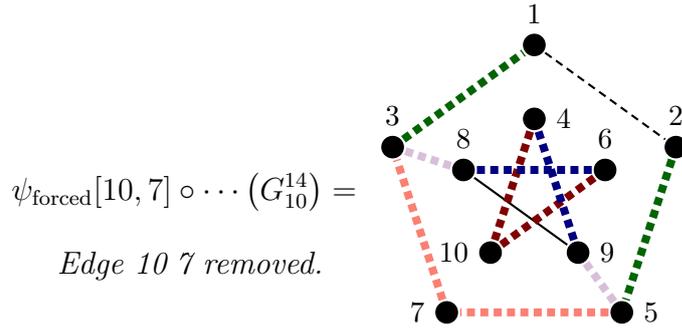
It is straightforward to verify that 1-4-7-10-8-9-5-3-6-2 is a Hamiltonian cycle in the original graph.

Example 3.48. The Petersen graph, the smallest NHNB cubic graph, is reduced to K_2 after applying the reduction found by Algorithm 3.1.

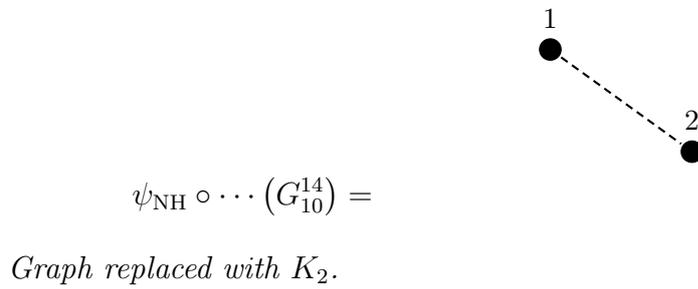


$$\text{GRAPHREDUCTION}(G_{10}^{19}) = \psi_{\text{NH}} \circ \psi_{\text{forced}}[10, 7] \circ \psi_{\text{pinwheel}}[2, 5, 6] \circ \psi_{\text{star}}[1, 2, 3, 4].$$

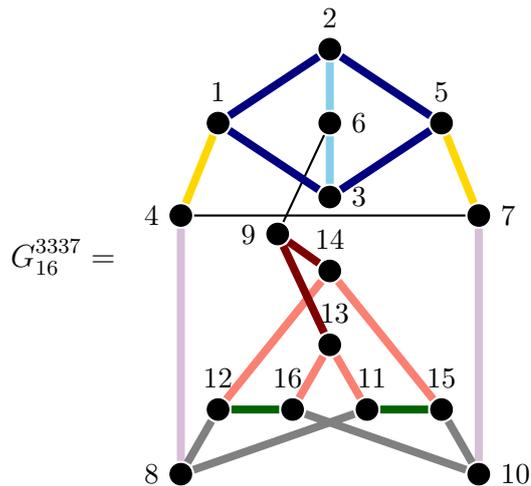




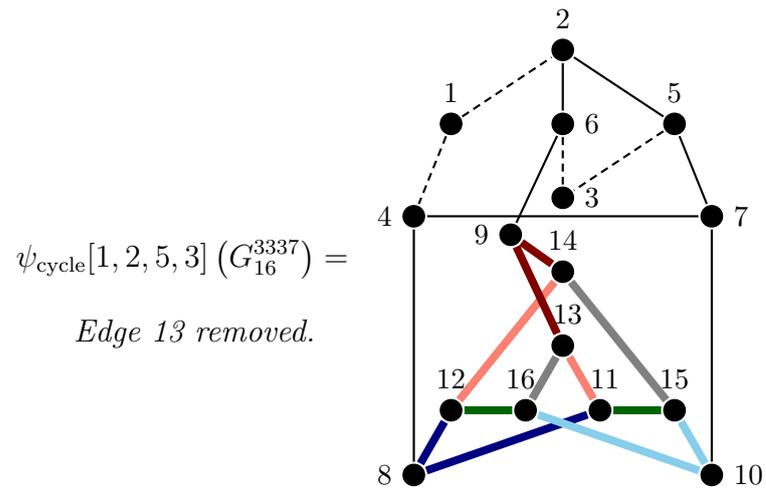
At this stage Algorithm 3.1 detects more than two forced edges at either vertex 3 or 5 and so it applies ψ_{NH} :



Example 3.49. The smallest NHNB cubic graph just partially reduced by Algorithm 3.1 (G_{16}^{3337}). Only a single reduction step is found before the algorithm terminates.



$\text{GRAPHREDUCTION}(G_{16}^{3337}) = \psi_{\text{cycle}}[1, 2, 5, 3].$



Chapter 4

Extending the Base Model

In Chapter 2 we examined a number of linear models for HCP and TSP and concluded that the Base Model is the strongest amongst them in two senses. First, for the non-Hamiltonian HCP instances tested, the Base Model identifies a proper superset of those which the other models identify. Second, for the TSP instances tested, the gaps obtained by the Base Model are on average the smallest amongst the considered models. Indeed, of the 800 TSP instances tested, only eight instances were found for which the Base Model is outperformed, in each case by the SST model.

Rather than trying to further reduce the graphs as done in Chapter 3, an alternative avenue to improve detection of non-Hamiltonian graphs is to seek to tighten the Base Model itself. In this way we aim to induce infeasibility more often for non-Hamiltonian graphs. Additionally, we aim to improve the bounds obtained for TSP instances as this also constitutes a measure of improvement. To this end, we have considered a variety of new kinds of constraints, some of which offered improvement while others appeared to be redundant. In this chapter, we describe the new constraints for which an improvement is observed for the instances considered. The new constraints are grouped into several categories, and for each category we define an extension of the Base Model with the additional constraints. In

particular, we will consider extensions based on the SST model, the presence of forced edges, the presence of 3-cuts, and an eigenvalue of Hamiltonian permutation matrices.

Some of the new constraints exploit features that may only be present in some graphs, but all the constraints are presented in such a way that they reduce to an empty set of constraints when the features are absent, ensuring that the models are well-defined for any graph. It should be noted that the constraints proposed in this chapter are not designed to be minimal in a redundancy sense, although we will remove redundant constraints when such redundancies are obvious. With only one exception, the extended models do not have a higher time complexity than the Base Model. That is, the number of variables and constraints remains $\mathcal{O}(n^3)$ for sparse graphs and $\mathcal{O}(n^4)$ for dense graphs. For the one model that does have a higher time complexity than the Base Model, it will be shown that the set of $\mathcal{O}(n^4)$ constraints responsible may be replaced by a stronger set of $\mathcal{O}(n^3)$ constraints.

Throughout this chapter we test the extended models on the two HCP problem sets NHNB20 and NHNB20PR, and on the two TSP problem sets ATSP16A and ATSP16AC. NHNB20, introduced in Section 2.2.2, is the set of all 2099 non-Hamiltonian non-bridge cubic graphs up to order 20, an index of which may be found in Appendix A.1. NHNB20PR, introduced in Section 3.6, is the set of 87 graphs to which the 443 partially reduced instances of NHNB20 are isomorphic. The TSP problem sets are the ATSP16A and ATSP16AC sets constructed in Section 2.2.4, each containing 400 instances. Recall that each instance of ATSP16A is a complete instance that is based on an underlying cubic graph. For each instance in ATSP16A, there is a corresponding cubic instance in ATSP16AC where only the edges in the underlying cubic graph are used. Note that, for any instance of ATSP16A and the corresponding instance in ATSP16AC, those edges in common for both instances have the same costs.

We conclude this introduction by recalling the Base Model and the results of the Base Model on the four problem sets. The following sections then introduce the extended models along with their results on the problem sets, showing the improvements gained. Then, in Section 4.5, we define a combined model that uses constraints from all the extended models. We will demonstrate that this combined model is stronger than any of its constituent models, in the sense that instances exist for which the combined model outperforms all the other extended models considered. Finally, in Section 4.6, we introduce a method that produces a set of subgraphs for any given HCP instance, and uses the combined model on these subgraphs to attempt to infer non-Hamiltonicity of the original instance. We will show that this approach is successful for almost all instances of NHNB20 and NHNB20PR.

Recall that the Base Model is defined in terms of variables $x_{r,ia}^k$ for all vertices $k, i = 1, \dots, n$, steps $r = 0, \dots, n-1$, and adjacent vertices $a \in N(i)$. The value of $x_{r,ia}^k$ is intended to be 1 if the arc $i \rightarrow a$ is used r steps after vertex k in the Hamiltonian cycle, and 0 otherwise. For convenience, we restate the (relaxed) linear constraints of the Base Model, from Section 2.1.4. Unless otherwise restricted, the indices i, j , and k range from 1 to n and that the indices r and s range from 0 to $n-1$.

$$\sum_{a \in N(i)} x_{r,ia}^k - \sum_{a \in N(i)} x_{r-1,ai}^k = 0 \quad \forall i, k, r; r \neq 0 \quad (4.1)$$

$$\sum_{a \in N(i)} x_{r,ia}^k - \sum_{a \in N(k)} x_{n-r,ka}^i = 0 \quad \forall i, k, r; r \neq 0 \quad (4.2)$$

$$\sum_{r=0}^{n-1} x_{r,ia}^k - \sum_{r=0}^{n-1} x_{r,ia}^j = 0 \quad \forall i, j, k; a \in N(i); k \neq j \quad (4.3)$$

$$\sum_{k=1}^n x_{r,ia}^k - \sum_{k=1}^n x_{s,ia}^k = 0 \quad \forall i, r, s; a \in N(i); s \neq r \quad (4.4)$$

$$\sum_{r=0}^{n-1} \sum_{a \in N(i)} x_{r,ia}^k = 1 \quad \forall i, k \quad (4.5)$$

$$\sum_{k=1}^n \sum_{a \in N(i)} x_{r,ia}^k = 1 \quad \forall i, r \quad (4.6)$$

$$x_{0,ia}^k = 0 \quad \forall i, k; a \in N(i); i \neq k \quad (4.7)$$

$$x_{r,ia}^k \geq 0 \quad \forall k, r; a \in N(i). \quad (4.8)$$

When used in a TSP sense, recall from Section 2.2.3 that we may define the objective function, which we seek to minimise, to be

$$\sum_{i=1}^n \sum_{j \in N(i)} c_{ij} x_{0,ij}^i. \quad (4.9)$$

We now summarise the results of the Base Model on the problem sets NHNB20 and NHNB20PR in Table 4.1, the former of which were presented in Section 2.2.2. Similarly, results of the Base Model on ATSP16A and ATSP16AC from Section 2.2.5 are summarised in Table 4.2. As in previous chapters, all results in this chapter were generated using the CPLEXTM Callable Library version 12.5 [42]. For the HCP instances we report the number of graphs for which the Base Model is infeasible, and for the TSP instances we report the sum and mean of the gaps. Recall that for a TSP instance and a given model, the gap is defined to be the difference between the length of the optimal tour and the lower bound obtained by that model. Also recall from Definition 2.11 that for the non-Hamiltonian instances of ATSP16AC, where no optimal tour exists, we define the gap to be the difference between the length of the optimal tour of the corresponding complete instance of ATSP16A, and the lower bound obtained by the model on the ATSP16AC instance. Finally, recall that the TSP instances were specifically constructed to induce large gaps between the solution found by the Base Model and the length of the optimal tour in the complete instances; indeed, no instances in these sets have zero gap for the Base Model, with the minimum gap being approximately 48.7 for both sets.

In the upcoming extended models, we report not only infeasibility and gaps, but also the improvements relative to the Base Model. That is, for HCP instances we report the number of instances that are feasible for the Base Model but infeasible for the extended model, if any. For TSP instances, we

Table 4.1: Results of the Base Model on (a) NHNB20 and (b) NHNB20PR, by order n .

(a) NHNB20			(b) NHNB20PR		
n	Graphs	Infeasible	n	Graphs	Infeasible
10	1	0	12	1	0
12	1	0	13	1	1
14	6	1	14	7	3
16	33	6	15	5	4
18	231	52	16	9	4
20	1827	418	17	23	3
All	2099	477	18	17	0
			19	6	3
			20	18	0
			All	87	18

Table 4.2: Results of the Base Model on the 200 Hamiltonian-derived and 200 NHNB-derived instances in each of (a) ATSP16A and (b) ATSP16AC.

(a) ATSP16A		
Subset	Sum of gaps	Mean
Ham.-derived	16 864.2	84.3
NHNB-derived	289 064.2	1445.3
All	305 928.4	764.8

(b) ATSP16AC		
Subset	Sum of gaps	Mean
Ham.-derived	16 864.2	84.3
NHNB-derived	288 979.2	1444.9
All	305 843.4	764.6

report the number of instances for which the optimal solution *changed*, and the mean improvement in the gap for those changed instances. Specifically, we consider the solution to have changed for a TSP instance, if in the given extended model there is not a feasible solution with the same $x_{r,ia}^k$ values as those in the optimal feasible solution from the Base Model.

4.1 Merging SST with the Base Model

As seen in Section 2.2.5, there are four instances from the ATSP16A problem set (and their corresponding four instances in the ATSPC16AC cubic problem set) for which the SST model outperforms the Base Model. It follows that the constraints in SST prevent some linear combinations of cycles and subcycles that are not prevented by constraints in the Base Model. Therefore, a natural extension to the Base Model is to include variables and constraints analogous to those in the SST model. We begin by mapping the x_{ij} variables from SST to the $x_{r,ia}^k$ variables of the Base Model and including the appropriately reformulated constraints from SST in the Base Model.

Recall that SST is defined in terms of the following variables:

- x_{ij} , intended to be 1 if the arc $i \rightarrow j$ is used in the cycle, and 0 otherwise.
- y_{ij} , intended to be 1 if, starting from vertex 1, vertex j comes later than vertex i in the cycle, and 0 otherwise.
- f_{ij}^v , intended to be 1 if, starting from vertex 1, the arc $i \rightarrow v$ is used prior to visiting vertex j , and 0 otherwise.

While the Base Model contains no natural analogues to the y and f variables of SST, the x_{ij} variables of SST can easily be expressed in terms of the $x_{r,ia}^k$ variables from the Base Model. Specifically, inspecting the objective functions of the two models it is clear that we can express the variables x_{ij} of SST as

$$x_{ij} = x_{0,ij}^i.$$

Hence the constraints from SST, based on the more general constraints for potentially non-complete graphs, (2.25), (2.29), (2.43), (2.44), (2.50) and (2.58) – (2.66) may be reformulated for the Base Model variables as follows. Unless otherwise restricted, all indices range from 1 to n .

$$\sum_{j \in N(i)} x_{0,ij}^i = 1 \quad \forall i \quad (4.10)$$

$$\sum_{i \in N(j)} x_{0,ij}^i = 1 \quad \forall j \quad (4.11)$$

$$y_{ij} + y_{ji} = 1 \quad \forall i, j; 1 \neq i \neq j \quad (4.12)$$

$$y_{ij} \geq x_{0,1i}^1 \quad \forall j; i \in N(1); 1 \neq i \neq j \quad (4.13)$$

$$y_{ji} \geq x_{0,i1}^i \quad \forall j; i \in N(1); 1 \neq i \neq j \quad (4.14)$$

$$0 \leq x_{0,ij}^i \leq 1 \quad \forall i, j; i \neq j \quad (4.15)$$

$$y_{ij} \geq 0 \quad \forall i, j; 1 \neq i \neq j \quad (4.16)$$

$$y_{ij} + x_{0,ji}^j + y_{jl} + y_{li} \leq 2 \quad \forall i, l; j \in N(i); 1 \neq i \neq j \neq l \quad (4.17)$$

$$y_{ij} + 0 + y_{jl} + y_{li} \leq 2 \quad \forall i, l; j \notin N(i); 1 \neq i \neq j \neq l \quad (4.18)$$

$$0 \leq f_{ij}^v \leq x_{0,iv}^i \quad \forall i, j; v \in N(i); 1 \neq i \neq v \neq j \quad (4.19)$$

$$\sum_{v \in N(i) \setminus \{1, j\}} f_{ij}^v + x_{0,ij}^i = y_{ij} \quad \forall i; j \in N(i); 1 \neq i \neq j \quad (4.20)$$

$$\sum_{v \in N(i) \setminus \{1\}} f_{ij}^v + 0 = y_{ij} \quad \forall i; j \notin N(i); 1 \neq i \neq j \quad (4.21)$$

$$x_{0,1v}^1 + \sum_{i \in N(v) \setminus \{1, j\}} f_{ij}^v = y_{vj} \quad \forall j; v \in N(1); 1 \neq v \neq j \quad (4.22)$$

$$0 + \sum_{i \in N(v) \setminus \{j\}} f_{ij}^v = y_{vj} \quad \forall j; v \notin N(1); 1 \neq v \neq j. \quad (4.23)$$

The intention is now to combine the Base Model constraints (4.1) – (4.8) with the reformulated SST constraints (4.10) – (4.23). However, there are some redundancies. Clearly, (4.15) follows from (4.8) and (4.6) where $r = 0$. Additionally, (4.10) and (4.11) follow from Lemma 2.13. Hence, adding the non-redundant constraints above to the Base Model, we obtain a new model which we call Base-SST.

Definition 4.1 (Base-SST). Minimise (4.9), subject to (4.1) – (4.8), (4.12) – (4.14) and (4.16) – (4.23). If the costs c_{ij} are not provided, find any solution subject to these constraints.

Table 4.3 shows the results of Base-SST on the problem sets NHNB20 and NHNB20PR. As can be seen, there are no additional instances in these sets for which Base-SST obtains infeasibility, relative to the Base Model.

Table 4.3: Results of Base-SST on (a) NHNB20 and (b) NHNB20PR, by order n . The table also shows the improvement in solved instances relative to the Base Model.

(a) NHNB20				(b) NHNB20PR			
n	Graphs	Inf.	Imprv.	n	Graphs	Inf.	Imprv.
10	1	0	0	12	1	0	0
12	1	0	0	13	1	1	0
14	6	1	0	14	7	3	0
16	33	6	0	15	5	4	0
18	231	52	0	16	9	4	0
20	1827	418	0	17	23	3	0
All	2099	477	0	18	17	0	0
				19	6	3	0
				20	18	0	0
				All	87	18	0

Table 4.4 shows the results of Base-SST on the problem sets ATSP16A and ATSP16AC. It can be seen that, unlike for the HCP instances, there is a clear improvement over the Base Model in these instances. Indeed, an improvement is observed in 183 of the 400 instances for both problem sets.

4.1.1 Base-SST model with multiple starting vertices

As seen above, adding the reformulated SST constraints tightens the Base Model. However, the y and f variables used of the SST constraints are intended to describe only a cycle starting at vertex 1. In contrast, the variables of the Base Model are intended to describe the same cycle n times, from each possible starting vertex. Therefore, a natural extension of Base-SST is

Table 4.4: Results of Base-SST on the 200 NHNB-derived and 200 Hamiltonian-derived instances in each of (a) ATSP16A and (b) ATSP16AC. The table indicates the number of instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

(a) ATSP16A				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	16 667.5	83.3	101/200	1.947
NHNB-derived	288 895.7	1444.5	82/200	2.054
All	305 563.2	763.9	183/400	1.995

(b) ATSP16AC				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	16 667.6	83.3	101/200	1.947
NHNB-derived	288 810.8	1444.1	82/200	2.054
All	305 478.3	763.7	183/400	1.995

to consider higher-dimensional y and f variables, defined for each possible starting vertex, as below. Note that for consistency with the Base Model variables, where the superscript k denotes the starting vertex, the positions of the indices in the extended y and f variables have been altered.

- y_{ij}^k , intended to be 1 if, starting from vertex k , vertex j comes later than vertex i in the cycle, and 0 otherwise, for $i, j, k = 1 \dots n$; $i \neq j \neq k$.
- $f_{ia,j}^k$, intended to be 1 if, starting from vertex k , the arc $i \rightarrow a$ is used prior to visiting vertex j , and 0 otherwise, for $i, j, k = 1 \dots n$; $a \in N(i)$; $i \neq a \neq j \neq k$.

Constraints (4.12) – (4.14) and (4.16) – (4.23) can now be extended to use these new variables as follows. Since this extension involves effectively just replacing every instance of the index 1 with k in the original constraints, correctness follows from the correctness of Base-SST. Unless otherwise restricted, the indices i, j, k and l range from 1 to n .

$$y_{ij}^k + y_{ji}^k = 1 \quad \forall k, i, j; k \neq i \neq j \quad (4.24)$$

$$y_{ij}^k \geq x_{0,ki}^k \quad \forall k, j; i \in N(k); k \neq i \neq j \quad (4.25)$$

$$y_{ji}^k \geq x_{0,ik}^i \quad \forall i, j; i \in N(k); k \neq i \neq j \quad (4.26)$$

$$y_{ij}^k + x_{0,ji}^j + y_{jl}^k + y_{li}^k \leq 2 \quad \forall k, i, l; j \in N(i); k \neq i \neq j \neq l \quad (4.27)$$

$$y_{ij}^k + 0 + y_{jl}^k + y_{li}^k \leq 2 \quad \forall k, i, l; j \notin N(i); k \neq i \neq j \neq l \quad (4.28)$$

$$y_{ij}^k \geq 0 \quad \forall k, i, j; k \neq i \neq j \quad (4.29)$$

$$0 \leq f_{ia,j}^k \leq x_{0,ia}^i \quad \forall k, i, j; a \in N(i); k \neq i \neq a \neq j \quad (4.30)$$

$$\sum_{a \in N(i) \setminus \{k,j\}} f_{ia,j}^k + x_{0,ij}^i = y_{ij}^k, \quad \forall k, i; j \in N(i); k \neq i \neq j \quad (4.31)$$

$$\sum_{a \in N(i) \setminus \{k\}} f_{ia,j}^k + 0 = y_{ij}^k \quad \forall k, i; j \notin N(i); k \neq i \neq j \quad (4.32)$$

$$x_{0,ki}^k + \sum_{b \in N(i) \setminus \{k,j\}} f_{bi,j}^k = y_{ij}^k \quad \forall k, j; i \in N(k); k \neq i \neq j \quad (4.33)$$

$$0 + \sum_{b \in N(i) \setminus \{j\}} f_{bi,j}^k = y_{ij}^k \quad \forall k, j; i \notin N(k); k \neq i \neq j. \quad (4.34)$$

We remark that (4.28) contains $\mathcal{O}(n^4)$ constraints in the event that the graph is sparse, in contrast to the Base Model which has $\mathcal{O}(n^3)$ constraints in total for sparse graphs. This increase in time complexity is undesirable, however it will be shown in Section 4.1.2 that we can replace both (4.27) and (4.28) with a stronger set of $\mathcal{O}(n^3)$ equality constraints.

We now define the model Base-SST- k to use these modified constraints, where k signifies the use of every starting vertex:

Definition 4.2 (Base-SST- k). Minimise the objective function (4.9), subject to (4.1) – (4.8) and (4.24) – (4.34). If the costs c_{ij} are not provided, find any solution subject to these constraints.

Unfortunately, as with Base-SST, Base-SST- k is not infeasible for any additional instances of NHHB20 or NHHB20PR relative to the Base Model. However, Base-SST- k offers significant improvements in a TSP sense relative

to Base-SST. Table 4.5 shows the results of Base-SST- k on ATSP16A and ATSP16AC, where improvements are given relative to the Base Model. Unlike for Base-SST, for which fewer than half of the instances show an improvement, Base-SST- k induces an improved gap in 348 instances of ATSP16A and ATSP16AC, with the mean improvement in gaps more than three times as large compared to Base-SST, demonstrating the value of considering the different starting points.

Table 4.5: Results of Base-SST- k on the 200 NHNB-derived and 200 Hamiltonian-derived instances in each of (a) ATSP16A and (b) ATSP16AC. The table indicates the number of instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

(a) ATSP16A				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	15 351.9	76.8	188/200	8.044
NHNB-derived	288 363.1	1441.8	160/200	4.382
All	303 715.0	759.3	348/400	6.360

(b) ATSP16AC				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	15 351.9	76.8	188/200	8.044
NHNB-derived	288 278.1	1441.4	160/200	4.382
All	303 630.1	759.1	348/400	6.360

4.1.2 Extended Base-SST model

A further extension to Base-SST is possible by adding linking constraints for the new y and f variables:

$$y_{ij}^k = y_{jk}^i \quad \forall k, i, j; k < i < j \text{ or } j < k < i \quad (4.35)$$

$$f_{ia,j}^k + f_{ia,k}^j = x_{0,ia}^i \quad \forall k, i, j; a \in N(i); k < j; k \neq i \neq a \neq j. \quad (4.36)$$

To show the correctness of the new constraints it is sufficient to show that, for any Hamiltonian cycle, the constraints are satisfied if the variables are set

according to their interpretations, which we show in Proposition 4.4 below.

For use in the upcoming proposition and the remainder of this section, we introduce the following definition.

Definition 4.3 (Vertex ordering). A *vertex ordering*, denoted $[v_0, v_1, \dots, v_{k-1}]$, indicates an ordered sequence of vertices in a cyclic sense. That is, vertex v_i occurs at some point after v_{i-1} on a cycle, but before v_{i+1} for all $i = 0 \dots, k-1$, where the subscripts are taken mod k .

Proposition 4.4. Let $G = (V, E)$ be a graph. Constraints (4.35) and (4.36) are satisfied for any solution of Base-SST- k corresponding to a (directed) Hamiltonian cycle H in G .

Proof. We first show that (4.35) holds. Let $i, j, k \in V$ be distinct and consider the vertex ordering of these vertices in H . There are just two possible vertex orderings; $[k, i, j]$ if i precedes j when starting at k , and $[k, j, i]$ otherwise. See Figure 4.6 for a visualisation. By the stated interpretation of the y variables, in the case of $[k, i, j]$ we should set $y_{ij}^k = 1$. By cyclicity, it is clear that we should also set $y_{jk}^i = y_{ki}^j = 1$. In the case of $[k, j, i]$ however, $y_{ij}^k = 0$ since i does not precede j , if starting at k . Similarly, $y_{jk}^i = y_{ki}^j = 0$. Thus regardless of the direction of H and the choice of distinct vertices, we have

$$y_{ij}^k = y_{jk}^i = y_{ki}^j \quad \forall k \neq i \neq j. \quad (4.37)$$

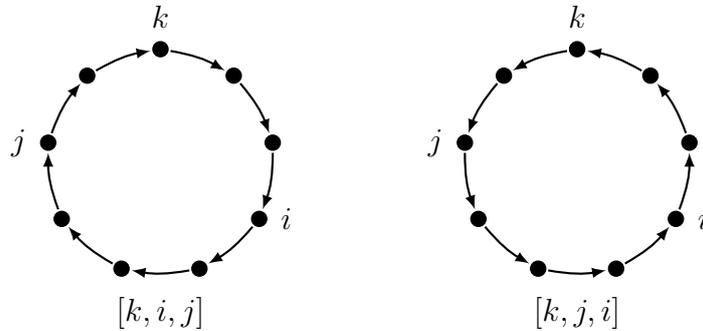


Figure 4.6: An example of two directed Hamiltonian cycles showing both possible vertex orderings of the vertices i, j and k .

Clearly, (4.37) implies (4.35). However, it can also be shown that (4.35), along with (4.24), implies (4.37) despite the latter not imposing ordering requirements on the indices. Without loss of generality, choose three vertices numbered 1, 2 and 3. It is sufficient to show that (4.35), together with the other constraints in Base-SST- k , implies

$$y_{23}^1 = y_{31}^2 = y_{12}^3 \quad (4.38)$$

$$y_{32}^1 = y_{13}^2 = y_{21}^3. \quad (4.39)$$

Immediately from (4.35) we have the two equalities when the indices satisfy $k < i < j$ and $j < k < i$, respectively,

$$y_{23}^1 = y_{31}^2 \quad (4.40)$$

$$y_{31}^2 = y_{12}^3. \quad (4.41)$$

This implies (4.38). Next, by (4.24) in Base-SST- k , we can exchange the variables in (4.40) and (4.41) as follows:

$$1 - y_{32}^1 = 1 - y_{13}^2 \quad (4.42)$$

$$1 - y_{13}^2 = 1 - y_{21}^3. \quad (4.43)$$

It is clear that (4.42) and (4.43) imply (4.39). Therefore, (4.35) implies (4.37).

Finally we show that (4.36) holds for the Hamiltonian cycle H . Let $i \rightarrow a$ be any arc in G . By the stated interpretation of the $x_{0,ia}^i$ variables, we can set $x_{0,ia}^i = 1$ if the arc $i \rightarrow a$ is used in H , and set $x_{0,ia}^i = 0$ otherwise. In the latter case, (4.30) will constrain $f_{ia,j}^k$ and $f_{ia,k}^j$ to be zero regardless of the choice of k and j , so (4.36) holds.

It remains to consider the case that $x_{0,ia}^i = 1$. Since a must immediately follow i , there are again two possible vertex orderings of the vertices k, i, a and j ; either $[i, a, j, k] = [k, i, a, j]$ or $[i, a, k, j] = [j, i, a, k]$. In the former case, the arc $i \rightarrow a$ is used before j if starting at k , so we can set $f_{ia,j}^k = 1$

and $f_{ia,k}^j = 0$. In the latter case we can similarly set $f_{ia,j}^k = 0$ and $f_{ia,k}^j = 1$. Therefore (4.36) holds in either case. \square

Additionally to the linking constraints (4.35) and (4.36), we may also replace the inequality constraints (4.27) and (4.28) with a stronger set of equality constraint as follows:

$$y_{ij}^1 + y_{il}^j + y_{jl}^1 + y_{li}^1 = 2 \quad \forall i, j, l; 1 < i < j < l. \quad (4.44)$$

We remark that in contrast to (4.27) and (4.28) from Base-SST- k , which together comprise $\mathcal{O}(n^4)$ inequality constraints, (4.44) has only $\mathcal{O}(n^3)$ equality constraints.

Proving that (4.44) is stronger than (4.27) and (4.28) is non-trivial. First we consider a more general version of (4.44);

$$y_{ij}^k + y_{il}^j + y_{jl}^k + y_{li}^k = 2 \quad \forall k, i, j, l; k \neq i \neq j \neq l. \quad (4.45)$$

We will first prove in Proposition 4.5 that (4.45) is satisfied for all solutions corresponding to Hamiltonian cycles and is stronger than (4.27) and (4.28). Following this, Theorem 4.6 shows that (4.44) and (4.45) are equivalent.

Proposition 4.5. *Let $G = (V, E)$ be a graph. Then:*

- (i) *The constraints (4.27) and (4.28) are redundant in the presence of (4.45) and the other Base-SST- k constraints.*
- (ii) *The constraints (4.45) are satisfied for any solution of Base-SST- k corresponding to a Hamiltonian cycle H in G .*

Proof. By (4.25) and the non-negativity constraints (4.8) we have

$$0 \leq x_{0,ji}^j \leq y_{il}^j,$$

so the left hand sides of (4.27) and (4.28) are both bounded from above by

(4.45) as follows:

$$\begin{aligned} y_{ij}^k + x_{0,ji}^j + y_{jl}^k + y_{li}^k &\leq y_{ij}^k + y_{il}^j + y_{jl}^k + y_{li}^k = 2 \\ y_{ij}^k + 0 + y_{jl}^k + y_{li}^k &\leq y_{ij}^k + y_{il}^j + y_{jl}^k + y_{li}^k = 2. \end{aligned}$$

Therefore the constraints (4.27) and (4.28) are redundant, hence (i) is proved.

Next, we show that (4.45) is satisfied for the cycle H . Consider four distinct vertices i, j, k and l in V . There are six possible vertex orderings of these vertices depending on the cycle H : $[k, i, j, l]$, $[k, i, l, j]$, $[k, j, i, l]$, $[k, j, l, i]$, $[k, l, i, j]$ and $[k, l, j, i]$. Setting each of the y variables in (4.45) according to their interpretations, we tabulate the values for the six possible vertex orderings:

Vertex ordering	y_{ij}^k	y_{il}^j	y_{jl}^k	y_{li}^k	Sum
$[k, i, j, l]$	1	0	1	0	2
$[k, i, l, j]$	1	1	0	0	2
$[k, j, i, l]$	0	1	1	0	2
$[k, j, l, i]$	0	0	1	1	2
$[k, l, i, j]$	1	0	0	1	2
$[k, l, j, i]$	0	1	0	1	2

In every case the sum of the four variables is 2. Therefore the solution corresponding to H always satisfies (4.45) regardless of the ordering of the vertices on the cycle. \square

We remark that the equalities of (4.45) may be especially stronger than the inequalities of (4.27) and (4.28) when the arc $j \rightarrow i$ is not used or not present. In that case, the only potentially positive terms remaining on the left hand sides of (4.27) and (4.28) are y_{ij}^k , y_{jl}^k and y_{li}^k , whereas (4.45) has an additional non-negative term on the left hand side, namely y_{il}^j .

Theorem 4.6. *The equalities in (4.45) are implied by the subset of $\binom{n-1}{3}$ equalities given in (4.44) and the constraints (4.24) and (4.35).*

Proof. This proof consists of two parts. We will first prove that (4.45) is

equivalent to

$$y_{ij}^k + y_{il}^j + y_{jl}^k + y_{li}^k = 2 \quad \forall k, i, j, l; k < i < j < l, \quad (4.46)$$

which is identical to (4.45) except the indices are ordered. Following this, we will prove that k can be fixed to be 1.

To show the equivalence of (4.45) and (4.46), we will demonstrate that given any particular equation from (4.46), we can derive additional constraints that have the same form but a different ordering of the indices. In particular, we will show the derivation of two such additional constraints, which respectively correspond to two cyclic permutations of the indices; $(i j)$ and $(i j l k)$. Together, these are a generating set for the group of all permutations on the four indices (that is, the symmetric group S_4 .) Hence, we will conclude that we can derive any constraint of (4.45) from an appropriate constraint of (4.46).

Fix any k, i, j , and l , such that $k < i < j < l$. Then the corresponding equality from (4.46) is

$$y_{ij}^k + y_{il}^j + y_{jl}^k + y_{li}^k = 2. \quad (4.47)$$

By (4.24) and (4.35), which were shown in Proposition 4.4 to imply (4.37), we may rotate the indices of any given y term. In this way we take (4.47) and rotate the indices clockwise in the second term:

$$y_{ij}^k + y_{lj}^i + y_{jl}^k + y_{li}^k = 2. \quad (4.48)$$

Then by (4.24), we obtain

$$(1 - y_{ji}^k) + (1 - y_{jl}^i) + (1 - y_{lj}^k) + (1 - y_{li}^k) = 2, \quad (4.49)$$

Next, we multiply both sides by -1 and subtract 4:

$$y_{ji}^k + y_{jl}^i + y_{lj}^k + y_{li}^k = 2. \quad (4.50)$$

Now we swap the third and fourth terms:

$$y_{ji}^k + y_{jl}^i + y_{il}^k + y_{lj}^k = 2. \quad (4.51)$$

It can be seen that the steps in (4.48) – (4.51) correspond to the cyclic permutation $(i j)$ on the indices of (4.47).

Next, we may take (4.51) and rotate the indices of the first, third and fourth terms, respectively, anti-clockwise, clockwise and clockwise:

$$y_{kj}^i + y_{jl}^i + y_{lk}^i + y_{jk}^l = 2. \quad (4.52)$$

Finally, we rotate the positions of the first, fourth and second terms:

$$y_{jl}^i + y_{jk}^l + y_{lk}^i + y_{kj}^i = 2. \quad (4.53)$$

The steps in (4.48) – (4.53) can be seen to correspond to the cyclic permutation $(i j l k)$ on the indices of (4.47). Thus by the group properties of S_4 for which $\{(i j), (i j l k)\}$ is a generating set, all possible permutations of (4.45) are implied by (4.46) in the presence of (4.35) and the constraints in Base-SST- k .

Finally, we prove that any equality from (4.46) can be derived from equalities in (4.44). That is, we can effectively fix k to be 1 without weakening the constraint set (4.46).

Consider again (4.47) for any choice of $k > 1$; that is, $1 < k < i < j < l$. We will show that (4.47) follows from the following four equalities in (4.44):

$$y_{ij}^1 + y_{il}^j + y_{jl}^1 + y_{li}^1 = 2 \quad (4.54)$$

$$y_{ki}^1 + y_{kl}^i + y_{il}^1 + y_{lk}^1 = 2 \quad (4.55)$$

$$y_{kj}^1 + y_{kl}^j + y_{jl}^1 + y_{lk}^1 = 2 \quad (4.56)$$

$$y_{ki}^1 + y_{kj}^i + y_{ij}^1 + y_{jk}^1 = 2. \quad (4.57)$$

Then, by adding (4.54) and (4.55) and subtracting (4.56) and (4.57), we

obtain

$$\begin{aligned} & y_{ij}^1 + y_{il}^j + y_{jl}^1 + y_{li}^1 + y_{ki}^1 + y_{kl}^i + y_{il}^1 + y_{lk}^1 \\ & - y_{kj}^1 - y_{kl}^j - y_{jl}^1 - y_{lk}^1 - y_{ki}^1 - y_{kj}^i - y_{ij}^1 - y_{jk}^1 = 0, \end{aligned}$$

and after simplifying,

$$y_{il}^j + y_{kl}^i - y_{kl}^j - y_{kj}^i + (y_{li}^1 + y_{il}^1) - (y_{kj}^1 + y_{jk}^1) = 0. \quad (4.58)$$

By (4.24), $y_{li}^1 + y_{il}^1 = y_{kj}^1 + y_{jk}^1 = 1$, so (4.58) reduces to

$$y_{il}^j + y_{kl}^i - y_{kl}^j - y_{kj}^i = 0. \quad (4.59)$$

Also by (4.24), we can replace the negated terms of (4.59) as follows:

$$y_{il}^j + y_{kl}^i + (y_{lk}^j - 1) + (y_{jk}^i - 1) = 0.$$

Finally, by rotating the indices and simplifying, we obtain

$$y_{ij}^k + y_{ij}^j + y_{jl}^k + y_{li}^k = 2,$$

which is identical to (4.47). □

Having established the correctness of (4.35), (4.36) and (4.44), we now define an extension of Base-SST- k which we name Base-SST- k -Ext.

Definition 4.7 (Base-SST- k -Ext). Minimise (4.9), subject to (4.1) – (4.8), (4.24) – (4.26), (4.29) – (4.36) and (4.44). If the costs c_{ij} are not provided, find any solution subject to these constraints.

As with Base-SST and Base-SST- k , Base-SST- k -Ext is not infeasible for any additional instances of NHNB20 or NHNB20PR relative to the Base Model. However, there are additional improvements in a TSP sense, which are shown in Table 4.7. Indeed, an additional 10 instances for each of ATSP16A and ATSP16AC display improvement, and the mean reductions in the gaps of each case are also significantly improved.

Table 4.7: Results of Base-SST- k -Ext on the 200 NHNB-derived and 200 Hamiltonian-derived instances in each of (a) ATSP16A and (b) ATSP16AC. The table indicates the number of instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

(a) ATSP16A				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	14 756.9	73.8	193/200	10.919
NHNB-derived	288 170.2	1440.9	165/200	5.418
All	302 927.1	757.3	358/400	8.383

(b) ATSP16AC				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	14 756.9	73.8	193/200	10.919
NHNB-derived	288 085.2	1440.4	165/200	5.418
All	302 842.1	757.1	358/400	8.383

The additional improvements offered by Base-SST- k -Ext are particularly pleasing given that the model has $\mathcal{O}(n^4)$ fewer constraints than Base-SST- k . As noted, unlike Base-SST- k , Base-SST- k -Ext has the same time complexity as the Base Model. Thus, in the combined model to be introduced in Section 4.5, we can include the constraints of Base-SST- k -Ext to take advantage of this significant improvement without increasing the time complexity of the model.

As mentioned in the chapter introduction, there are eight TSP instances for which SST outperforms the Base Model. Specifically, these instances, identified in Section 2.2.5, comprise four instances from the problem set ATSP16A and their corresponding four instances from ATSP16AC. Since we have included the SST constraints in the three models developed in this section, it follows that SST cannot outperform any of these extended models on these four instances. Rather, the combination of SST and Base Model constraints in Base-SST, Base-SST- k and Base-SST- k -Ext leads to significant additional improvement on these four instances, which we highlight in

Table 4.8. Note that the gaps obtained for these four instances in ATSP16A are identical to the gaps obtained for the four corresponding instances in ATSP16AC, so we only report gaps for the former.

Table 4.8: Gaps for each of the Base Model, Base-SST, Base-SST- k and Base-SST- k -Ext on the four instances from ATSP16A for which SST outperforms the Base Model.

ID	Base Model	SST	Base-SST	Base-SST- k	Base-SST- k -Ext
92	66.2	62.7	57.6	49.6	49.3
105	77.2	75.1	66.3	65.4	64.9
259	1465.7	1462.5	1455.1	1440.8	1438.6
338	1444.1	1434.5	1427.9	1425.2	1424.8

We now conclude this section with two visualisations of the relative improvements obtained by Base-SST, Base-SST- k and Base-SST- k -Ext. In Figure 4.9 we plot four points for each instance in ATSP16A. The points have the gap obtained from the SST model as an x -coordinate, and the gaps obtained from the Base Model, Base-SST, Base-SST- k and Base-SST- k -Ext as y -coordinates, with the four points for each instance connected by a vertical line. The further that points lie below the solid line $y = x$, the bigger the improvement over the SST model. This can be compared to Figure 2.11, which for each instance only includes the points for the Base Model. The four instances for which the SST model outperforms the Base Model are displayed in dark red.

In Figure 4.10 there are two ternary plots containing a point for each instance of ATSP16A. For each instance, we consider first the improvement in gap from the Base Model to Base-SST, then the improvement from Base-SST to Base-SST- k , and finally the improvement from Base-SST- k to Base-SST- k -Ext. Then for each instance, we plot a point where the three coordinates are the proportions of the total improvement in gap comprising the respective individual improvements. For example, if the three improvements were 5, 15 and 10 for a total improvement of 30, we would plot the point $(\frac{1}{6}, \frac{1}{2}, \frac{1}{3})$.

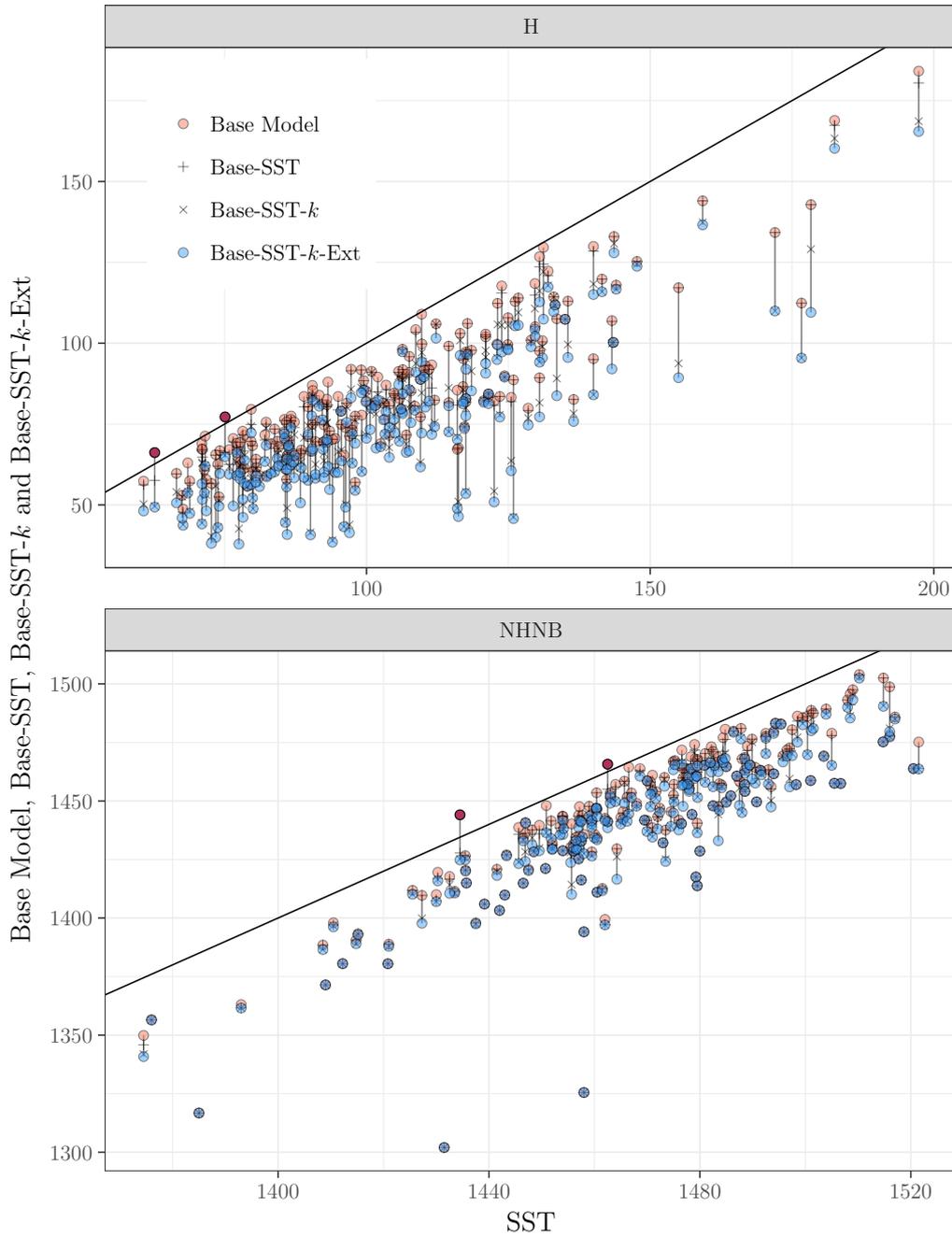


Figure 4.9: Gaps for the Hamiltonian-derived and NHNB-derived instance of ASTP16A under the Base Model, Base-SST, Base-SST- k and Base-SST- k -Ext versus the gaps for SST. The solid line $y = x$ corresponds to the given model and SST having the same gap.

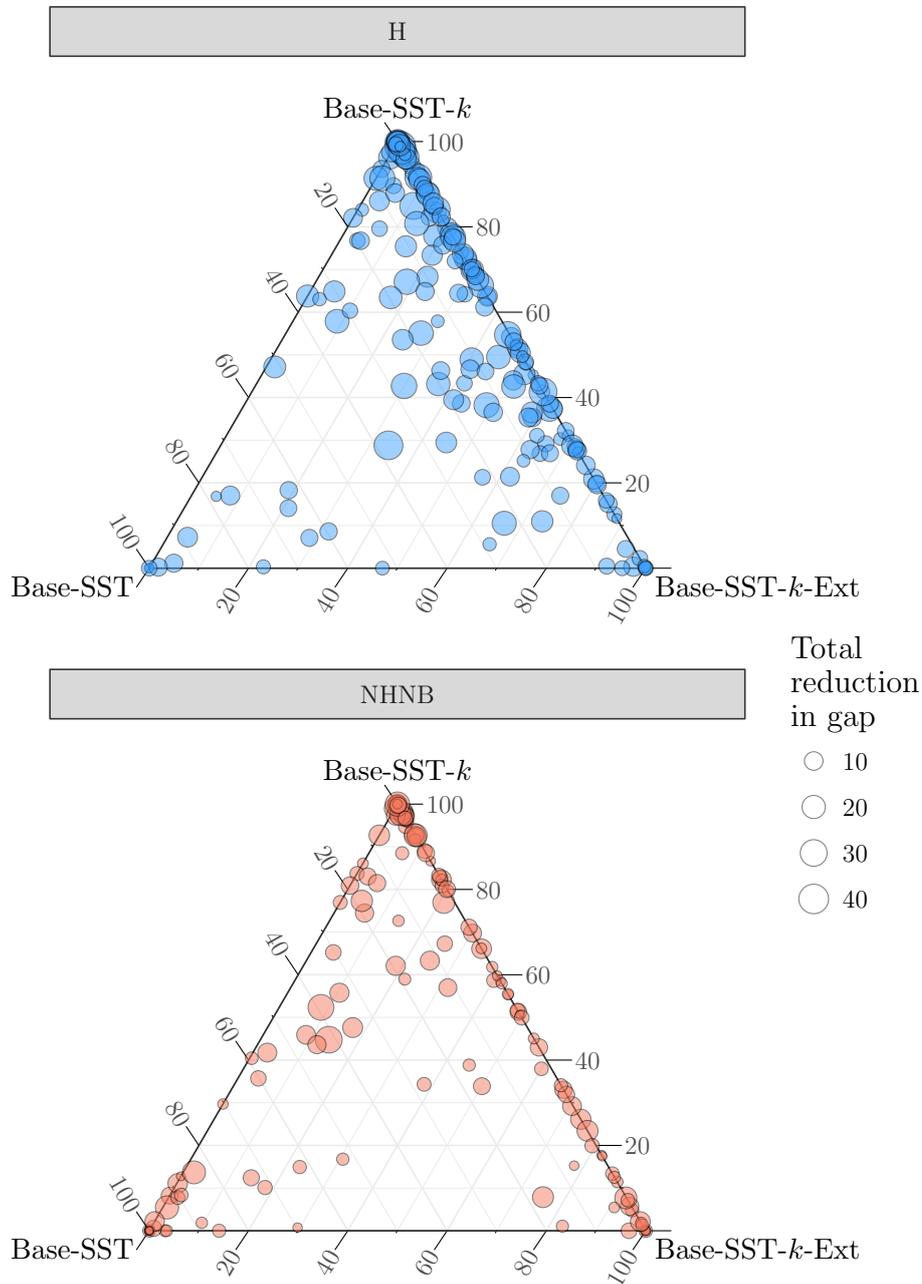


Figure 4.10: Ternary plots showing the proportion of the total reduction in gap that can be attributed to Base-SST, Base-SST- k and Base-SST- k -Ext relative to the Base Model, for the Hamiltonian-derived and NHNB-derived instances of ATSP16A.

In Figure 4.10 the size of each point also corresponds to the size of total reduction in gap. As can be seen, the majority of instances have negligible improvement attributable to Base-SST relative to the Base Model. In contrast, there are many instances for which a majority of the improvement can be attributed to Base-SST- k , with most of the remaining improvement attributable to Base-SST- k -Ext.

We do not include figures equivalent to Figures 4.9 and 4.10 for the set ATSP16AC as, for the extended models considered in this section, they are visually almost identical to those for ATSP16A.

4.2 Constraints involving forced edges

Suppose a feasible solution has been obtained from the Base Model, but does not correspond to a Hamiltonian cycle. Such a solution necessarily contains some $x_{r,ia}^k$ values strictly between 0 and 1. This may be interpreted as multiple edges being traversed when leaving a vertex. For example, Figure 4.11 shows part of a feasible solution from the Base Model on a non-Hamiltonian subcubic graph resulting from the reduction algorithm in Chapter 3. It can be seen that, considering the starting vertex k shown, multiple edges are used even in the initial step ($r = 0$). Clearly this cannot be the case for a solution corresponding to a Hamiltonian cycle but, in general, this feature is difficult to prevent through linear constraints on relaxed variables, because we do not know *a priori* which edges should be used.

Figure 4.11 shows the evolution of this feasible solution, relative to this starting point, on a subset of three vertices and their six incident edges from the graph. We make some remarks about these values: First, it can be seen that, summing the values over all steps, each of the vertices has exactly one unit on outgoing arcs, which follows from (4.5). Second, for each vertex, the sum of values on outgoing arcs is always equal to the sum on incoming

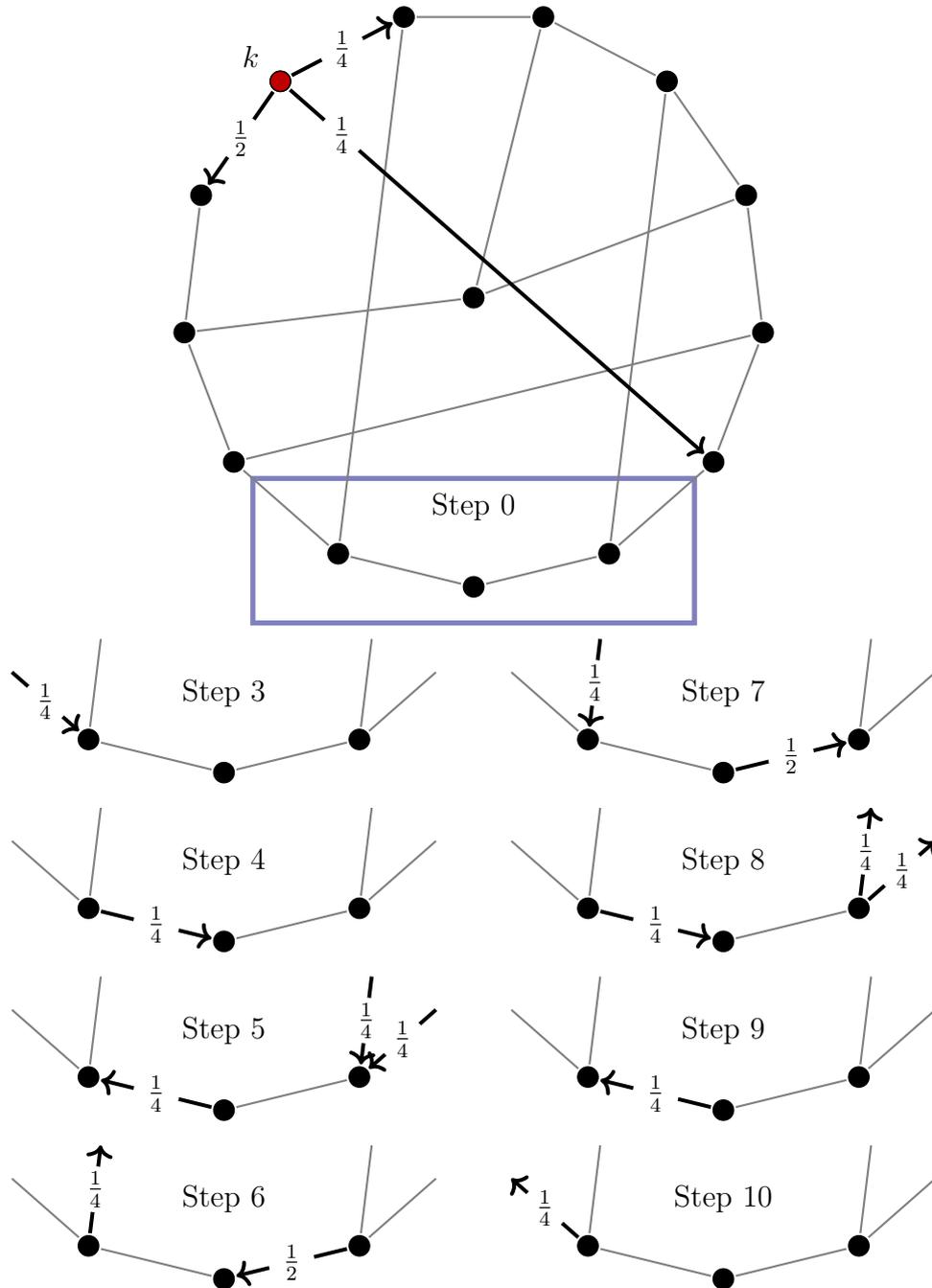


Figure 4.11: Visualisation of part of one feasible solution of the Base Model for a non-Hamiltonian subcubic graph (top, produced by GRAPHREDUCTION on G_{20}^{71268}). We consider the variables $x_{r,ia}^k$ where the starting vertex k is shown in red. The arc labels give the non-zero values of $x_{r,ia}^k$ for arc $i \rightarrow a$ in the given step r . For steps $r > 0$ it is instructive to only show a subset of the edges (from the blue rectangle), skipping steps $r = 1, 2, 11, 12, 13$ where these edges have only zero values.

arcs in the previous step, which follows from (4.1). Third, note the unwanted feature that some edges are used more than once at different steps, sometimes in both directions.

Clearly, it is desirable to prevent solutions with the kind of behaviour seen in Figure 4.11, and fortunately there are instances in which this is possible. Specifically, where we know that any particular edge *must* be used in the solution, we can impose additional constraints on the linear program. Recall from Definition 3.18 that we define *forced edges* to be those that we have determined to be Hamiltonian edges; that is, edges we know must be present in every Hamiltonian cycle of the graph, should any Hamiltonian cycles exist. Consider a graph $G = (V, E)$ with forced edges $F \subseteq E$. We may then impose constraints (4.60) – (4.62), which prevent some unwanted behaviour from occurring in feasible solutions.

$$x_{0,ia}^i + x_{0,ai}^a = 1 \quad \forall i; ia \in F \quad (4.60)$$

$$x_{r,ia}^k = \sum_{b \in N(i) \setminus \{a\}} x_{r-1,bi}^k \quad \forall i, k; ia \in F; r \neq 0 \quad (4.61)$$

$$x_{r,ia}^k = \sum_{j \in N(a) \setminus \{i\}} x_{r+1,aj}^k \quad \forall i, k; ia \in F; r \neq n-1. \quad (4.62)$$

These constraints, respectively, are motivated by the following observations about any forced edge $ia \in F$:

- (i) The edge ia must be used, either as the arc $i \rightarrow a$ or the arc $a \rightarrow i$.
- (ii) If the vertex i was entered in the previous step from a vertex other than a , then arc $i \rightarrow a$ must be used in the current step.
- (iii) Similarly to (ii), if the arc $i \rightarrow a$ is used in the current step, then in the next step it is not possible to return to vertex i .

An obvious subset of F is the edges incident to degree 2 vertices, which includes the two bottom edges of the graph as shown in Figure 4.11. Including constraints (4.60) – (4.62) would help to prevent the undesired behaviour in

the solution displayed in this figure. In particular, the value of $\frac{1}{4}$ that enters the degree-2 vertex in step 4 would be prevented from returning over the same arc in step 5 by (4.62). Similarly, the values of $\frac{1}{2}$ and $\frac{1}{4}$ entering the degree-2 vertex in steps 6 and 8 respectively would be prevented from returning over those arcs. In fact, after imposing these additional constraints, with F set to the edges incident to degree 2 vertices, the Base Model no longer has any feasible solution for the graph in Figure 4.11; precisely the desired outcome for a non-Hamiltonian graph.

Proposition 4.8. *Constraints (4.60) – (4.62) are satisfied for any solution of the Base Model corresponding to a Hamiltonian cycle H in G , where G has a set of forced edges F .*

Proof. Let ia be a forced edge in F . By definition, the edge ia must be used in H ; that is, either arc $i \rightarrow a$ or $a \rightarrow i$ is used. Without loss of generality, let vertex u be the vertex, other than a , adjacent in an undirected sense to i in H . Similarly, let the vertex v be the vertex, other than i , adjacent in an undirected sense to a in H . In a directed sense, then, H contains either the path $u \rightarrow i \rightarrow a \rightarrow v$ or the path $v \rightarrow a \rightarrow i \rightarrow u$.

If we set the $x_{r,ia}^k$ variables according to their interpretation, it is straightforward to show that (4.60) is satisfied: If arc $i \rightarrow a$ is used, then $x_{0,ia}^i = 1$ and $x_{0,ai}^a = 0$. Otherwise if $a \rightarrow i$ is used, then $x_{0,ia}^i = 0$ and $x_{0,ai}^a = 1$. In both cases the sum is exactly 1.

For constraints (4.61) and (4.62), first consider the case where arc $a \rightarrow i$ is used in H . Then it is clear that $x_{r,ia}^k = 0$ for all k and r , and so the left hand side of (4.61) and (4.62) are zero. Similarly, it is clear that for all k and r , we have $x_{r,bi}^k = 0$ if $b \neq a$, and $x_{r,aj}^k = 0$ if $j \neq i$. Hence the right hand side of (4.61) and (4.62) are zero as well, and so both constraints are satisfied.

Next consider the case where arc $i \rightarrow a$ is used in H , with the path $u \rightarrow i \rightarrow a \rightarrow v$. Let k be the starting vertex of H . Then suppose that $i \rightarrow a$ is step s of

H . If we set the $x_{r,ia}^k$ variables according to their interpretation, we have the following:

$$x_{r,ia}^k = \begin{cases} 1 & \text{if } r = s, \\ 0 & \text{otherwise.} \end{cases}$$

$$x_{r,bi}^k = \begin{cases} 1 & \text{if } r = s - 1 \pmod n, \text{ and } b = u, \\ 0 & \text{otherwise.} \end{cases}$$

$$x_{r,aj}^k = \begin{cases} 1 & \text{if } r = s + 1 \pmod n, \text{ and } j = v, \\ 0 & \text{otherwise.} \end{cases}$$

Now consider the LHS of (4.61). It will be equal to one if $r = s$ and will be zero otherwise. Every term in the RHS of (4.61) is of the type $x_{r,bi}^k$. Recall that only one such term is equal to one, when $r = s - 1 \pmod n$ and $b = u$. Suppose that $s > 0$. Then the RHS will contain such a term when $r = s$ but not for any other value of r . Hence the RHS will be equal to one if and only if $r = s$, and will be zero otherwise. This is identical to the LHS and hence (4.61) is satisfied by H when $s > 0$.

Then consider the case when $s = 0$. By definition this can only occur when $k = i$. In this case, the LHS of (4.61) is always zero since the case when $r = 0$ is excluded. Likewise, the RHS of (4.61) is always zero because the term $x_{n-1,ui}^k$ never occurs. Hence (4.61) is satisfied by H in all cases.

Next, consider the LHS of (4.62). It will be equal to one if $r = s$ and will be zero otherwise. Every term in the RHS of (4.62) is of the type $x_{r,aj}^k$. Recall that only one such term is equal to one, when $r = s + 1 \pmod n$ and $j = v$. Suppose that $s < n - 1$. Then the RHS will contain such a term when $r = s$ but not for any other value of r . Hence the RHS will be equal to one if and only if $r = s$, and will be zero otherwise. This is identical to the LHS and hence (4.62) is satisfied by H when $s < n - 1$.

Finally, consider the case when $s = n - 1$. By definition this can only

occur when $k = a$. In this case, the LHS of (4.62) is always zero since the case when $r = n - 1$ is excluded in (4.62). Likewise, the RHS of (4.62) is always zero because the term x_{0,a_j}^k never occurs. Hence (4.62) is satisfied by H in all cases. \square

We now define the model Base-Forced.

Definition 4.9 (Base-Forced). Minimise the objective function (4.9), subject to (4.1) – (4.8) and (4.60) – (4.62). If the costs c_{ij} are not provided, find any solution subject to these constraints.

Note that in order to take advantage of the new constraints in Base-Forced we must find a set of forced edges F . Recall from Lemma 3.19 that edges whose removal results in a graph that is not 2-connected are necessarily Hamiltonian, so in the results that follow we will use the same construction of F as in Chapter 3, which can be found in polynomial time:

$$F = \{uv \in E \mid G_{E \setminus \{uv\}} \text{ is not 2-connected}\}.$$

Table 4.12 shows the results of Base-Forced on the problem sets NHNB20 and NHNB20PR. It is notable that, unlike in any of the extended models based on SST, for Base-Forced there are 52 and 8 additional instances, relative to the Base Model, with infeasible LPs from the respective problem sets.

Table 4.13 shows the results of Base-Forced on the set ATSP16AC. Note that ATSP16A is not included here as all instances in that set are complete and hence do not contain any forced edges. As can be seen, in almost all of the 43 instances of ATSP16AC containing forced edges an improvement is found.

Table 4.12: Results of Base-Forced on (a) NHNB20 and (b) NHNB20PR, by order n . We restrict our consideration to the instances that contain forced edges, the numbers of which are shown in the $|F| > 0$ columns. For these instances, the table shows the improvement relative to the Base Model.

(a) NHNB20					(b) NHNB20PR				
n	Graphs	$ F > 0$	Inf.	Imprv.	n	Graphs	$ F > 0$	Inf.	Imprv.
10	1	0			12	1	1	0	0
12	1	0			13	1	1	1	0
14	6	2	1	0	14	7	7	6	3
16	33	15	6	0	15	5	5	4	0
18	231	117	52	0	16	9	8	6	2
20	1827	979	470	52	17	23	23	4	1
All	2099	1113	529	52	18	17	4	0	0
					19	6	6	4	1
					20	18	18	1	1
					All	87	73	26	8

Table 4.13: Results of Base-Forced on the 200 NHNB-derived and 200 Hamiltonian-derived instances of ATSP16AC. The table indicates the number of instances for which F is not empty, and thus additional constraints are present. The table also includes the number of such instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

Subset	Sum of gaps	Mean	$ F > 0$	Changed	Mean red.
Ham.-derived	16 844.4	84.2	3	3	6.585
NHNB-derived	288 782.0	1443.9	40	35	5.635
All	305 626.4	764.1	43	38	5.710

4.3 Constraints based on 3-cuts

Recall the subtour elimination constraints from the DFJ formulation (Definition 2.1), which ensure that any induced subgraph is entered and exited at least once by a solution:

$$\sum_{i \in S} \sum_{j \notin S} (x_{ij} + x_{ji}) \geq 2 \quad \forall S \subset V, 0 < |S| < n. \quad (4.63)$$

As for other constraints based on x_{ij} variables, in the Base Model these constraints may be expressed as:

$$\sum_{i \in S} \sum_{a \in N(i) \setminus S} (x_{0,ia}^i + x_{0,ai}^a) \geq 2 \quad \forall S \subset V, 0 < |S| < n. \quad (4.64)$$

Note that we do not intend to add the constraints in (4.64) to the Base Model, as there are exponentially many. Furthermore, Conjecture 2.12 implies that all these constraints are already satisfied for the Base Model. However, if we know *a priori* that an induced subgraph with vertices S may only be entered and exited exactly once by any Hamiltonian cycle, the inequality in (4.63) may be tightened to a strict equality. One particular case in which we know that the subgraph induced by S may only be entered and exited once is when S is connected to $V \setminus S$ by an edge cut set of size no greater than 3. This follows since, in such a case, there are not enough edges in the cut set to enter and exit S more than once. In this section we develop equality constraints to take advantage of this property.

Consider first a 1-cut, which by definition only occurs in bridge graphs. It was proved in [28] that the Base Model is always infeasible for bridge graphs. Hence, we do not consider 1-cuts. Next consider a 2-cut. Note that in this case, both edges in the 2-cut are forced edges. Hence from (4.60) we can immediately obtain (4.64) with equality on any 2-cut. As such, we do not consider 2-cuts here either, as these are handled in the Base-Forced model. In this section then, we restrict our focus to 3-cuts only. The combined

effect of forced edge constraints and 3-cut constraints will be considered in Section 4.5.

Note that not all 3-cuts need be considered. For instance, in the cases where the 3-cut isolates a single vertex, (4.64) reduces to (4.5). Hence, we exclude this situation. We also exclude the case where the 3-cut contains a 2-cut, since, as mentioned earlier, the 2-cut case is handled by Base-Forced. Therefore, in the following set of constraints, we only consider minimal 3-cuts that do not isolate a single vertex. Denote the set of all such 3-cuts by \mathcal{C}_3 . Then we define the 3-cut constraints as follows:

$$x_{0,ab}^a + x_{0,ba}^b + x_{0,cd}^c + x_{0,dc}^d + x_{0,ef}^e + x_{0,fe}^f = 2, \quad \forall \{ab, cd, ef\} \in \mathcal{C}_3. \quad (4.65)$$

The validity of (4.65) follows immediately from the subtour elimination constraints (4.64). Regarding the number of constraints $|\mathcal{C}_3|$, consider the result of Lehel et al. [51] that the number of 3-cuts in any simple graph with n vertices is bounded from above by $\lfloor \frac{3n}{2} \rfloor - 2$. Since \mathcal{C}_3 is a subset of all 3-cuts, it follows that (4.65) consists of $\mathcal{O}(n)$ equality constraints. Furthermore, fast polynomial-time algorithms exist for finding small edge cuts in any graph [47].

We now define the Base-3-Cut model.

Definition 4.10 (Base-3-Cut). Minimise the objective function (4.9), subject to (4.1) – (4.8) and (4.65). If the costs c_{ij} are not provided, find any solution subject to these constraints.

Table 4.14 shows the results of Base-3-Cut on the problem sets NHNB20 and NHNB20PR. Note that \mathcal{C}_3 is non-empty for almost all of the instances in these sets, so additional constraints are imposed in nearly all cases. Relative to the Base Model, there are 49 and 4 additional instances with infeasible LPs from the respective problem sets. We note that this includes 5 instances and 1 instance, respectively, that do not have infeasible LPs in Base-Forced. A full breakdown of the overlaps of instances solved for the various models

in this chapter will be given at the end of Section 4.5.

Table 4.14: Results of Base-3-Cut on (a) NHNB20 and (b) NHNB20PR, by order n . We restrict our consideration to the instances that have a non-empty set of 3-cuts as defined in this section, the numbers of which are shown in the $|\mathcal{C}_3| > 0$ columns. For these instances, the table shows the improvement relative to the Base Model.

(a) NHNB20					(b) NHNB20PR				
n	Graphs	$ \mathcal{C}_3 > 0$	Inf.	Imprv.	n	Graphs	$ \mathcal{C}_3 > 0$	Inf.	Imprv.
10	1	0			12	1	1	0	0
12	1	1	0		13	1	1	1	0
14	6	6	1	0	14	7	7	3	0
16	33	33	6	0	15	5	5	4	0
18	231	229	52	0	16	9	9	6	2
20	1827	1820	467	49	17	23	23	4	1
All	2099	2089	526	49	18	17	16	0	0
					19	6	6	4	1
					20	18	18	0	0
					All	87	86	22	4

Table 4.15 shows the results of Base-3-Cut on the problem sets ATSP16A and ATSP16AC. Note that \mathcal{C}_3 is non-empty for most of the Hamiltonian-derived instances, and all of the NHNB-derived instances. In the majority of these cases there is a substantial reduction in the gap, considerably larger than that obtained by the extended models considered thus far. Indeed, the gaps for 29 of the Hamiltonian-derived instances were reduced to zero; that is, the solutions found correspond to the optimal tours. This is notable as none of the models considered previously in this thesis obtained optimal tours for any of the instances in ATSP16A or ATSP16AC. For reference, then, we give the IDs of these 29 instances; 4, 5, 6, 7, 8, 9, 10, 11, 13, 15, 16, 17, 18, 19, 20, 21, 22, 30, 48, 50, 51, 55, 66, 68, 76, 82, 108, 163, and 165. Edge lists and weights for these instances may be found in Appendix B.

Table 4.15: Results of Base-3-Cut on the 200 NHNB-derived and 200 Hamiltonian-derived instances of ATSP16AC. The table indicates the number of instances for which \mathcal{C}_3 is not empty, and thus additional constraints were present. The table indicates the number of such instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

Subset	Sum of gaps	Mean	$ \mathcal{C}_3 > 0$	Changed	Mean red.
Ham.-derived	10 428.8	52.1	165	161	39.971
NHNB-derived	284 734.8	1423.7	200	168	25.264
All	295 163.6	737.9	365	329	32.461

4.4 Constraints based on an eigenvalue of Hamiltonian permutation matrices

Consider a graph G , with adjacency matrix A , containing a (directed) Hamiltonian cycle H with a corresponding permutation matrix P . That is, the element P_{jk} is 1 if the arc $j \rightarrow k$ is used in H , and 0 otherwise. Since G is undirected, the reverse cycle to H is also present with corresponding permutation matrix $P^{-1} = P^T$.

In 2012, Weber [70] proved the following result:

Theorem 4.11 (Weber [70]). *Let P be an $n \times n$ doubly-stochastic matrix. Then P is a permutation matrix corresponding to a cycle graph if and only if the complex exponential $e^{\frac{2\pi}{n}i}$ is an eigenvalue of P .*

For the sake of neatness we define θ to be $\frac{2\pi}{n}$ throughout the remainder of this chapter. We now define a vector v , which we prove in Proposition 4.12 to be an eigenvector of P corresponding to the eigenvalue $e^{\theta i}$. For convenience, we use h_j to denote the number of steps after vertex 1 that vertex j occurs in the Hamiltonian cycle H , where h_1 is fixed to be zero. Let the entries of v then be given by

$$v_j = e^{h_j \theta i}. \quad (4.66)$$

Proposition 4.12. *The vector v , whose elements v_j are given by (4.66), satisfies*

$$Pv = e^{\theta i}v. \quad (4.67)$$

Proof. Recall that P is a permutation matrix corresponding to a Hamiltonian cycle H . Suppose that vertex $k \neq 1$ follows vertex j in H . That is, $h_k = h_j + 1$, and $P_{jk} = 1$. Now consider the element in the j th position of the left hand side of (4.67). Since the j th row of P contains all zeros except for P_{jk} ,

$$\begin{aligned} [Pv]_j &= v_k \\ &= e^{h_k \theta i} \\ &= e^{(h_j+1)\theta i} \\ &= e^{\theta i}v_j. \end{aligned} \quad (4.68)$$

Hence (4.67) is satisfied element-wise for all elements j whose subsequent vertex in H is not 1. We now consider this final case. If $k = 1$, then clearly $h_j = n - 1$, and

$$\begin{aligned} [Pv]_j &= v_1 \\ &= e^{h_1 \theta i} \\ &= e^{0\theta i} \\ &= e^{\theta i}e^{(n-1)\theta i} \\ &= e^{\theta i}v_j. \end{aligned} \quad (4.69)$$

By (4.68) and (4.69), (4.67) is satisfied. \square

Given a graph with the adjacency matrix A , and the permutation matrix P corresponding to the Hamiltonian cycle H , define

$$S = A - P - P^T.$$

Clearly, S is a 0-1 matrix. For any given vertex j , the corresponding j th row of S will contain $\deg(j) - 2$ unit entries, all contained within the positions corresponding to the neighbours of vertex j . In particular, we focus on the cases where the degree of j is either 2 or 3. By Proposition 4.12,

$$\begin{aligned} Sv &= Av - Pv - P^T v \\ &= Av - e^{\theta i} v - e^{-\theta i} v \\ &= Av - 2 \cos \theta v \\ &= (A - 2 \cos \theta I) v. \end{aligned}$$

If the degree of j is 2, then the j th row of S has all zeros, thus $[Sv]_j = 0$ and we obtain

$$\begin{aligned} [A - 2 \cos \theta I]_j v = 0, & \quad \forall j = 1, \dots, n; \\ & \quad \deg(j) = 2. \end{aligned} \tag{4.70}$$

Alternatively, if the degree of j is 3, then the j th row of S has exactly one unit, whose element must be in a column corresponding to one of the three vertices in $N(j)$. Therefore,

$$\begin{aligned} [A - 2 \cos \theta I]_j v \in \left\{ e^{h_k \theta i} \mid k \in N(j) \right\}, & \quad \forall j = 1, \dots, n; \\ & \quad \deg(j) = 3. \end{aligned} \tag{4.71}$$

It will be shown that the vector v , and hence the left hand sides of (4.70) and (4.71) may be expressed by a (complex) linear combination of $x_{r,ia}^k$ variables from the Base Model. However, since the ordering of vertices in the desired Hamiltonian cycle is not known *a priori*, we cannot assume to know the individual values of h_k in the set on the right hand side of (4.71). Rather, we may give lower and upper bounds on each h_k based on the shortest path between vertex 1 and k , which can easily be calculated in polynomial time [20].

Let μ_k^1 denote the length of the shortest path between vertex 1 and k , where μ_1^1 is defined to be zero. For convenience, we also define $\hat{\mu}_k^1$ to be

identical to μ_k^1 in all cases except for $k = 1$ where we define $\hat{\mu}_1^1 = n$. It is clear that h_k , the position of vertex k on the Hamiltonian cycle relative to vertex 1, can be bounded from above and below, as

$$\mu_k^1 \leq h_k \leq (n - \hat{\mu}_k^1). \tag{4.72}$$

Note that in the case that $k = 1$, the definition of $\hat{\mu}_k^1$ ensures that both the lower and upper bounds of (4.72) will be 0. Note also that it is not possible for the left hand side of (4.72) to be greater than $\frac{n}{2}$, since in such a case the graph would be non-Hamiltonian by the following lemma.

Lemma 4.13. *Let G be an undirected graph and let k be a vertex in G . Then G is non-Hamiltonian if $\mu_k^1 > \frac{n}{2}$.*

Proof. Suppose a Hamiltonian cycle H exists in G , and that $\mu_k^1 > \frac{n}{2}$. Then vertex k follows more than $\frac{n}{2}$ steps after vertex 1 in H . Likewise, since G is undirected, vertex 1 follows more than $\frac{n}{2}$ steps after vertex k in H . Thus the length of H must be greater than n , and hence it is not a Hamiltonian cycle. By contradiction, G is non-Hamiltonian. \square

Using (4.72) we can then replace the right hand side of (4.71) with a superset as follows, which can be calculated in advance using just the shortest paths in G . For brevity, we do not repeat here the conditions on j from (4.71).

$$[A - 2 \cos \theta I]_j v \in \left\{ e^{l\theta i} \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\}. \tag{4.73}$$

In order to derive linear constraints suitable for use with the Base Model, we now consider a construction of the vector v in terms of the $x_{r,ia}^k$ variables of the Base Model, and write linear constraints based on the real and imaginary parts of (4.70) and (4.73).

Let the $x_{r,ia}^k$ variables be set according to their interpretations for the Hamiltonian cycle H ; that is, 1 precisely if the arc $i \rightarrow a$ is used after starting at vertex k and visiting r vertices, and 0 otherwise. If we set $k = 1$, then by

definition of h_j , an arc out of j must be used after visiting h_j vertices, thus

$$\sum_{a \in N(j)} x_{h_j, ja}^1 = 1,$$

and we multiply both sides by $e^{h_j \theta i}$ to obtain

$$e^{h_j \theta i} \sum_{a \in N(j)} x_{h_j, ja}^1 = e^{h_j \theta i}. \quad (4.74)$$

Furthermore, for all $a \in N(j)$ and any $r \neq h_j$ it is clear that

$$x_{r, ja}^1 = 0,$$

and thus,

$$\sum_{\substack{r=0 \\ r \neq h_j}}^{n-1} e^{r \theta i} \sum_{a \in N(j)} x_{r, ja}^1 = 0. \quad (4.75)$$

Adding (4.74) and (4.75), and recalling (4.66), we arrive at a linear expression for v_j in terms of the $x_{r, ia}^k$ variables:

$$\sum_{r=0}^{n-1} e^{r \theta i} \sum_{a \in N(j)} x_{r, ja}^1 = e^{h_j \theta i} = v_j. \quad (4.76)$$

Applying (4.72) to (4.76) we can express the set of valid values for each of these linear combinations as:

$$\sum_{r=0}^{n-1} e^{r \theta i} \sum_{a \in N(j)} x_{r, ja}^1 \in \left\{ e^{l \theta i} \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\}. \quad (4.77)$$

Next, using (4.76), the left hand sides of both (4.70) and (4.73) may be expressed as:

$$\begin{aligned} \text{LHS} &= \sum_{k=1}^n [A - 2 \cos \theta I]_{jk} v_k \\ &= \left(\sum_{k \in N(j)} v_k \right) - 2 \cos \theta v_j \\ &= \sum_{k \in N(j)} \sum_{r=0}^{n-1} e^{r \theta i} \sum_{a \in N(k)} x_{r, ka}^1 - 2 \cos \theta \sum_{r=0}^{n-1} e^{r \theta i} \sum_{a \in N(j)} x_{r, ja}^1 \end{aligned}$$

$$\begin{aligned}
 &= \sum_{r=0}^{n-1} e^{r\theta i} \left(\sum_{k \in N(j)} \sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta \sum_{a \in N(j)} x_{r,ja}^1 \right) \\
 &= \sum_{r=0}^{n-1} e^{r\theta i} \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right). \quad (4.78)
 \end{aligned}$$

Finally, by (4.78), we can give linear constraints based on the real and imaginary parts of (4.70) and (4.73) for vertices j with degree 2 or 3, respectively, as well as bounds for based on (4.77).

Linear constraints based on (4.70), where $j = 1, \dots, n$, and $\deg(j) = 2$, may be written as:

$$\sum_{r=0}^{n-1} \cos(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) = 0 \quad (4.79)$$

$$\sum_{r=0}^{n-1} \sin(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) = 0. \quad (4.80)$$

Linear constraints based on (4.73), where $j = 1, \dots, n$, and $\deg(j) = 3$, may be written as:

$$\begin{aligned}
 &\min \left\{ \cos(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\} \\
 &\leq \sum_{r=0}^{n-1} \cos(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) \quad (4.81) \\
 &\leq \max \left\{ \cos(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\}
 \end{aligned}$$

$$\begin{aligned}
 &\min \left\{ \sin(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\} \\
 &\leq \sum_{r=0}^{n-1} \sin(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) \quad (4.82) \\
 &\leq \max \left\{ \sin(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\}.
 \end{aligned}$$

Linear constraints based on the bounds (4.77), for all $j = 1, \dots, n$ regardless

of the degree of j , may be written as:

$$\begin{aligned} & \min \left\{ \cos(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\} \\ & \leq \sum_{r=0}^{n-1} \cos(r\theta) \sum_{a \in N(j)} x_{r,ja}^1 \\ & \leq \max \left\{ \cos(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\} \end{aligned} \tag{4.83}$$

$$\begin{aligned} & \min \left\{ \sin(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\} \\ & \leq \sum_{r=0}^{n-1} \sin(r\theta) \sum_{a \in N(j)} x_{r,ja}^1 \\ & \leq \max \left\{ \sin(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\}. \end{aligned} \tag{4.84}$$

Note that in (4.81) – (4.84), the sets over which the minimum and maximum values are found could theoretically be empty, precisely where $\mu_k^1 > \frac{n}{2}$ for some k . To handle such cases, we define, for (4.81) – (4.84), the minimum of an empty set to be ∞ , and the maximum of an empty set to be $-\infty$. This will have the effect of forcing the model to be infeasible, which is appropriate since such a graph must be non-Hamiltonian by Lemma 4.13.

Since constraints (4.79) – (4.84) were constructed based on an eigenvalue and eigenvector pair that is guaranteed to exist for any Hamiltonian cycle, it follows that these constraints will be satisfied for any solution to the Base Model that corresponds to a Hamiltonian cycle. Thus we define the model Base-Spectral:

Definition 4.14 (Base-Spectral). Minimise (4.9), subject to (4.1) – (4.8) and (4.79) – (4.84). If the costs c_{ij} are not provided, find any solution subject to these constraints.

Table 4.16 shows the results of Base-Spectral on the sets NHNB20 and NHNB20PR. As can be seen, there are no additional instances in these sets for which Base-Spectral obtains infeasibility, so we focus instead on the TSP instances.

Table 4.16: Results of Base-Spectral on (a) NHNB20 and (b) NHNB20PR, by order n . The table also shows the improvement in solved instances relative to the Base Model.

(a) NHNB20				(b) NHNB20PR			
n	Graphs	Inf.	Imprv.	n	Graphs	Inf.	Imprv.
10	1	0	0	12	1	0	0
12	1	0	0	13	1	1	0
14	6	1	0	14	7	3	0
16	33	6	0	15	5	4	0
18	231	52	0	16	9	4	0
20	1827	418	0	17	23	3	0
All	2099	477	0	18	17	0	0
				19	6	3	0
				20	18	0	0
				All	87	18	0

Table 4.17 shows the results of Base-Spectral on the sets ATSP16A and ATSP16AC. We note that for ATSP16A, which comprises complete ATSP instances, the only additional constraints are (4.83) and (4.84). In contrast, for ATSP16AC, which comprises cubic ATSP instances, constraints (4.81) and (4.82) are applicable in addition to (4.83) and (4.84). As can be seen, there are no instances from ATSP16A for which the optimal solution changed relative to the Base Model. This suggests, perhaps, that the constraints (4.83) and (4.84) do not provide any additional benefit, at least in isolation. However, for ATSP16AC there are two instances for which the solution did change, albeit with only a very slight improvement in the gap.

Given the very small improvement in gaps for these two instances of ATSP16AC, we wanted to ensure that these improvements were not perhaps due to numerical inaccuracy, and so we investigated these instances further. We verified that the solutions of the Base Model for these two instances are, indeed, infeasible in Base-Spectral, and that this infeasibility could not be attributed to any numerical inaccuracy in the double-precision floating-point format used. The two instances have IDs 288 and 352, and the ratios of the improvement in gap to the original lower bounds are 1.3×10^{-7}

Table 4.17: Results of Base-Spectral on the 200 NHNB-derived and 200 Hamiltonian-derived instances in each of (a) ATSP16A and (b) ATSP16AC. The table indicates the number of instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

(a) ATSP16A				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	16 864.2	84.3	0/200	
NHNB-derived	289 064.2	1445.3	0/200	
All	305 928.4	764.8	0/400	

(b) ATSP16AC				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	16 864.2	84.3	0/200	
NHNB-derived	288 969.2	1444.9	2/200	4.8×10^{-4}
All	305 843.4	764.6	2/400	4.8×10^{-4}

and 1.2×10^{-6} , respectively. Both instances may be found in Appendix B. Since a small improvement is found for these instances, it follows that the constraints are not redundant, and so we reasoned that, for some carefully chosen costs, the improvement in gap could be made starker.

We used the following technique to modify the costs. First, we compared the solution from the Base Model to that of Base-Spectral, and noted which x variables in the objective function had changed. Then, we made small increases and decreases to the costs, with the intention that the new solution from Base-Spectral would be more costly relative to that from the Base Model, while ensuring the total sum of costs was unchanged. We continued this process iteratively, each time comparing the two solutions and adjusting the costs, until the method ceased to yield further improvement. At the end of this process, we scaled and rounded the costs to the integer range 0 to 100, which is the same range as other instances in ATSP16AC. For Base-Spectral, the modified instance based on that with ID 288 has a lower bound of 705.958 compared to 705.653 for the Base Model; a difference of 0.305 or

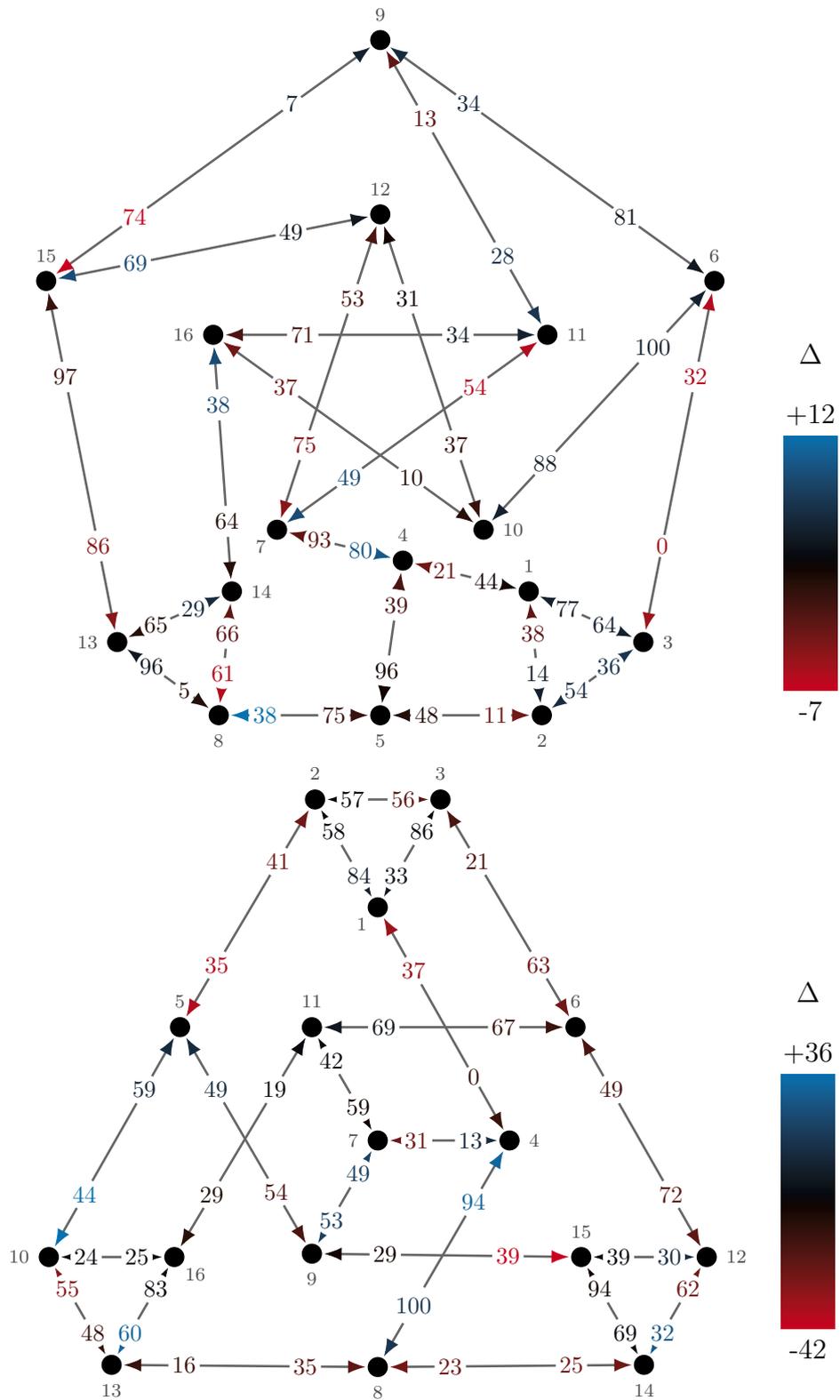


Figure 4.18: Instances of ATSP16AC with IDs 288 (top) and 352 (bottom), modified to increase the contrast between Base-Spectral and the Base Model. Costs are shown on each arc closest to the vertex that the arc enters. Colour gives an indication of the increase or decrease of costs relative to the costs of the original instances.

ratio of 4.3×10^{-4} . For the modified instance based on that with ID 352, Base-Spectral has a lower bound of 599.809 compared to 595.586 for the Base Model; a difference of 4.22 or a ratio of 7.1×10^{-3} . Note that in each case the ratio is improved by three orders of magnitude. We display these two modified instances along with their new arc costs in Figure 4.18.

4.5 Results of combined extensions

We have seen that each of the models Base-SST- k -Ext, Base-Forced, Base-3-Cut and Base-Spectral are improvements upon the Base Model. A logical question is whether additional improvements could be gained by combining all four of these models. Note that while each of these models is well-defined for any graph G , some of the models only offer improvements for graphs with certain properties. For example, some additional constraints will only be present in graphs that contain forced edges, 3-cuts or vertices of certain degrees.

We now define the model Base-Combined, as follows:

Definition 4.15. Minimise (4.9), subject to (4.1) – (4.8), (4.24) – (4.26), (4.29) – (4.36), (4.44), (4.60) – (4.62), (4.65) and (4.79) – (4.84). If the costs c_{ij} are not provided, find any solution subject to these constraints.

For the reader's convenience, we repeat the objective function,

$$\sum_{i=1}^n \sum_{j \in N(i)} c_{ij} x_{0,ij}^i, \quad (4.9)$$

and each of the linear constraints of Base-Combined below. Unless otherwise restricted, the indices i, j, k and l range from 1 to n , and r and s range from 0 to $n - 1$. The set of forced edges is denoted by F and the set of minimal 3-cuts not isolating a single vertex is denoted by \mathcal{C}_3 .

Constraints from the Base Model:

$$\sum_{a \in N(i)} x_{r,ia}^k - \sum_{a \in N(i)} x_{r-1,ai}^k = 0 \quad \forall i, k; r \neq 0 \quad (4.1)$$

$$\sum_{a \in N(i)} x_{r,ia}^k - \sum_{a \in N(k)} x_{n-r,ka}^i = 0 \quad \forall i, k; r \neq 0 \quad (4.2)$$

$$\sum_{r=0}^{n-1} x_{r,ia}^k - \sum_{r=0}^{n-1} x_{r,ia}^j = 0 \quad \forall j, k \neq j; ia \in E \quad (4.3)$$

$$\sum_{k=1}^n x_{r,ia}^k - \sum_{k=1}^n x_{s,ia}^k = 0 \quad \forall r, s \neq r; ia \in E \quad (4.4)$$

$$\sum_{r=0}^{n-1} \sum_{a \in N(i)} x_{r,ia}^k = 1 \quad \forall i, k \quad (4.5)$$

$$\sum_{k=1}^n \sum_{a \in N(i)} x_{r,ia}^k = 1 \quad \forall i, r \quad (4.6)$$

$$x_{0,ia}^k = 0 \quad \forall k; i \neq k; ia \in E \quad (4.7)$$

$$x_{r,ia}^k \geq 0 \quad \forall k, r; ia \in E. \quad (4.8)$$

Additional constraints from Base-SST- k -Ext:

$$y_{ij}^k + y_{ji}^k = 1 \quad \forall k, i, j; k \neq i \neq j \quad (4.24)$$

$$y_{ij}^k \geq x_{0,ki}^k \quad \forall k, j; i \in N(k); k \neq i \neq j \quad (4.25)$$

$$y_{ji}^k \geq x_{0,ik}^i \quad \forall i, j; i \in N(k); k \neq i \neq j \quad (4.26)$$

$$y_{ij}^k \geq 0 \quad \forall k, i, j; k \neq i \neq j \quad (4.29)$$

$$0 \leq f_{ia,j}^k \leq x_{0,ia}^i \quad \forall k, i, j; a \in N(i); k \neq i \neq a \neq j \quad (4.30)$$

$$\sum_{a \in N(i) \setminus \{k,j\}} f_{ia,j}^k + x_{0,ij}^i = y_{ij}^k \quad \forall k, i; j \in N(i); k \neq i \neq j \quad (4.31)$$

$$\sum_{a \in N(i) \setminus \{k\}} f_{ia,j}^k + 0 = y_{ij}^k \quad \forall k, i; j \notin N(i); k \neq i \neq j \quad (4.32)$$

$$x_{0,ki}^k + \sum_{b \in N(i) \setminus \{k,j\}} f_{bi,j}^k = y_{ij}^k \quad \forall k, j; i \in N(k); k \neq i \neq j \quad (4.33)$$

$$0 + \sum_{b \in N(i) \setminus \{j\}} f_{bi,j}^k = y_{ij}^k \quad \forall k, j; i \notin N(k); k \neq i \neq j \quad (4.34)$$

$$y_{ij}^k = y_{jk}^i \quad \forall k, i, j; k < i < j \text{ or } j < k < i \quad (4.35)$$

$$f_{ia,j}^k + f_{ia,k}^j = x_{0,ia}^i \quad \forall k, i, j; a \in N(i); k < j; k \neq i \neq a \neq j \quad (4.36)$$

$$y_{ij}^1 + y_{il}^j + y_{jl}^1 + y_{li}^1 = 2 \quad \forall i, j, l; 1 < i < j < l. \quad (4.44)$$

Additional constraints from Base-Forced:

$$x_{0,ia}^i + x_{0,ai}^a = 1 \quad \forall i; ia \in F \quad (4.60)$$

$$x_{r,ia}^k = \sum_{b \in N(i) \setminus \{a\}} x_{r-1,bi}^k \quad \forall i, k; ia \in F; r \neq 0 \quad (4.61)$$

$$x_{r,ia}^k = \sum_{j \in N(a) \setminus \{i\}} x_{r+1,aj}^k \quad \forall i, k; ia \in F; r \neq n-1. \quad (4.62)$$

Additional constraints from Base-3-Cut:

$$x_{0,ab}^a + x_{0,ba}^b + x_{0,cd}^c + x_{0,dc}^d + x_{0,ef}^e + x_{0,fe}^f = 2 \quad \forall \{ab, cd, ef\} \in \mathcal{C}_3. \quad (4.65)$$

Additional constraints from Base-Spectral for all j such that $\deg(j) = 2$;

$$\sum_{r=0}^{n-1} \cos(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) = 0 \quad (4.79)$$

$$\sum_{r=0}^{n-1} \sin(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) = 0, \quad (4.80)$$

for all j such that $\deg(j) = 3$;

$$\begin{aligned} & \min \left\{ \cos(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\} \\ & \leq \sum_{r=0}^{n-1} \cos(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) \\ & \leq \max \left\{ \cos(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\} \end{aligned} \quad (4.81)$$

$$\begin{aligned} & \min \left\{ \sin(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\} \\ & \leq \sum_{r=0}^{n-1} \sin(r\theta) \sum_{k \in N(j)} \left(\sum_{a \in N(k)} x_{r,ka}^1 - 2 \cos \theta x_{r,jk}^1 \right) \\ & \leq \max \left\{ \sin(l\theta) \mid \min_{k \in N(j)} \mu_k^1 \leq l \leq \max_{k \in N(j)} (n - \hat{\mu}_k^1); l \in \mathbb{Z} \right\}, \end{aligned} \quad (4.82)$$

and for all j ;

$$\begin{aligned} & \min \left\{ \cos(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\} \\ & \leq \sum_{r=0}^{n-1} \cos(r\theta) \sum_{a \in N(j)} x_{r,ja}^1 \\ & \leq \max \left\{ \cos(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\} \end{aligned} \quad (4.83)$$

$$\begin{aligned} & \min \left\{ \sin(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\} \\ & \leq \sum_{r=0}^{n-1} \sin(r\theta) \sum_{a \in N(j)} x_{r,ja}^1 \\ & \leq \max \left\{ \sin(l\theta) \mid \mu_j^1 \leq l \leq (n - \hat{\mu}_j^1); l \in \mathbb{Z} \right\}. \end{aligned} \quad (4.84)$$

Table 4.19 shows the results of Base-Combined relative to the Base Model on the problem sets NHNB20 and NHNB20PR. As expected, all of the instances that are infeasible in any of the extended models are infeasible for Base-Combined as well. However, there is one additional instance from NHNB20PR that is feasible for all the individual models, but for which the combination of all the models induces infeasibility. We display this instance in Figure 4.20. This instance indicates that Base-Combined prevents some feasible solutions, not corresponding to Hamiltonian cycles, that lie in the intersection of feasible solutions in the other extended models. In other words, using Base-Combined for a given instance can give a stronger result than taking the best outcome from the individual extended models.

Table 4.21 shows the results of Base-Combined relative to the Base Model on the problem sets ATSP16A and ATSP16AC. There are 358 and 379 instances, respectively, for which the optimal solution changed relative to the Base Model. We note that this set of instances is the union of the respective sets from the individual extended models. It is worthwhile, then, to compare the reduction in gap for Base-Combined on these instances to the best of the reductions for the individual extended models. Table 4.22 shows the means of the gaps for Base-Combined compared to the best gaps obtained by any of

Table 4.19: Results of Base-Combined on (a) NHNB20 and (b) NHNB20PR, by the order n . The table also shows the improvement in solved instances relative to the Base Model.

(a) NHNB20				(b) NHNB20PR			
n	Graphs	Inf.	Imprv.	n	Graphs	Inf.	Imprv.
10	1	0	0	12	1	0	0
12	1	0	0	13	1	1	0
14	6	1	0	14	7	6	3
16	33	6	0	15	5	4	0
18	231	52	0	16	9	6	2
20	1827	475	57	17	23	6	3
All	2099	534	57	18	17	0	0
				19	6	4	1
				20	18	1	1
				All	87	28	10

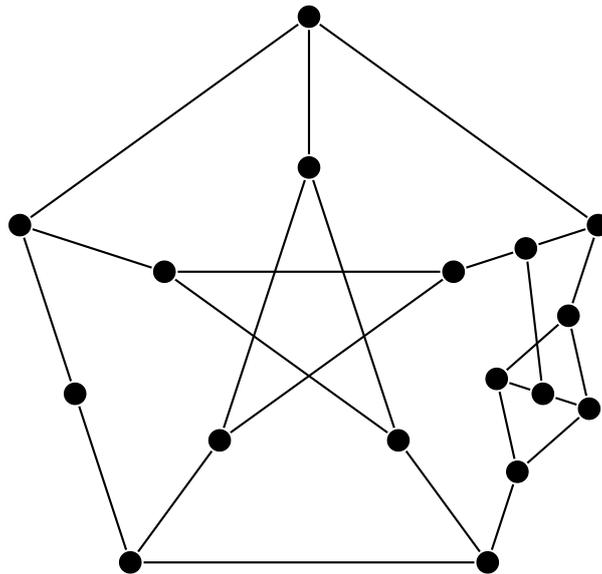


Figure 4.20: The instance of NHNB20PR that induced infeasibility in Base-Combined but not any of the individual extended models. It is the reduced graph of G_{20}^{71235} and has NHNB20PR ID 83.

the individual models for each instance. Note that for the complete instances in ATSP16A, Base-Combined effectively contains constraints from only Base-SST- k -Ext and the relatively weak Base-Spectral. It is not unexpected then that in all cases, there is no improvement over the result obtained for Base-SST- k -Ext. In contrast, for the cubic instances of ATSP16AC, there is a significant improvement in gap (greater than 0.1) found for 154, or 44% of the instances considered that had not already been solved to optimality.

Table 4.21: Results of Base-Combined on the 200 NHNB-derived and 200 Hamiltonian-derived instances in each of (a) ATSP16A and (b) ATSP16AC. The table indicates the number of instances for which the optimal solution changed relative to the Base Model, and the mean reduction in gap for these instances.

(a) ATSP16A				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	14 756.9	73.8	193/200	10.536
NHNB-derived	288 170.2	1440.9	165/200	4.470
All	302 927.1	757.3	358/400	7.503

(b) ATSP16AC				
Subset	Sum of gaps	Mean	Changed	Mean red.
Ham.-derived	9794.9	49.0	197/200	35.346
NHNB-derived	284 412.2	1422.1	182/200	22.835
All	294 207.1	735.5	379/400	29.091

Recall that there are 29 Hamiltonian-derived instances of ATSP16AC for which the optimal solution for Base-3-Cut corresponded to the optimal tour. For Base-Combined, there is one additional instance for which the optimal tour is obtained, bringing the total number up to 30. In other words, the information exploited by any individual extended model is not sufficient to obtain the optimal tour for this instance, but their combination is. This offers further support for the merit of the Base-Combined model. To illustrate the performance of each of the different models, Table 4.23 shows the gaps for each model considered in this chapter on this instance, which has ID 31 and

Table 4.22: A comparison of Base-Combined with the other extended models for the instances of (a) ATSP16A and (b) ATSP16AC in which the optimal solution changed relative to the Base Model. For each instance, we find the best gap obtained over each of the individual extended models, and list the mean of these in the column labelled *Mean best*. We then list the mean of the gaps found for Base-Combined in the column labelled *Base-Combined*. Finally the improvement in mean is listed.

(a) ATSP16A

Subset	Changed	Mean best	Base-Combined	Improvement
Ham.-derived	193	73.2	73.2	0
NHNB-derived	165	1445.0	1445.0	0
All	358	705.5	705.5	0

(b) ATSP16AC

Subset	Changed	Mean best	Base-Combined	Improvement
Ham.-derived	197	50.0	48.4	1.618
NHNB-derived	182	1423.8	1422.4	1.423
All	379	709.7	708.2	1.524

is displayed in Figure 4.24. Note that this instance has no forced edges, so Base-Forced is no stronger than the Base Model. It does contain four 3-cuts, and Base-3-Cut is very effective, though constraints from the other models are required to reduce the gap all the way to zero.

Table 4.23: Gaps for various models on ATSP16AC instance with ID 31.

Model	Gap
SST	136.5
Base Model	82.6
Base-SST	82.6
Base-SST- k	78.3
Base-SST- k -Ext	75.9
Base-Forced	82.6
Base-3-Cut	3.0
Base-Spectral	82.6
Base-Combined	0

Each of the extended models considered in this chapter exploit some information or features that may or may not be present in a given instance.

In some instances then, it may be helpful to exploit one feature, while in another instance this may not provide any benefit. To illustrate this concept, we present Euler diagrams in Figures 4.25 and 4.26 that indicate the number of instances for which each extended model is *effective* on the four problem sets. For the instances in NHNB20 and NHNB20PR, we consider an extended model to be effective if it is infeasible but the Base Model is feasible. For the instances in ATSP16A and ATSP16AC, we consider a model to be effective if the optimal solution found by the Base Model is no longer feasible. In each Euler diagram the universal set is taken to be the set of instances that are effective under Base-Combined, and we only include those models that are effective on at least one instance.

Recall that for the Base Model, 477 instances of NHNB20 are infeasible, while an extra 57 instances are infeasible for Base-Combined. In Figure 4.25(a) we consider these 57 instances. As discussed previously, of the individual extended models, only Base-Forced and Base-3-Cut are effective, but it is interesting to note that there are instances for which one but not the other is effective. Similarly, recall that for the Base Model, 18 instances of NHNB20PR are infeasible, while an extra 10 instances are infeasible for Base-Combined. In Figure 4.25(b) we consider these 10 instances. As before, of the individual extended models, only Base-Forced and Base-3-Cut are effective on these instances, again with some instances effective in only one but not the other. Note also the one instance effective for Base-Combined that is not effective for either Base-Forced or Base-3-Cut, shown previously in Figure 4.20.

In Figure 4.26(a) we consider the 358 instances of ATSP16A for which Base-Combined is effective. As discussed previously, only Base-SST, Base-SST- k and Base-SST- k -Ext are effective on any of these instances. In Figure 4.26(b) we consider the 379 instances of ATSP16AC for which Base-Combined is effective. In this case, each of the extended models are effective

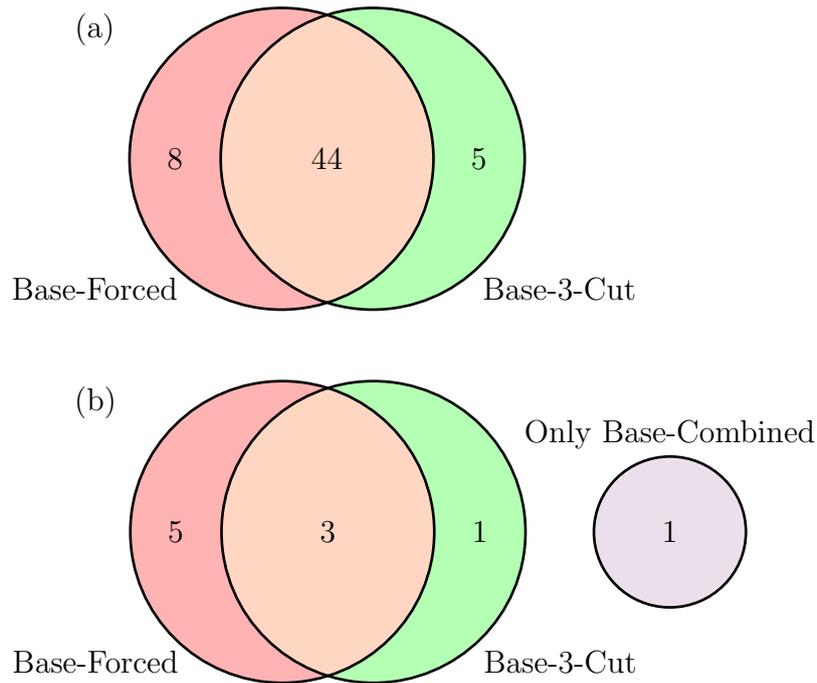


Figure 4.25: Euler diagrams of the (a) 57 instances from NHNB20, and (b) 10 instances from NHNB20PR, for which Base-Combined is effective relative to the Base Model. Zones show which individual extended models are effective.

on at least one instance, so they are each included in the Euler diagram. It is notable that the 379 instances are partitioned into many distinct zones (thirteen), indicating how each of the extended models contributes to the effectiveness of Base-Combined on this problem set. Interestingly, the two instances for which Base-Spectral is effective are contained entirely in the intersection of instances effective for Base-SST and Base-3-Cut.

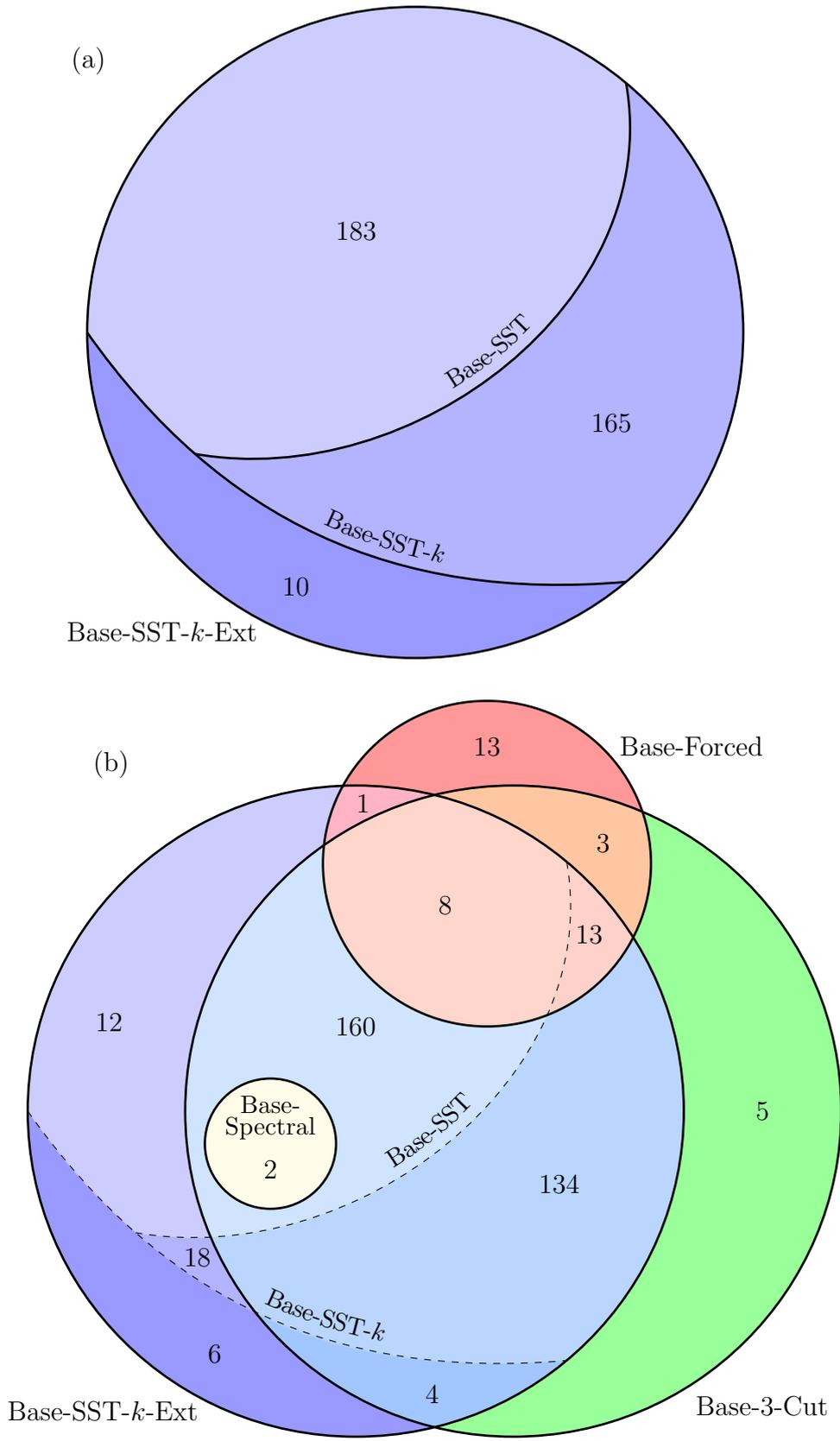


Figure 4.26: Euler diagrams of the (a) 358 instances from ATSP16A, and (b) 379 instances from ATSP16AC, for which Base-Combined is effective relative to the Base Model. Zones show which individual extended models are effective.

4.6 Detecting non-Hamiltonicity of graphs by using LP models on their subgraphs

Throughout this chapter we have considered both TSP and HCP instances. The TSP instances have been useful for providing a higher fidelity test set for the models. However, as we are primarily interested in detecting non-Hamiltonicity in HCP instances, we now conclude this chapter with a more elaborate approach to solving instances of NHNB20 and NHNB20PR, many of which are not detected as non-Hamiltonian even by the combined model. We will use this method with Base-Combined to successfully detect non-Hamiltonicity of almost all of the instances considered.

Observing that the two most effective extensions to the Base Model in an HCP sense are Base-Forced and Base-3-Cut, it follows that the graph features exploited by these extended models are very useful for inducing infeasibility of the LPs. However, not all of the instances considered possess these features; in particular, only 1113 of the 2099 instances in NHNB20, and 73 of the 87 instances in NHNB20PR contain forced edges by the definition used in Base-Forced. Therefore we consider the following straightforward method to take any subcubic HCP instance and construct a corresponding set of smaller instances, each having forced edges.

Given any graph $G = (V, E)$, consider the set of subgraphs obtained by the following approach. For each edge $uv \in E$, we produce the subgraph $(V, E \setminus \{uv\})$, which we denote by G_{-uv} . If the subgraph G_{-uv} is non-Hamiltonian, it is apparent that the edge uv must be present in all Hamiltonian cycles of G (if any exist). Thus, if we are able to determine that some of these subgraphs G_{-uv} are non-Hamiltonian for a subset of the edges $S \subseteq E$, we may verify that the edges in S are compatible with the presence of a Hamiltonian cycle in G . Specifically, since each edge of S lies in all Hamiltonian cycles of G , a necessary condition for G to be Hamiltonian is that

the subgraph induced by S must be isomorphic to a subgraph of the cycle graph C_n . Note that a graph is isomorphic to a subgraph of C_n if and only if it has at most n vertices, a girth of either n or ∞ , and a maximum vertex degree of 2. If this condition is not met, then G must be non-Hamiltonian. When combined with any given heuristic for detecting non-Hamiltonicity in the subgraphs G_{-uv} , we refer to this method of detecting non-Hamiltonicity in G as the *subgraph method*.

For a subcubic graph G , such as any of the instances from NHHB20 or NHHB20PR, there are $\mathcal{O}(n)$ edges and the given heuristic is run for each corresponding subgraph. In general, then, the subgraph method comes at the expense of an additional factor of $\mathcal{O}(n)$ in time complexity for subcubic graphs. However, an advantage of the method comes from the fact that if G is subcubic, then each subgraph produced by the subgraph method will necessarily contain forced edges by the definition used in Base-Forced.

In Table 4.27 we show the results of applying the subgraph method with both the Base Model and Base-Combined acting as the underlying heuristic, compared to the results of the two models without using the subgraph method. As one might expect, both models perform much better with the subgraph method, at the expense of this $\mathcal{O}(n)$ factor in additional time complexity, but the contrast is especially stark for Base-Combined which exploits more structural properties of the subgraphs. Indeed, using Base-Combined with the subgraph method detects non-Hamiltonicity in 99.0% of graphs from NHHB20, and 98.9% of graphs from NHHB20PR.

Table 4.27: Results of the Base Model and Base-Combined, using the subgraph method on (a) NHNB20 and (b) NHNB20PR, by order n . The columns labelled *Without* and *With* show the number of instances for which the given model is infeasible respectively with and without using the subgraph method.

(a) NHNB20

n	Graphs	Base Model		Base-Combined	
		Without	With	Without	With
10	1	0	0	0	0
12	1	0	1	0	1
14	6	1	4	1	6
16	33	6	27	6	33
18	231	52	191	52	229
20	1827	418	1418	475	1809
All	2099	477	1641	534	2078

(b) NHNB20PR

n	Graphs	Base Model		Base-Combined	
		Without	With	Without	With
12	1	0	1	0	1
13	1	1	1	1	1
14	7	3	7	6	7
15	5	4	5	4	5
16	9	4	9	6	9
17	23	3	23	6	23
18	17	0	13	0	16
19	6	3	6	4	6
20	18	0	18	1	18
All	87	18	83	28	86

Chapter 5

Conclusions and future work

We now conclude this thesis with a summary of the gains that have been made, and the future work arising from the research presented.

In Chapter 2 we compared various relaxed formulations of HCP. In order to make these comparisons, we considered NHNB20, the set of all non-Hamiltonian non-bridge cubic graphs with up to 20 vertices. We also constructed two sets of TSP instances, ATSP16A and ATSP16AC, to enable finer comparisons to be made. We concluded that the Base Model was the most powerful of the models considered in the majority of instances in these sets. Indeed, the Base Model dominated the other models in terms of identifying non-Hamiltonian graphs in NHNB20. In particular, the Base Model detected non-Hamiltonicity in approximately 23% of the instances of NHNB20.

In Chapter 3 we investigated techniques for reducing the HCP instances, without altering their Hamiltonicity. We identified a number of graph reductions, each of which is applicable on any graph containing particular features. We described an algorithm, GRAPHREDUCTION, that searches for a sequence of such reductions for a given graph. This is so effective that in many cases, the sequences of reductions found reduce the corresponding instances to trivially Hamiltonian or trivially non-Hamiltonian graphs. In particular, the algorithm is capable of reducing approximately 73% of the

instances from NHNB20 to a trivially non-Hamiltonian graph, and partially reducing an additional 21% of the instances. Furthermore, approximately 10% of these partially reduced instances can be immediately identified as non-Hamiltonian by the Base Model.

In Chapter 4 we considered several extensions of the Base Model and quantified their improved effectiveness. We then combined each of these extensions into a single model which we called Base-Combined. Base-Combined was shown to be considerably stronger than the Base Model, and indeed, stronger than even taking the best result from each of its constituent models. Finally, we introduced the subgraph method which, when paired with Base-Combined, is effective in solving almost all remaining instances of NHNB20, but at the cost of increasing the time complexity by a factor of $\mathcal{O}(n)$.

We now summarise the cumulative results of applying each of the above methods in turn on NHNB20. Following that, we outline the directions of future research that have arisen from each of the chapters in this thesis.

5.1 Summary of results

Given the methods described in this thesis, there is a natural approach for attempting to establish the non-Hamiltonicity of a graph. First, we apply the Base-Combined LP (Section 4.5) to see if the graph induces infeasibility. If not, we use GRAPHREDUCTION (Algorithm 3.1) to see if the graph can be reduced to a trivially non-Hamiltonian graph. If a partially reduced graph is obtained instead, we apply Base-Combined again on this reduced graph. Finally, if we have still not been successful in identifying non-Hamiltonicity, we use the subgraph method (Section 4.6) with Base-Combined.

Table 5.1 shows the outcome of the above approach for the instances of NHNB20. After each successive method is applied, the table shows the number of instances that have not yet been identified as non-Hamiltonian. As

can be seen, after all of our methods are applied, only 12 instances of NHNB20 remain unidentified as non-Hamiltonian. This is a dramatic improvement over the original Base Model for which 1622 graphs were not identified.

Since the approach described is guaranteed to terminate in polynomial time for cubic graphs, this constitutes a certificate of non-Hamiltonicity for 2087 out of the 2099 instances of NHNB20.

Table 5.1: The number of instances of NHNB20, by order n , that remain unidentified as non-Hamiltonian after each successive method is applied as described in Section 5.1.

n	Graphs	Base- Combined	Graph Reduction	(Red) Base- Combined	Subgraph method
10	1	1	0	0	0
12	1	1	0	0	0
14	6	5	0	0	0
16	33	27	2	2	0
18	231	179	38	34	1
20	1827	1352	506	452	11
Total	2099	1565	546	488	12

5.2 Future work arising from Chapter 2

Conjectures 2.12 and 2.22 are obvious topics for future research. Conjecture 2.12 would imply Conjecture 2.22, and all empirical evidence points to both being true.

The result of Theorem 2.23 is also very interesting from the perspective of the NP-hard graph toughness problem; determining whether a given graph is tough or non-tough. In particular, the feasibility of DFJ constitutes a new, polynomial-time verifiable, sufficient condition for graph toughness. Similar to in this thesis wherein we try to improve the detection of non-Hamiltonicity with polynomial-time methods, we could instead focus on improving the detection of tough graphs with polynomial-time methods such as the feasibility of appropriate LP models. This presents an interesting challenge; unlike for

the LP models we sought to tighten in Chapter 4, in this scenario we would seek rather to weaken the models as much as possible, without permitting non-tough graphs to induce feasibility.

5.3 Future work arising from Chapter 3

An obvious line of future work is to identify more reductions for inclusion in the graph reduction algorithm. One such family of reductions could be to consider more specific subgraphs than just triangles and diamonds. Such a choice of subgraph would need to be chosen by a suitable survey of graphs to see which are the most common. It would also be beneficial to try to identify other classes of incompatible edge sets. This could be achieved by identifying new measures of edge equivalence besides edge orbits.

Another potentially fruitful approach would be to further develop the graph reduction algorithm as a heuristic for solving HCP in its own right. We would first apply as many reductions as possible, and when no further reductions can be made, systematically remove edges and then see if the graph can now then be reduced to a trivial Hamiltonian or non-Hamiltonian graph. In the former case, the problem is solved, and in the latter case, we can return to the original graph and list that edge as forced, and then iterate. This procedure could also be combined with linear programming techniques, such as the Base-Combined model, to assist in the detection of forced edges.

5.4 Future work arising from Chapter 4

Broadly speaking, there are two different ways to improve the effectiveness of the techniques in Chapter 4. The first would be to further extend the models considered, by adding new constraints that take advantage of more graph properties. The second would be to consider ways that we can modify the

instances to take further advantage of the constraints we already have. For example, the constraints in Base-Forced and Base-3-Cut, which exploit the features of forced edge and 3-cuts respectively, were very effective but only on the graphs in which these graph features were present. Hence, a possible avenue for future research is to investigate techniques for introducing forced edges or 3-cuts into graphs without either altering the Hamiltonicity (in an HCP instance) or changing the length of the optimal tour (in a TSP sense). For example, one way to introduce a 3-cut is to replace any degree-3 vertex with a triangle, or some other appropriate graph, such that the original three edges form a 3-cut that separates the introduced subgraph from the rest of the graph.

Many of the new constraints in the extended models only involve $x_{r,ia}^k$ variables where $k = i$ and $r = 0$. Given the benefits gained so far, it stands to reason that finding new linking constraints on the other $x_{r,ia}^k$ variables might lead to additional improvement. One possible idea in this direction is to try to impose constraints on the powers of the permutation matrix P corresponding to a Hamiltonian cycle, as considered in Section 4.4. Although we only considered P in that section in order to obtain constraints on other variables, in fact, it can be easily seen that we can represent any element of any power of P linearly in terms of the $x_{r,ia}^k$ variables as follows.

$$[P^r]_{ki} = \sum_{a \in N(i)} x_{r,ia}^k \quad \forall r = 0, \dots, n-1. \quad (5.1)$$

Powers of P higher than $n-1$ may be obtained by recognising that $P^n = I$ for any Hamiltonian cycle. Thus (5.1) allows us to impose constraints on powers of P .

One potentially useful property on powers of P is the following: If P is a permutation matrix corresponding to a Hamiltonian cycle in a graph with n vertices, it can be shown that for $r = 1, \dots, n$, the matrix P^r will be a permutation matrix consisting of cycles of length $\frac{n}{\gcd(r,n)}$. Using linear

constraints to demand that powers of P contain cycles of the desired length is difficult; indeed, no easier than HCP itself, where we want a cycle of length n in the first power of P . We did, however, investigate the following set of constraints based on the cyclic properties of powers of P . For all r such that $\frac{n}{\gcd r, n} \neq 3$; we can prevent P^r from containing 3-cycles through the linear constraints

$$\begin{aligned} [P^r]_{ij} + [P^r]_{ik} + [P^r]_{ji} \\ + [P^r]_{jk} + [P^r]_{ki} + [P^r]_{kj} \leq 2 \end{aligned} \quad \forall i, j, k \in \{1 \dots n\}; i < j < k. \quad (5.2)$$

In investigating these constraints, we found many instances where particular feasible solutions from the Base Model violated (5.2) for some powers of r . However, imposing (5.2) never led to an improvement in gap for any TSP instances tested, nor to additional infeasible instances in the non-Hamiltonian graphs tested. Nonetheless, constraints such as (5.2), in combination with other carefully designed constraints for powers of P , could yield significant improvements.

Appendix A

Non-Hamiltonian non-bridge cubic graph sets

This appendix provides two sets of HCP instances used throughout the thesis. In Appendix A.1 we give a list of GENREG IDs for the instances in NHNB20; the cubic non-Hamiltonian non-bridge graphs up to 20 vertices in size, defined in Section 2.2.2. In Appendix A.2 we provide GENREG IDs and edge lists for the instances in NHNB20PR; the set of partially reduced graphs of NHNB20 after applying the graph reduction algorithm presented in Algorithm 3.1.

For both lists of instances, the GENREG ID refers to the graph number, starting at 1, produced by the quality GENREG software by Meringer [56], when the `genreg` executable is called to produce all cubic graphs of that size. For example, to produce the 510 489 cubic (3-regular) graphs of size 20 vertices, the command `genreg 20 3 -a` is used. The Hamiltonicity of all instances was verified with the exact algorithm of Chalaturnyk [14].

For convenience, both sets in GENREG's ASCII format may be downloaded from the *FHCP Dissertations* page on the Flinders Hamiltonian Cycle Project website: <http://fhcp.edu.au>.

A.1 NHNB20 GENREG IDs

There are 2099 non-Hamiltonian non-bridge cubic graphs up to 20 vertices in size, with the GENREG IDs as listed below. We also indicate the instances for which the graph reduction algorithm in Algorithm 3.1 is able to find a reduction; a plus (+) following an ID indicates that the instance is partially reduced, while an asterisk (*) indicates that the instance is completely reduced to a trivially non-Hamiltonian graph. There are respectively 443 and 1537 instances of NHNB20 with partial and complete reductions.

10 vertices (1 graph):

19*

12 vertices (1 graph):

63*

14 vertices (6 graphs):

120* 123* 251* 372* 388* 421*

16 vertices (33 graphs):

237* 240* 410* 416* 547* 552* 582* 824* 830* 831* 842* 852* 971*
 1066* 1281* 1386* 1792* 1828* 1840* 1864* 1998* 2031* 2235* 2911* 2923* 3009*
 3112* 3123* 3138* 3300* 3337+ 3427* 3453

18 vertices (231 graphs):

1066* 1069* 1245* 1251* 1397* 1402* 1440* 1567* 1697* 1703* 1704* 1715* 1726*
 1863* 1866* 2033* 2038* 2210* 2215* 2412* 2469+ 2748* 3030* 3031* 3032* 3058*
 3074* 3107* 3121* 3145* 3472* 3556* 3564* 3646* 3649* 3707* 4189* 4195* 4203*
 4212* 4213* 4238* 4250* 4279* 4489* 4535* 4536* 4537* 4557* 4652+ 5112* 5132*
 5190* 5459* 5460* 5461* 6099* 6105* 6814* 6932* 6933* 6934* 6964* 6965* 6966*
 6967* 6968* 6969* 6970* 6971* 7018* 7027+ 7037* 7038* 7039+ 7119* 7120* 7121*
 7122* 7147* 7229* 7305* 7389* 7578* 7640* 7648* 7649* 7675* 7679* 7683* 7710*
 7899* 8045* 8151* 8420* 8430* 8625* 8746* 8864* 9134* 9147* 9249* 9379* 9506*
 9719* 9907* 10094* 10937* 10976* 10994* 11010* 11041* 11133* 11360* 11424* 11526* 11969*
 12006* 12018* 12043* 12201* 12300* 12952* 13068* 14794* 15633* 15971* 15996* 16009* 16029*
 16238* 16239* 16240* 16241* 16331* 16332* 16353* 16432* 16611* 16612* 16613* 16617* 16664*
 16781* 17340* 17499* 17576* 17641* 17766* 17796* 17914* 18069+ 18139* 18214* 18567+ 18597*
 18608* 18632* 18758+ 18902* 18921* 18978* 19026* 19153* 19271+ 19337* 20388* 20633* 20740*
 20766* 20795* 21027+ 21493* 22141+ 22181* 25534* 28010* 28478* 28485* 28488* 28544* 28579*
 28624* 28803* 28884+ 29269+ 29446* 29479* 29498+ 29499+ 29500* 29501+ 29502+ 29777* 29824*
 30289* 30554+ 30555* 30556+ 30557* 30558+ 30560+ 30599* 30675* 33494* 33547* 33587* 33737*
 33798 33827+ 34034* 34065+ 34468+ 34621+ 34742* 34770 34858* 34877* 34901 34934 35117
 35141 35533 36973 37070 37124 37193 38297 40847+ 40849 40852*

20 vertices (1827 graphs):

8602* 8605* 8783* 8789* 8938* 8943* 8981* 9108* 9238* 9244* 9245* 9256* 9267*
 9407* 9410* 9583* 9588* 9770* 9775* 9986* 10043+ 10336* 10568* 10624* 10625* 10626*
 10652* 10668* 10701* 10715* 10739* 11081* 11090* 11222* 11242* 11333* 11336* 11405* 11631*
 11912* 11918* 11926* 11935* 11936* 11962* 11975* 12006* 12235* 12291* 12292* 12293* 12294*
 12300* 12304* 12319* 12416+ 12417* 12929* 12949* 13021* 13268* 13301* 13302* 13303* 13532*

13862*	13865*	13986*	13992*	14753*	14759*	14880*	14886*	14887*	14888*	14889*	14923*	14924*
14925*	14926*	14927*	14928*	14929*	14930*	14931*	14977*	14985*	14996*	15007*	15008*	15009+
15094*	15095*	15096*	15097*	15123*	15208*	15286*	15371*	15574*	15639*	15647*	15648*	15681*
15685*	15689*	15716*	15942*	15945*	16117*	16123*	16267*	16272*	16308*	16560*	16566*	16567*
16578*	16589*	16877*	16882*	17165*	17174*	17326*	17331*	17397*	17896*	17902*	17910*	17919*
17920*	17946*	17959*	17990*	18203*	18208*	18369*	18375*	18654*	18663*	18813*	18818*	18884*
19385*	19391*	19399*	19408*	19409*	19435*	19448*	19479*	19642*	19645*	19943*	19949*	20093*
20099*	20345*	20356*	20603+	20830*	21016+	21056*	21057*	21058*	21121*	21197*	21203+	21556+
21569+	21633*	21706+	21730+	21792*	21899+	22087*	22092*	22242*	22935*	22946*	24207+	24261*
24262*	24263*	24267*	24273+	24298+	24465+	24547*	24682+	24940*	25061*	25149*	25218+	25868*
26304*	26305*	26306*	27203*	27204*	27205*	27206*	27207*	27208*	27209*	27210*	27211*	27212*
27213*	27214*	27455*	27456*	27457*	27458*	27459*	27495*	27545*	27550*	27581*	27586*	27631*
27649*	27666*	27702*	27771*	27806*	27834*	28015+	28034*	28045*	28046*	28047*	28048*	28159*
28160*	28161+	28162*	28163+	28164*	28267*	28344*	28448*	28503*	28504*	28505*	28506*	28510*
28537*	29056*	29344*	29350*	29368+	29459*	29519*	29534*	29712*	29946*	29949*	30057*	30060*
30213*	30219*	30494*	30500*	30750+	30993+	31419*	31985*	31993*	32006*	32052*	32070*	32087*
32123*	32224*	32233*	32248*	32417*	32423*	32515*	32518*	32821*	32858*	32861*	32863*	32885*
32902*	32959*	33147*	33283*	33288*	33321*	33568*	33574*	33575*	33586*	33597*	33797*	33942*
34021*	34022*	34023*	34027*	34077*	34220+	34882*	35029*	35059*	35194*	35468*	35773*	35774*
35775*	37189*	37195*	38348*	38505*	38757*	38783*	38838*	38839*	38840*	38865*	38878*	38911*
38925*	38948*	39023*	39024*	39025*	39026*	39080*	39081*	39082*	39083*	39084*	39085*	39086*
39087*	39088*	39089*	39090*	39229*	39245*	39256+	39267*	39268*	39269*	39270+	39379*	39380*
39381*	39382*	39407*	39489*	39719*	39720*	39721*	39722*	39726*	39777*	39911*	40103*	40593*
40785*	40871*	40889*	40894*	40936*	40958*	41017*	41082*	41141*	41145*	41149*	41183*	41203*
41314*	41317*	41596+	41710*	41728*	41874*	42420+	42463*	42476*	42505*	42727*	42877*	42883*
42887*	42888*	42889*	42890*	42891*	42892*	42893*	42894*	42895*	42896*	42897*	42898*	42899*
42900*	42925*	42926*	42927*	42943*	42944*	42945*	42972*	42977*	43006*	43025*	43042+	43049*
43050*	43051*	43174*	43318+	43403*	43473+	43752+	43761+	43772+	43880+	44016*	44021*	44304+
44530+	45443*	45618+	48031+	48114*	48127*	48129*	48180*	48274*	48278*	48384*	48725*	48839*
48840*	48841*	49097*	49337*	49382+	50083*	50485*	50935*	50936*	50937*	50938*	51552*	51553*
51554*	51579*	51580*	51581*	51582*	51583*	51584*	51585*	51586*	51587*	51588*	51589*	51671+
52039*	53516+	53778*	53789*	53790*	55422*	55933+	56973*	57130*	57408*	58570*	58579*	58580*
58767*	58768*	58769*	59264+	59806*	59830*	59884*	59885*	59886*	59910*	59920*	59953*	59967*
59990*	60204*	60256+	62899*	67169*	67186*	67396*	67397*	67398*	67429*	67435*	67532*	67605*
67627*	67643*	67675*	69036*	69052+	69084*	69479*	70252*	70258*	70298*	70299*	70300*	70320*
70321*	70322*	70323*	70324*	70325*	70326*	70327*	70328*	70329*	70330*	70331*	70332*	70333*
70334*	70335*	70336*	70337*	70560*	70561*	70562*	70563*	70564*	70565*	70566*	70567*	70568*
70569*	70570*	70571*	70572*	70573*	70574*	70575*	70576*	70577*	70578*	70579*	70580*	70581*
70582*	70583*	70584*	70585*	70586*	70587*	70588*	70589*	70590*	70591*	70592*	70593*	70594*
70595*	70596*	70597*	70598*	70599*	70600*	70601*	70602*	70603*	70604*	70605*	70606*	70607*
70608*	70609*	70893*	70917*	71121*	71122*	71123*	71170+	71171+	71172+	71230*	71231*	71232+
71233*	71234*	71235+	71236*	71237+	71238+	71239+	71240*	71241+	71242+	71243*	71244+	71268+
71300*	71415*	71907*	71911*	71912*	71913*	71914+	71915*	71916*	71917*	71918*	71919*	71920*
71921*	71922*	71923*	71924*	71925+	71926*	71927+	71928*	71976+	71988*	72082*	72087*	72101*
72103*	72112*	72115*	72116*	72117+	72118*	72119+	72240+	72338+	72738*	72971*	72987*	73011*
73012+	73290*	73899*	73907+	73916+	73918*	74752*	74772*	74784*	75369*	77114*	77368*	77398*
77410*	77416+	77509*	77878*	77901*	78010*	78139*	78140*	78517*	79742*	79974*	79975*	80023*
80160*	80169*	80175*	80189*	80190*	80199*	80214*	80220*	80221*	80234*	80251*	80295*	80649*
80722*	80830*	80970*	80993*	81032*	81039*	81093*	81099*	81376*	81495*	81576*	81586*	81595*
81596*	81630*	81638*	81643*	81644*	81651*	81680*	81688*	81695*	81786*	81791*	81805*	81821*
81886*	82068*	82140*	82141*	82236+	82277+	82507*	82679+	83062*	83063*	83064*	83065*	83066*
84038*	84186*	84294*	84563*	84573*	84690*	84830*	84980*	85195+	85711*	85741*	85755*	85777*
86050*	86123*	86623*	86660*	86672*	86699*	86889*	86932*	86933*	86934*	87038+	87480*	88390*
89071*	89273*	89274*	89275+	89352*	89353*	89354*	89378*	89458*	89533*	89616*	89800*	89860*
89867*	89868*	89893*	89897*	89901*	89928*	90728*	90868*	90972*	91236*	91246*	91400*	91627*
91747*	92184*	92221*	92233*	92260*	92400*	92628+	92747*	93144*	93287*	93317*	93352*	93470*
93587*	94071*	94745*	94746*	94848+	94939*	95983*	95987*	96002*	96006*	96011*	96033*	96064*
96123*	96124*	96173*	96174*	96175+	96235*	96445*	96474*	96647*	96781*	96880*	97141*	97151*
97376*	97597*	97701*	98168*	98205*	98217*	98244*	98494*	98611*	98805*	99302*	99332*	99346*
99368*	99529*	99651*	99771*	99985*	100178*	100374*	101236*	101275*	101293*	101309*	101340*	101432*
101575*	101792*	101900*	102086*	102607*	102738*	103040*	103052*	103180*	103203*	103353*	103570*	103759*
103858*	104044*	104912*	104950*	104962*	104987*	105021*	105100*	105242*	105426*	106332*	106469*	108357*
108867*	109290*	110867*	112685*	112703*	113405*	113444*	113462*	113478*	113509*	113601*	113857*	113858*
113859*	113860*	113975*	113976*	113977*	113978*	114096*	114097*	114098*	114099*	114124*	114198*	114296*
114514*	114515*	114516*	114520*	114567*	114782*	115659*	115838*	115919*	116179*	116191*	116284*	116289*
116305*	116620*	116643*	116743*	117083*	117245*	117378*	117424*	117626*	117736*	117844*	118040*	118215*
118393*	119202*	119241*	119259*	119275*	119306*	119398*	119530*	119597*	119827*	119877*	119948*	120159*
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127438*	127526*	127625*	128063+	128100*	128112*	128137*	128283*	128462+	128561+	128987*	129024*	129036*
129063*	129235*	129297*	129481*	129651+	129748*	131170*	131260*	131439*	131606+	132404*	132527*	134268*
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156690*	156844+	157264*	157333*	157365*	157378*	157399+	157522*	157950*	158943+	161433*	165994*	166000*
166082*	166145*	166178*	166204*	167396+	167422*	167760*	168443*	168558*	168850*	169151*	170803*	170836*

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 174789+ 174918* 174928* 174930* 174931* 174932* 174933* 175683* 175698* 175721* 175722* 175977* 176089+
 177006* 177632* 177633* 177634+ 177635* 177636+ 177637* 177638* 177639+ 177641* 177642* 177643+ 177653*
 177654* 177655* 177669* 177793* 177802* 178017* 178127* 178143* 178166* 178167* 179254* 179256* 179257*
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 194487+ 194491* 194596* 196149+ 196150+ 196151* 196152* 196967* 197189* 197427* 197513* 197527* 197545*
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 200679* 200743* 201079* 201109* 201120* 201144* 201298* 201384* 201468* 201618+ 201744+ 201879+ 202523+
 202555+ 202571+ 202585+ 202613+ 202687+ 202782* 202857* 203109* 203192* 203255* 203259* 203350* 203559+
 203637+ 203967* 203978* 204002* 204136* 204215+ 204745+ 204844+ 206349+ 207340* 207395+ 207424+ 207436+
 207457+ 207656+ 207741+ 207760* 207833* 208000+ 208003* 208044* 208151* 208705* 208856* 208933* 208995+
 209091+ 209142* 209171* 209254* 209332* 209467+ 209536+ 209872+ 209902+ 209913+ 209937+ 210057+ 210089*
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 212216* 212295* 212351* 212544* 212553* 212622* 212693* 212743* 212865* 212981* 213100* 213707* 213739*
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 215068+ 215089+ 215202+ 215285+ 215343* 215578* 215656* 215718* 215722* 215812* 216001+ 216111+ 216176*
 217298+ 217400+ 217878+ 219722+ 220429+ 223296* 226842* 226899* 227152* 227193* 227244* 227255* 227331*
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 232370+ 232470+ 233428* 233535+ 233630+ 233728+ 234254+ 234286+ 234302+ 234315+ 234342+ 234412+ 234498+
 234775* 234869+ 235163+ 235415+ 236835+ 238741+ 238807* 238863* 238867* 238950* 239092+ 239729+ 244064*
 244128+ 244227+ 244329+ 244421+ 244509+ 246245+ 246334+ 246729* 246869+ 246874+ 246934+ 246983+ 247004+
 247022+ 247089* 247289+ 247377* 247420* 247440* 253182+ 253379+ 253474+ 254298+ 254502+ 254738+ 255389+
 255703+ 255786* 256054+ 256761+ 257382+ 258408* 260741+ 264223+ 267396+ 268521+ 269104+ 270280* 287129*
 287176* 287418+ 287441* 287450* 287468* 288629+ 288800+ 288887+ 288997+ 289991+ 296754+ 296802* 297985+
 298024+ 306924+ 311109+ 311887+ 319062+ 327104* 327161+ 327579* 327660* 327749+ 328042* 332900* 333264*
 333295* 333320* 333329* 333442* 333609* 333662* 333687* 333731+ 333985+ 334076* 334104* 334118+ 334119+
 334120* 334121+ 334122+ 334437* 334438+ 334439+ 334440+ 334441* 334442+ 334752* 334962* 335385* 337526+
 338019* 338854* 339126+ 339160* 339385+ 339405+ 339412+ 339429+ 339583+ 341155* 341201+ 341516+ 342307*
 342351+ 343102+ 343247+ 343250+ 343379+ 343404+ 343482+ 343567+ 343580+ 345988* 345989* 345990* 345991*
 345992* 346054+ 346104+ 346192+ 346203* 346204* 346205* 346206* 346207* 346334+ 346358* 346359* 346360*
 346361+ 346362+ 346363+ 346364+ 346365+ 346366+ 346367+ 346368+ 346369* 346370+ 346371+ 346372+ 346373+
 346374+ 346375* 346376+ 346377+ 346378+ 346379+ 346380+ 346381+ 346382+ 346383+ 346384+ 346385+ 346386+
 346387+ 346388+ 346389+ 346390+ 346391+ 346392+ 346393+ 346394+ 346395* 346396* 347133* 348925* 348992*
 349065+ 349087+ 349204+ 349236+ 349291+ 349300* 349301+ 349309+ 349315* 349316+ 349323+ 349337+ 349519+
 350322+ 350339+ 353410+ 353469+ 353551* 353552+ 353553+ 355890+ 356755* 357734+ 357795+ 358211+ 358279*
 358448* 358449+ 358450* 358451+ 358452+ 358453+ 358454+ 358455+ 358456* 358457* 358458+ 358459+ 358461+
 358462+ 358463+ 358464+ 358465* 358466* 358467+ 358468+ 358469+ 358470+ 358471+ 358472+ 358476* 358477*
 358478+ 358479+ 358480+ 358481+ 358482+ 358483+ 358484+ 358485+ 358486+ 358487+ 358488* 358489* 358490+
 358491+ 358492+ 358493* 358506* 358567+ 358675+ 358766+ 358806+ 358843+ 358844* 358848+ 358908+ 358919+
 359301+ 359378+ 359379* 359380+ 359381+ 361236* 361500+ 367771+ 376442+ 376498+ 376786+ 377178+ 379913+
 383925+ 385630+ 385965+ 391322+ 392099+ 393918* 400138* 404228* 404260* 404577+ 404727+ 405059* 405120+
 405454+ 410763* 411046+ 411965* 412677* 413133* 413174* 413325* 413365* 413423+ 413662* 413670* 413715+
 414174* 414497+ 414514* 414737* 414790* 414828* 414980* 415007* 415069* 415122* 415178* 415570* 415698+
 415824* 415856+ 416707+ 417120* 417162+ 417355+ 417721+ 417798* 417830+ 417930* 417982+ 418009+ 418224*
 418273* 418288* 418801* 418847* 418976+ 422384* 422473+ 424159+ 424367+ 424399+ 424400* 424401+ 424541+
 425973* 426002+ 426126* 426173* 426198* 426389+ 426400* 427045* 427071+ 427207* 427232* 427355* 427395*
 427417* 427596* 427633* 427665* 427786* 428012+ 428031* 428525* 429718* 429732* 429763* 429780* 429950*
 429962* 429990* 430005* 430028* 430135* 430352* 430366* 430633* 430655* 430805* 431491* 434209* 434218*
 434232* 434253* 434405* 434417* 434644* 436326* 436338* 436558* 436638* 436748* 437336* 439826* 439993*
 440009* 451500* 451510* 451522* 451538* 451658* 451672* 452512* 452518* 452528* 452541* 452654* 452667*
 452678* 452691* 452702* 453194* 453197* 453259* 453299* 453309* 453371* 453570* 453645* 454046* 454156*
 455252* 455548* 455865* 458069* 458181* 458184* 460746* 461487* 462692* 468366* 468368* 468386* 468428*
 468429* 468581* 468582* 468610* 468851* 468863* 470354* 470360* 470469* 470475* 470481* 470674* 474063*
 474064* 474227* 474575* 476227* 495446+ 504707* 504708* 504713* 504724* 504725* 504730* 504756* 504757*
 504758* 504759* 504803* 504912* 505618* 505657+ 510433+

A.2 NHNB20PR edge lists

Of the 443 instances of NHNB20 which are partially reduced by Algorithm 3.1, there are 87 unique partially reduced instances up to isomorphism (determined with the graph canonicalisation routines in *nauty* [55]). These 87 instances are given in this

section, along with the GENREG IDs of the 443 instances in NHHB20 to which they correspond. The first number given is the assigned instance ID followed by an edge list consisting of pairs of vertices in base 20 (vigesimal); the first through tenth vertices are represented by 0 through 9, the eleventh vertex is represented by A and so on until a maximum of J for the 20th vertex, where present. Below this line is an indented list of NHHB20 GENREG IDs that are reduced to this instance by Algorithm 3.1. Instances are numbered by the first time they are produced as NHHB20 is processed in order of graph size then GENREG ID, with this first produced instance also determining the given vertex labelling.

```

1  01 03 14 15 24 25 36 37 46 58 69 7A 7B 8C 8D 9E 9F AC AE BD BF CF DE
   16 vertices: 3337
   18 vertices: 18069 18567 18758 29269 29498 29499 30554 30556
   20 vertices: 42420 59264 127438 128063 128462 128561 156844 157399 173333 174039 174040 174041
                   174779 174789 176089 177634 177636 194487 198032 198385 202523 202555 202571 202585
                   202613 202687 203559 203637 204844 207395 207424 207436 209091 209872 209902 209913
                   209937 210344 232303 232370 238741 247289 333985 334118 334119 334438 334439 337526
                   343247 343250 343379 343404 343567 346104 349236 349291 349316 353410 353469 358766
                   358919 359301 359378
2  01 02 13 14 23 25 36 46 47 58 59 6A 7B 7C 8B 8D 9C 9E AD AE BE CD
   18 vertices: 2469
   20 vertices: 10043 21203 21556 21569 21706 21730 21899 24682 25218 30750 30993 48031
                   85195 92628 413423
3  01 02 14 15 24 26 35 37 48 59 6A 6B 7A 7C 8C 8D 9B 9D AD BC
   18 vertices: 4652
   20 vertices: 12416 24465 28161 34220 43752 43761 43772 53516 87038 94848 413715
4  01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7A 89 AB
   18 vertices: 7027
   20 vertices: 14996 39245 39256 55933 71170 71171 71172 71976 72117 72338 73907 82679
5  01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 89 AD BD BE CD CE
   18 vertices: 7039
   20 vertices: 15009 39270 71237 71238 71242 72119 73012 73916 77416 89275 96175 414497
6  01 02 03 14 15 24 26 35 37 47 58 69 6A 7B 8C 8D 9C 9E AD AF BE BF CF DE
   18 vertices: 19271 21027 22141 28884 29501 29502 30558 30560
   20 vertices: 129651 131439 131606 137371 137814 140064 140462 158943 167396 172579 174046 174048
                   174051 174787 174788 177639 177643 196150 197982 199476 214726 214953 214964 215068
                   215089 215202 220429 234254 234286 234302 234315 234342 234412 235163 239729 244329
                   246245 246869 246874 246934 246983 247022 253474 264223 267396 288800 288997 311109
                   327161 327749 333731 334121 334122 334440 334442 339405 339412 339429 349301 349309
                   349323 353552 353553 358843 358848 359380 359381
7  01 03 14 15 24 25 36 37 46 58 69 79 7A 8B 8C 9D AE AF BE BG CF CH DG DH EH FG
   18 vertices: 33827
   20 vertices: 201744 207457 209536 254738 319062 346363 346373 358449 358458
8  01 05 13 14 23 24 37 48 57 59 67 6E 8A 8B 9C 9D AC AE BD BF CF DE
   18 vertices: 34065
   20 vertices: 204215 208995 210057 298024 311887 346374 346388 358459 358461
9  01 02 03 14 24 25 36 37 48 5D 69 6A 79 7A 8B 8C 9F AG BD BF CE CG DG EF
   18 vertices: 34468
   20 vertices: 206349 207741 211596 349519 358806
10 01 03 14 15 24 25 36 37 48 59 6A 6B 7C 7D 8A 8C 9B 9E AF BC DG DH EG EH FG FH
   18 vertices: 34621
   20 vertices: 207656 208000 211444 357734 361500 392099 404727
11 01 02 03 14 15 26 38 39 46 48 57 59 6A 7B 8C 9D AE AF BE BG CF CH DG DH EH FG
   18 vertices: 40847
   20 vertices: 346054 350339 385630
12 01 02 13 14 23 25 36 45 47 58 67 69 7A 8B 8C 9D 9E AF AG BD BF CE CG DG EF
   20 vertices: 18663
13 01 02 13 14 23 25 36 46 47 57 58 69 7A 8B 8C 9D 9E AF AG BD BF CE CG DG EF
   20 vertices: 19949
14 01 02 13 14 23 25 36 46 47 58 59 68 7A 7B 8C 9D 9E AD AF BE BG CF CG DG EF
   20 vertices: 20356
15 01 02 13 14 23 25 36 46 47 58 59 6A 78 7B 8C 9B 9D AB AC CD
   20 vertices: 20603

```

16 01 02 13 14 23 25 36 46 47 58 59 6A 7A 7B 8C 8D 9E 9F AG BC BE CF DE DG FG
20 vertices: 21016

17 01 02 13 14 23 25 36 47 48 59 5A 67 68 7B 8C 9D 9E AF AG BD BF CE CG DG EF
20 vertices: 24207

18 01 02 13 14 23 25 36 47 48 59 5A 67 69 7A 8B 8C 9D AB BD CD
20 vertices: 24273

19 01 02 13 14 23 25 36 47 48 59 5A 67 69 7B 8A 8B 9C AD BC CD
20 vertices: 24298

20 01 02 13 14 23 25 36 47 48 59 5A 6B 6C 79 7B 8A 8C 9C AD BD
20 vertices: 28015

21 01 02 13 14 23 25 36 47 48 59 5A 6B 6C 79 7B 8C 8D 9C AE AF BG DE DF EG FG
20 vertices: 28163

22 01 02 13 14 23 25 36 47 48 59 5A 6B 6C 7B 7D 8C 8E 9F AF AG BE CD DF EG
20 vertices: 29368

23 01 02 13 14 25 26 35 36 47 48 57 69 7A 8B 8C 9D 9E AF AG BD BF CE CG DG EF
20 vertices: 41596

24 01 02 13 14 25 26 35 37 46 48 58 69 7A 7B 8C 9D 9E AD AF BE BG CF CG DG EF
20 vertices: 43042

25 01 02 14 15 24 26 35 37 48 59 68 6A 79 7B 8B 9A AC BC
20 vertices: 43318

26 01 02 13 14 25 26 35 37 46 48 59 6A 79 7B 8C 8D 9E AF AG BC BF CG DE DF EG
20 vertices: 43473

27 01 02 14 15 24 26 35 37 48 59 6A 6B 7C 7D 8C 8E 9A 9F AC BE BF DE DF
20 vertices: 43880

28 01 02 13 14 25 26 35 37 47 48 58 69 6A 7B 8C 9D 9E AF AG BD BF CE CG DG EF
20 vertices: 44304

29 01 02 13 14 25 26 35 37 47 48 59 67 6A 8B 8C 9D 9E AF AG BD BF CE CG DG EF
20 vertices: 44530

30 01 02 13 14 25 26 35 37 47 48 59 6A 6B 79 8C 8D 9E AC AF BD BG CG DF EF EG
20 vertices: 45618

31 01 02 13 14 25 26 35 37 48 49 58 6A 6B 78 7C 9D 9E AD AF BE BG CF CG DG EF
20 vertices: 49382

32 01 06 13 14 23 25 38 46 47 59 5A 6B 7C 8D 8E 9B 9D AC AE BE CD
20 vertices: 51671

33 01 02 13 14 25 26 37 38 47 49 57 58 6A 6B 8C 9D 9E AD AF BE BG CF CG DG EF
20 vertices: 60256

34 01 04 12 13 26 27 36 38 49 4A 5B 5C 6D 78 7D 8E 9B 9E AC AF BF CE DF
20 vertices: 69052

35 01 03 15 16 25 27 38 39 4A 4B 5C 6C 6D 7C 7E 8A 8D 9B 9E AE BD
20 vertices: 70258

36 01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 89 AB AD BE CF CG DF EF EG
20 vertices: 71232

37 01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 89 AC AD BE BF CG DE DF EG FG
20 vertices: 71235

38 01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 89 AD AE BD BF CE CF DG EG FG
20 vertices: 71239

39 01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 89 AD AE BD BF CE CG DG EF FG
20 vertices: 71241

40 01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 89 AD AE BF BG CD CF DG EF EG
20 vertices: 71244

41 01 02 13 14 25 26 37 38 49 4A 57 59 68 6B 7C 8A 9D AD BC BD
20 vertices: 71268

42 01 02 13 14 25 26 37 38 49 4A 57 59 6B 6C 7A 89 8B AD BE CF CG DF DG EF EG
20 vertices: 71914

43 01 02 14 15 26 27 38 39 46 48 5A 5B 69 78 7C 9D AC AE BD BE CF DF EF
20 vertices: 71923

44 01 02 14 15 26 27 38 39 46 48 5A 5B 69 78 7C 9D AC AE BD BF CF DE EF
20 vertices: 71925

45 01 02 13 14 25 26 37 38 49 4A 57 59 6B 6C 7A 89 8D AE BD BF CF CG DG EF EG
20 vertices: 71927

46 01 02 14 15 26 27 38 39 46 48 5A 5B 69 78 7C 9D AE AF BE BF CD CE DF
20 vertices: 71928

47 01 02 13 14 25 26 37 38 49 4A 57 59 6B 6C 7B 8A 8C 9D AD BD
20 vertices: 72240

48 01 03 15 16 27 28 39 3A 4B 4C 57 58 67 6D 8E 9B 9D AC AE BE CD
20 vertices: 82236

49 01 04 12 13 26 27 38 39 4A 4B 5C 5D 68 69 7A 7C 8E 9E AD BC BF DF EF
20 vertices: 82277

50 01 02 03 14 15 24 25 36 37 46 58 69 78 7A 8B 9C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 201618 201879 204745 209467 343482 343580 346361 346362 346368 358451 358455 358484
404577 411046

51 01 02 03 14 15 24 26 35 36 47 58 69 78 7A 8B 9C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 211992 215285 215578 255703 287418 346364 346370 358453 358472 383925

52 01 02 03 14 15 24 26 35 37 47 58 68 69 7A 8B 9C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 214134 233630 246334 339385 346365 346371 358456 358490 405454

53 01 02 03 14 15 24 26 35 37 47 58 69 6A 79 8B 8C 9D AE AF BE BG CF CH DG DH EH FG

20 vertices: 214304 214644 233535 233728 244227 247004 339126 346366 346367 346372 358452 358454
358470 376786 391322

54 01 02 03 14 15 24 26 35 37 48 59 67 68 7A 8B 9C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 216001 217878 256761 296754 346376 346379 358462 358478 379913

55 01 02 03 14 15 24 26 35 37 48 59 67 69 7A 8B 8C 9D AE AF BE BG CF CH DG DH EH FG
20 vertices: 216111 219722 255389 256054 260741 288629 346382 346383 346390 355890 358211 358471
358481 358483 377178

56 01 02 03 14 15 24 26 35 37 48 59 68 69 7A 7B 8C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 217298 217400 288887 289991 346378 346381 358464 358480 405120

57 01 02 03 14 15 24 26 37 38 47 56 58 69 7A 8B 9C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 232197 232470 341516 343102 346377 346380 358479 358485 385965

58 01 02 03 14 15 24 26 37 38 47 58 59 68 6A 7B 9C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 234498 236835 244421 341201 342351 346384 346389 350322 358486 358491 376442

59 01 02 03 14 15 24 26 37 38 47 58 59 6A 6B 79 8C 9D AE AF BG BH CE CG DF DH EH FG
20 vertices: 234869 244128 253182 339583 346385 346392 349337 358469 358482 358908

60 01 02 03 14 15 24 26 37 38 47 58 59 6A 6B 7C 8C 9D 9E AD AF BE BG CH DG EF FH GH
20 vertices: 235415 239092 244509 253379 254298 254502 269104 306924 346386 346387 346391 358463
358467 358487 376498

61 01 02 03 14 15 24 26 37 38 49 57 5A 67 6A 8B 8C 9D 9E AF BD BG CE CH DH EG FG FH
20 vertices: 257382 268521 297985 346393 346394 357795 358468 358492

62 01 02 03 14 15 26 27 38 39 46 48 57 5A 69 7B 8C 9D AE AF BE BG CF CH DG DH EH FG
20 vertices: 346192 346334 349065 349204 358675 367771

63 01 03 14 15 26 27 38 39 46 48 5A 5B 69 7A 7C 8D 9E AF BD BG CE CG DH EH FG FH
20 vertices: 349087 358567

64 01 03 14 15 24 25 36 37 46 58 69 79 7A 8B 8C 9D AD AE BF BG CH CI DJ EF EH FI GH GJ IJ
20 vertices: 415698

65 01 03 14 15 24 25 36 37 46 58 69 7A 7B 8A 8C 9A 9D BE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 415856

66 01 03 14 15 24 25 36 37 46 58 69 7A 7B 8C 8D 9A 9B AE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 416707

67 01 03 14 15 24 25 36 37 46 58 69 7A 7B 8C 8D 9E 9F AC AE BF BG CF DH DI EJ GH GI HJ IJ
20 vertices: 417162

68 01 02 03 14 15 24 25 36 37 46 58 69 7A 7B 8C 8D 9E 9F AC AG BD BH CH DG EI FI FJ GI HJ
20 vertices: 417355

69 01 03 14 15 24 25 36 37 46 58 69 7A 7B 8C 8D 9E 9F AE AG BF BH CI DI DJ EH FG GI HJ
20 vertices: 417721

70 01 03 14 15 24 25 36 37 48 59 68 69 7A 7B 8A 9C AD BE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 417830

71 01 03 14 15 24 25 36 37 48 59 68 6A 78 7B 9A 9C AD BE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 417982

72 01 05 13 14 23 24 37 48 57 59 67 6A 8B 8C 9A 9D AE BF BG CH CI DF DH EG EI FI GH
20 vertices: 418009

73 01 02 03 14 24 25 36 37 48 59 68 6A 79 7A 8B 9C AD BE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 418224

74 01 03 14 15 24 25 36 37 48 59 68 6A 7A 7B 8C 9D 9E AC BF BG CH DF DI EG EJ FJ GI HI HJ
20 vertices: 418976

75 01 03 14 15 24 25 36 37 48 59 6A 6B 7A 7C 8A 8B 9D 9E BF CG CH DG DI EH EJ FI FJ GJ HI
20 vertices: 422473

76 01 02 03 14 24 25 36 37 48 59 6A 6B 7A 7C 8D 8E 9F 9G AH BC BH CI DF DI EG EJ FJ GI HJ
20 vertices: 424159

77 01 02 03 14 24 25 36 37 48 5E 69 6A 79 7B 8C 8D 9G AG AH BG BI CE CH DF DI EI FH
20 vertices: 424367

78 01 03 14 15 24 25 36 37 48 59 6A 6B 7C 7D 8A 8C 9B 9E AF BC DG DH EG EI FH FI GJ HJ IJ
20 vertices: 424399

79 01 03 14 15 24 25 36 37 48 59 6A 6B 7C 7D 8A 8C 9B 9E AF BC DG DH EG EI FI FJ GJ HI HJ
20 vertices: 424401

80 01 05 13 14 23 24 37 48 59 5A 6B 6C 79 7B 8D 8E 9C AB AF CG DF DH EG EI FI GH HI
20 vertices: 424541

81 01 02 03 14 15 24 26 35 47 57 68 79 8A 8B 9A 9C AD BE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 426002

82 01 02 03 14 15 24 26 35 36 47 58 69 7A 8A 8B 9C 9D AE BG CF CG DH DI EF EH FI GH
20 vertices: 426389

83 01 02 03 14 15 24 26 35 37 47 68 79 8A 8B 9A 9C AD BE BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 427071

84 01 02 03 14 15 24 26 35 37 47 58 69 7B 89 8A 9C AH BD BE CF CG DF DH EG EI FI GH
20 vertices: 428012

85 01 03 14 15 24 26 37 38 49 5A 5B 6A 6B 79 7A 8C 8D 9E BF CG CH DI DJ EG EI FH FJ GJ HI
20 vertices: 495446

86 01 03 14 15 26 27 38 39 46 48 5A 5B 69 7C 7D 8C 9A AE BF BG CH DF DI EI EJ FJ GH GI HJ
20 vertices: 505657

87 01 02 03 14 15 26 27 38 39 46 4A 5B 5C 7E 7F 8B 8E 9C 9F AG AH BG CH DE DI FI GI
20 vertices: 510433

Appendix B

ATSP problem sets

This appendix contains the 400 ATSP instances of ATSP16A and ATSP16AC generated by the method described in Section 2.2.4. Each instance is arranged into a 24×3 array, labelled above with its instance ID and the optimal tour cost of the corresponding ATSP16A instance. In each row of the 24×3 array, the first element is an edge described by two vertices uv , and the second and third elements give the arc costs for $u \rightarrow v$ and $v \rightarrow u$ respectively. Vertices are represented in hexadecimal, with the first vertex being 0 and the 16th vertex being F.

Only the arc costs for the underlying cubic graph are given. For each complete instance of ATSP16A, all other arcs required to complete the graph have a cost of 1600. Alternatively, for each cubic instance of ATSP16AC, only the given edges are present. Instances 1 through 200 are derived from Hamiltonian graphs, while instances 201 through 400 are derived from non-Hamiltonian graphs. Underlined arc costs correspond to that arc being used in the optimal tour of the ATSP16A instance, and in the case of a non-Hamiltonian graph they indicate which arcs are in the optimal Hamiltonian path (with the cycle being formed in the complete graph using the additional arc with cost 1600 between the end and start of the optimal Hamiltonian path).

For convenience, the complete instances in TSPLIB [63] format may be downloaded from the *FHCP Dissertations* page on the Flinders Hamiltonian Cycle Project website: <http://fhcp.edu.au>.

An example is helpful in describing the format. Consider the instance with ID 1:

1 697
 01 26 41
 02 76 63
 03 98 79
 12 59 15
 ...

Having an ID between 1 and 200, this instance is derived from a Hamiltonian cubic graph. It has edges between the vertex 0 and 1, between vertex 0 and 2, et cetera.

The arc cost for 0→1 is 26 while the arc cost for 1→0 is 41. The optimal tour, of length 697, contains the arcs 2→0 and 0→1.

1	697	2	693	3	623	4	757	5	618	6	682	7	792	8	777	9	834	10	691
01	26 41	01	1 29	01	38 17	01	53 79	01	35 68	01	15 19	01	53 88	01	81 29	01	26 42	01	93 43
02	76 63	02	58 97	02	8 3	02	4 58	02	57 26	02	70 70	02	84 47	02	9 10	02	97 12	02	94 98
03	98 79	03	28 10	03	93 24	03	64 75	03	34 72	03	73 94	03	56 4	03	94 57	03	40 58	03	92 99
12	59 15	12	31 77	12	71 28	12	63 23	12	81 6	12	9 38	12	34 77	12	66 79	12	68 57	12	42 27
13	24 83	13	70 60	13	15 55	14	6 68	14	84 41	14	81 80	14	25 43	14	100 67	14	4 86	14	74 13
24	34 58	24	93 18	24	61 27	25	37 31	25	40 4	25	32 17	25	99 58	25	36 44	25	25 63	25	67 44
35	40 53	35	46 12	35	55 11	34	34 21	34	14 32	34	99 88	34	49 43	34	82 92	34	2 41	34	73 69
46	78 15	46	52 62	46	16 19	36	42 66	36	28 4	36	49 8	36	78 84	36	50 59	36	64 52	36	20 22
47	61 5	47	86 45	47	48 50	47	51 90	47	32 9	47	7 62	47	84 73	47	33 72	47	54 57	47	67 30
58	6 61	58	100 97	58	94 24	56	65 70	56	58 47	56	4 98	56	57 0	56	97 100	56	38 92	56	96 53
59	80 84	59	1 36	59	37 19	58	57 43	58	36 91	58	84 22	58	19 48	58	7 11	58	65 95	58	62 56
68	50 51	68	28 44	6A	64 6	69	68 1	69	12 12	69	2 48	69	79 40	69	44 70	69	99 5	69	15 17
6A	26 69	6A	98 69	6B	78 27	78	77 57	78	72 29	78	81 30	79	1 94	7A	9 88	7A	48 3	7A	20 67
79	99 7	7B	30 10	7C	7 38	7A	57 69	7A	54 21	7A	9 16	7A	35 8	7B	31 22	7B	90 85	7B	87 34
7B	40 7	7C	77 32	7D	80 74	8B	43 37	8B	63 29	8B	50 66	8B	53 44	89	12 6	8A	52 87	8A	89 92
8C	57 92	8D	36 98	8A	17 93	9B	63 38	9C	41 42	9C	5 95	8C	65 97	8C	97 19	8C	14 39	8C	39 40
9D	3 12	9E	17 12	8C	7 10	9C	20 12	9D	9 79	9D	88 50	9D	39 45	9D	61 96	9B	52 1	9B	19 89
AD	72 32	9F	93 11	9B	38 61	AC	83 45	AC	97 32	AE	65 72	AD	65 54	AB	7 38	9D	12 77	9D	96 7
AE	61 29	AB	41 33	9E	65 55	AD	92 8	AE	41 48	AF	23 87	AE	77 63	AD	12 49	AE	15 89	AE	8 81
BC	34 40	AE	45 46	AD	18 34	BE	98 69	BE	27 48	BC	81 65	BC	95 2	BE	81 85	BD	91 86	BF	50 7
BF	5 64	BF	0 57	BF	21 96	CF	52 76	BF	75 62	BE	63 16	BE	13 35	CE	53 39	CE	90 86	CD	6 16
CF	65 51	CD	20 92	CE	72 67	DE	55 2	DE	5 49	CF	48 49	CF	47 33	CF	75 23	CF	33 71	CE	10 4
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25	<u>95</u> <u>73</u>	25	<u>80</u> <u>68</u>	25	<u>26</u> 40	25	84 28	25	<u>31</u> 72	25	<u>15</u> 98	25	<u>14</u> 15	25	63 15	25	<u>60</u> <u>43</u>	25	<u>44</u> <u>75</u>
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36	<u>99</u> 65	36	70 84	36	4 <u>32</u>	36	<u>0</u> 72	36	73 61	36	69 59	36	35 7	36	23 <u>30</u>	36	<u>56</u> 39	36	64 1
47	<u>92</u> <u>55</u>	47	<u>48</u> 5	47	59 25	47	96 <u>68</u>	47	<u>60</u> <u>100</u>	47	<u>60</u> <u>11</u>	47	46 <u>28</u>	47	<u>90</u> 58	47	85 65	47	<u>21</u> 9
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7C	<u>48</u> 31	7C	13 79	7C	<u>97</u> <u>97</u>	7C	36 <u>56</u>	7C	<u>77</u> <u>72</u>	7C	70 92	7C	<u>81</u> <u>21</u>	7C	8 10	7C	1 88	7C	91 74
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89	<u>56</u> <u>10</u>	89	<u>56</u> <u>39</u>	89	<u>4</u> 2	89	37 95	8A	81 47	8A	<u>10</u> 17	8A	<u>86</u> 28	8A	70 9	8A	<u>85</u> <u>42</u>	8A	45 82
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9C	<u>58</u> <u>17</u>	9C	29 10	9E	6 41	9E	<u>10</u> 31	9A	<u>97</u> <u>22</u>	9C	75 <u>43</u>	9E	<u>92</u> 80	9B	<u>64</u> 68	9E	6 <u>43</u>	9A	<u>61</u> 81
AB	<u>96</u> 84	AD	47 <u>39</u>	AF	65 8	AF	15 93	9E	<u>32</u> 57	9D	<u>44</u> 18	9F	<u>99</u> <u>25</u>	9E	47 58	9F	10 49	9F	86 <u>11</u>
BE	<u>33</u> 67	BE	6 47	BC	<u>72</u> 9	BE	46 33	BC	97 3	AE	89 4	AC	82 49	AE	<u>99</u> 50	AB	65 <u>32</u>	BC	<u>25</u> 35
CF	<u>89</u> 72	BF	<u>99</u> 2	BE	<u>23</u> 27	BF	<u>35</u> 77	CF	<u>13</u> 29	BF	8 95	BD	<u>67</u> 71	BD	4 22	BD	72 64	BD	69 84
DE	67 48	CE	78 <u>61</u>	CF	11 98	CD	76 <u>26</u>	DE	80 <u>76</u>	CE	97 <u>50</u>	CE	42 <u>11</u>	CF	54 97	CE	14 22	CE	<u>67</u> 56
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EF	<u>83</u> 37	EF	32 <u>36</u>	DF	<u>60</u> 36	DF	10 <u>40</u>	EF	96 1	EF	63 <u>90</u>	EF	68 92	EF	54 <u>36</u>	EF	70 <u>30</u>	EF	66 65
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01	<u>28</u> 85	01	<u>62</u> 24	01	89 66	01	88 2	01	77 9	01	60 27	01	<u>98</u> 34	01	67 35	01	<u>92</u> 3	01	<u>100</u> <u>23</u>
02	<u>89</u> 21	02	70 42	02	<u>85</u> 70	02	<u>11</u> 96	02	<u>54</u> 86	02	<u>75</u> 38	02	<u>80</u> 36	02	<u>35</u> 20	02	<u>72</u> 51	02	7 81
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14	<u>92</u> 29	14	<u>32</u> 32	14	<u>2</u> 79	14	<u>72</u> <u>44</u>	14	<u>27</u> <u>91</u>	14	<u>57</u> <u>69</u>	14	61 85	14	<u>68</u> <u>31</u>	14	<u>36</u> <u>36</u>	14	<u>45</u> <u>17</u>
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BC	<u>91</u> 41	BD	57 6	BD	65 94	BD	56 99	BC	<u>62</u> 92	BE	73 <u>23</u>	BE	8 <u>44</u>	BF	<u>67</u> <u>72</u>	BF	64 <u>68</u>	BF	7 30
BF	87 0	CE	3 <u>14</u>	CF	<u>42</u> <u>27</u>	BE	63 87	BE	<u>95</u> 27	CF	<u>34</u> 84	BF	4 90	CD	<u>87</u> 71	DE	18 7	CE	9 99
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 8F 36 8 9C 19 15 9D 47 23 9B 18 24 9E 10 44 9E 53 29 9E 26 50 9F 70 18 9E 72 2 9D 74 66
 9C 12 10 9D 55 56 9E 83 27 9D 38 99 9E 10 44 9E 53 29 9E 26 50 9F 70 18 9E 72 2 9D 74 66
 9E 48 23 AE 0 70 AD 52 27 AE 18 93 AF 19 82 AF 62 9 AC 38 71 AC 50 38 9F 23 35 9E 40 74
 AD 63 2 BE 57 58 BE 89 49 BD 59 78 BD 45 9 BC 45 15 AE 61 38 AE 44 13 AC 27 42 AE 29 6
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 9E 5 61 9E 53 25 9F 93 36 AE 58 26 AF 32 94 AF 75 25 AE 26 33 AF 1 64 AF 12 54 9F 94 36
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 DF 37 93 DF 69 78 DF 50 52 EF 94 36 EF 39 58 EF 93 69 EF 33 54 DF 15 32 EF 48 66 DF 21 63

141	458	142	684	143	665	144	744	145	618	146	748	147	700	148	759	149	661	150	620
01	<u>6</u> 75	01	<u>21</u> 35	01	62 54	01	<u>67</u> 1	01	47 69	01	96 <u>11</u>	01	50 <u>93</u>	01	41 <u>79</u>	01	<u>60</u> 41	01	18 <u>41</u>
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14	<u>3</u> 83	14	<u>65</u> 77	14	28 <u>23</u>	14	<u>70</u> 63	14	<u>51</u> 54	14	16 86	14	59 93	14	99 <u>49</u>	14	<u>34</u> 79	14	<u>34</u> 69
25	20 <u>5</u>	25	61 <u>35</u>	25	76 35	25	57 <u>99</u>	25	17 87	25	57 <u>56</u>	25	52 <u>10</u>	25	<u>49</u> 60	25	66 <u>74</u>	25	<u>36</u> 82
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37	<u>80</u> 44	37	27 <u>2</u>	37	<u>13</u> 27	37	<u>20</u> 46	37	72 34	37	<u>63</u> 70	37	28 2	37	<u>16</u> 62	37	<u>68</u> 97	37	44 <u>75</u>
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7D	<u>25</u> 71	7D	41 94	7D	57 44	7D	84 92	7D	5 2	7D	<u>33</u> 7	7D	<u>93</u> 64	7D	25 33	7D	3 53	7C	48 <u>50</u>
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9C	22 <u>6</u>	9E	0 <u>58</u>	9E	81 <u>16</u>	9B	<u>57</u> 78	9C	<u>21</u> 44	9E	<u>38</u> 48	9F	31 77	9F	12 17	9F	<u>14</u> 34	9B	97 <u>35</u>
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AF	47 <u>15</u>	AE	<u>36</u> 95	AE	22 88	AF	<u>100</u> 62	AF	34 78	AF	42 <u>10</u>	AD	91 40	AD	66 59	AF	<u>32</u> 70	AE	<u>16</u> 70
BD	20 <u>34</u>	BC	82 71	BC	48 81	BE	<u>6</u> 54	BC	92 29	BE	80 <u>15</u>	BC	<u>67</u> 80	BE	10 74	BD	70 <u>1</u>	BE	89 <u>68</u>
BF	53 65	BD	84 <u>39</u>	BF	<u>66</u> 97	CD	<u>1</u> 18	BF	7 <u>18</u>	BF	15 93	BF	70 <u>1</u>	BF	<u>7</u> 56	BE	16 82	CF	46 <u>2</u>
DE	74 25	DF	23 <u>87</u>	DE	<u>61</u> 64	DF	<u>24</u> 54	DE	18 5	CE	94 40	DE	<u>16</u> 29	CE	<u>80</u> 74	CE	<u>77</u> 12	DF	<u>32</u> 85
EF	<u>46</u> 3	EF	80 17	DF	66 <u>16</u>	EF	42 9	DF	<u>18</u> 65	DF	<u>60</u> 2	EF	<u>88</u> 48	DF	5 <u>58</u>	DF	13 82	EF	18 80

151	563	152	657	153	713	154	620	155	658	156	630	157	698	158	710	159	640	160	641
01	52 29	01	70 12	01	<u>63</u> 66	01	<u>43</u> 14	01	69 85	01	84 <u>1</u>	01	92 <u>37</u>	01	28 55	01	79 <u>23</u>	01	9 66
02	<u>84</u> 86	02	22 <u>8</u>	02	91 34	02	46 69	02	<u>11</u> 93	02	46 82	02	<u>93</u> 96	02	7 24	02	52 74	02	94 88
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14	<u>24</u> 77	14	75 <u>3</u>	14	85 40	14	2 9	14	<u>70</u> 59	14	43 68	14	92 <u>29</u>	14	<u>29</u> 95	14	55 68	14	90 39
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37	80 31	37	<u>74</u> 96	37	66 <u>7</u>	37	69 66	37	21 <u>26</u>	37	44 55	37	<u>68</u> 39	37	41 18	37	51 50	37	60 <u>3</u>
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6C	32 64	6C	93 <u>54</u>	6C	95 <u>1</u>	6C	71 <u>53</u>	6C	88 <u>19</u>	6C	64 0	6C	54 <u>76</u>	6C	95 80	6C	<u>36</u> 65	6C	<u>70</u> 3
7A	88 <u>40</u>	7A	2 52	7A	3 <u>83</u>	7A	8 32	7A	8 83	7A	94 68	7A	40 78	7C	9 38	7D	<u>19</u> 19	7D	59 <u>28</u>
7C	<u>98</u> 8	7C	84 5	7D	71 20	7D	98 <u>72</u>	7D	29 57	7D	64 <u>93</u>	7D	<u>43</u> 17	7D	41 <u>50</u>	7E	88 <u>50</u>	7E	32 49
8D	73 <u>21</u>	8D	42 92	8C	95 22	8D	<u>54</u> 35	8D	<u>27</u> 24	8D	29 82	8E	61 <u>87</u>	8E	91 <u>47</u>	8D	0 68	8D	24 98
9B	<u>85</u> 95	9D	86 <u>31</u>	9B	94 26	9B	93 <u>63</u>	9B	65 10	9C	<u>55</u> 9	9C	<u>12</u> 12	9D	87 5	9C	73 35	9E	86 <u>93</u>
9D	58 59	9E	9 10	9E	5 83	9C	21 62	9E	<u>90</u> 43	9E	73 24	9F	35 6	9F	<u>13</u> 58	9F	<u>42</u> 98	9F	22 32
AE	63 2	AE	68 95	AE	28 <u>52</u>	AE	<u>79</u> 59	AE	28 4	AE	<u>2</u> 86	AF	<u>47</u> 89	AD	<u>55</u> 85	AC	25 <u>92</u>	AC	82 <u>76</u>
BF	58 37	BD	<u>57</u> 45	BD	9 96	BF	11 49	BF	68 <u>24</u>	BE	57 <u>21</u>	BD	94 7	AF	1 16	AE	<u>56</u> 34	AD	<u>3</u> 93
CF	<u>63</u> 36	BF	42 48	CF	<u>93</u> 96	CF	<u>77</u> 21	CF	<u>20</u> 39	BF	59 84	BE	<u>36</u> 67	BE	70 47	BD	33 23	BC	16 64
DE	97 <u>0</u>	CF	18 <u>34</u>	DF	<u>59</u> 38	DE	83 63	CF	52 61	CF	<u>63</u> 24	CE	68 29	BF	83 <u>76</u>	BF	2 <u>14</u>	BF	<u>17</u> 63
EF	22 <u>41</u>	EF	<u>18</u> 67	EF	39 83	EF	<u>64</u> 26	DF	<u>48</u> 97	DF	29 <u>62</u>	DF	97 46	CE	<u>51</u> 51	EF	86 47	EF	95 <u>22</u>

161	634	162	606	163	730	164	703	165	709	166	703	167	618	168	569	169	577	170	455
01	<u>71</u> 64	01	26 <u>6</u>	01	74 33	01	51 <u>32</u>	01	77 6	01	61 <u>41</u>	01	<u>7</u> 42	01	63 52	01	77 <u>11</u>	01	17 79
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14	<u>60</u> 86	14	77 82	14	74 <u>56</u>	14	95 97	14	<u>55</u> 9	14	27 <u>20</u>	14	65 96	14	<u>20</u> 82	14	98 <u>22</u>	14	<u>5</u> 41
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9B	25	60	9B	54	81	9E	94	92	9D	66	16	9E	32	91	9F	25	78	9F	79	1	9C	63	16	9B	55	35	9E	76	41
9E	98	36	9E	18	10	9F	93	83	AE	88	10	AD	75	49	AC	45	27	AC	65	58	AD	39	57	AE	84	23	AD	95	33
BF	30	17	AD	27	76	AE	56	99	BF	26	23	AE	94	47	AE	44	27	AE	83	61	AE	21	58	AF	24	6	AF	9	85
CD	84	24	BF	5	84	BD	92	37	CD	23	63	BE	5	65	BD	87	88	BD	21	85	BE	40	69	BD	34	5	BE	72	11
CE	1	86	CF	0	19	BF	27	7	CF	69	90	BF	21	27	BE	5	13	BF	96	83	CF	75	19	CE	1	29	BF	100	29
DF	8	100	DE	65	56	CF	44	22	DE	31	48	CF	15	56	CF	7	78	CF	77	32	DF	30	33	CF	2	88	CF	16	41
EF	10	81	EF	92	51	DE	63	6	EF	36	11	DF	79	50	DF	97	5	DE	37	12	EF	31	45	DF	68	39	DE	30	50

181	716	182	777	183	620	184	717	185	652	186	689	187	792	188	559	189	579	190	781										
01	87	82	01	81	66	01	30	16	01	13	99	01	86	8	01	69	42	01	86	51	01	50	8	01	74	60	01	24	27
02	2	40	02	40	17	02	62	41	02	31	11	02	54	63	02	77	13	02	72	91	02	25	12	02	25	12	02	99	9
03	17	11	03	44	76	03	56	42	03	26	31	03	36	46	03	37	95	03	31	38	03	30	24	03	15	5	03	92	6
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15	18	47	15	61	76	15	20	21	15	81	27	15	69	34	15	44	66	15	60	94	15	41	14	15	9	83	15	74	25
24	82	86	24	68	48	24	24	19	24	54	91	24	99	35	24	80	85	24	83	48	24	27	64	24	49	99	24	33	53
26	84	91	26	19	13	26	46	93	26	54	23	26	3	18	26	55	86	26	55	12	26	42	45	26	5	69	26	72	83
37	29	1	37	67	31	37	84	18	37	99	50	37	3	81	37	14	41	37	6	77	37	60	31	37	74	78	37	90	91
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5A	1	79	5A	34	74	5A	26	6	5A	7	50	5A	22	52	5A	16	74	5A	50	26	5B	95	10	5B	25	58	5B	94	44
6A	99	59	6A	94	88	6A	23	87	6A	83	61	6A	29	67	6B	28	92	6B	77	95	6A	0	3	6A	4	8	6C	74	31
6B	81	29	6B	15	17	6B	25	86	6B	86	94	6B	15	60	6C	90	31	6C	48	92	6C	79	43	6C	46	53	6D	70	33
7C	18	70	7C	55	48	7C	24	95	7C	89	32	7C	84	79	7B	2	74	7D	4	87	79	7	85	79	60	36	7A	81	83
89	73	65	8B	86	81	8C	51	93	8C	48	25	8D	78	54	8D	86	72	8B	42	36	7B	26	12	7B	76	44	7C	97	64
8D	52	92	8D	94	34	8D	55	76	8D	16	36	8E	99	77	8E	19	15	8E	65	83	8C	81	2	8C	95	1	8B	11	96
9E	33	50	9D	45	73	9B	19	77	9B	47	9	9B	93	23	9C	34	19	9C	66	45	8D	6	40	8D	5	70	8E	67	38
AF	42	57	9E	81	21	9E	84	10	9E	25	54	9D	58	70	9D	44	46	9E	1	14	9D	57	34	9E	66	63	9E	10	43
BC	35	34	AF	62	6	AD	35	27	AF	67	94	AE	37	19	AC	53	60	AB	45	60	AE	37	9	AD	22	2	9F	19	50
BD	54	62	BE	63	75	BF	32	92	BD	21	88	BC	1	47	AE	52	63	AF	54	76	BF	7	66	BF	23	32	AD	25	92
CE	11	87	CD	7	90	CF	68	31	CE	67	78	CF	26	8	BF	97	61	CF	41	77	CF	42	19	CF	89	66	BF	91	93
DF	4	66	CF	74	30	DE	31	15	DF	72	100	DF	24	14	DF	26	18	DE	59	39	DE	87	59	DE	75	20	CE	55	61
EF	57	74	EF	45	31	EF	34	86	EF	15	44	EF	16	22	EF	36	33	DF	70	40	EF	18	97	EF	26	74	DF	45	97

191	624	192	665	193	707	194	693	195	519	196	676	197	712	198	844	199	665	200	647										
01	86	54	01	34	98	01	26	83	01	91	64	01	72	23	01	39	44	01	76	61	01	78	91	01	16	15	01	17	74
02	43	48	02	53	88	02	16	12	02	37	41	02	31	4	02	44	37	02	31	20	02	75	65	02	63	100	02	96	86
03	97	11	03	75	37	03	10	65	03	43	41	03	29	22	03	99	8	03	94	97	03	7	51	03	97	64	03	98	91
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15	98	46	15	72	7	15	81	12	15	39	48	15	3	17	15	91	42	15	84	15	15	86	30	15	60	97	15	90	94
26	68	26	26	87	62	26	22	9	26	28	74	26	58	29	26	19	48	26	59	47	26	81	59	26	1	30	26	97	4
27	68	5	27	21	77	27	26	7	27	91	18	27	86	23	27	67	58	27	98	77	27	36	84	27	89	81	27	35	2
38	6	41	38	16	97	38	69	90																					

201	2072	202	2108	203	2150	204	2148	205	2065	206	2101	207	2095	208	2085	209	2094	210	2201
01	<u>20</u> <u>33</u>	01	<u>57</u> <u>10</u>	01	<u>46</u> <u>53</u>	01	<u>89</u> <u>40</u>	01	<u>62</u> <u>30</u>	01	<u>57</u> <u>46</u>	01	<u>92</u> <u>15</u>	01	<u>59</u> <u>62</u>	01	<u>6</u> <u>40</u>	01	<u>0</u> <u>24</u>
02	<u>80</u> <u>4</u>	02	<u>61</u> <u>33</u>	02	<u>72</u> <u>93</u>	02	<u>52</u> <u>38</u>	02	<u>10</u> <u>73</u>	02	<u>98</u> <u>49</u>	02	<u>13</u> <u>2</u>	02	<u>46</u> <u>26</u>	02	<u>8</u> <u>53</u>	02	<u>58</u> <u>69</u>
03	<u>4</u> <u>40</u>	03	<u>14</u> <u>11</u>	03	<u>61</u> <u>68</u>	03	<u>44</u> <u>27</u>	03	<u>84</u> <u>55</u>	03	<u>1</u> <u>93</u>	03	<u>48</u> <u>36</u>	03	<u>20</u> <u>32</u>	03	<u>38</u> <u>41</u>	03	<u>55</u> <u>73</u>
12	<u>85</u> <u>60</u>	12	<u>24</u> <u>43</u>	12	<u>94</u> <u>12</u>	12	<u>81</u> <u>58</u>	12	<u>38</u> <u>54</u>	12	<u>25</u> <u>35</u>	12	<u>55</u> <u>50</u>	12	<u>92</u> <u>77</u>	12	<u>57</u> <u>50</u>	12	<u>2</u> <u>66</u>
13	<u>10</u> <u>28</u>	13	<u>11</u> <u>63</u>	13	<u>43</u> <u>21</u>	13	<u>85</u> <u>64</u>	13	<u>4</u> <u>13</u>	13	<u>21</u> <u>64</u>	13	<u>98</u> <u>22</u>	13	<u>33</u> <u>44</u>	13	<u>100</u> <u>59</u>	13	<u>29</u> <u>39</u>
24	<u>68</u> <u>12</u>	24	<u>66</u> <u>56</u>	24	<u>54</u> <u>66</u>	24	<u>5</u> <u>61</u>	24	<u>54</u> <u>23</u>	24	<u>48</u> <u>47</u>	24	<u>56</u> <u>13</u>	24	<u>95</u> <u>18</u>	24	<u>58</u> <u>48</u>	24	<u>71</u> <u>19</u>
35	<u>80</u> <u>64</u>	35	<u>95</u> <u>54</u>	35	<u>86</u> <u>17</u>	35	<u>71</u> <u>83</u>	35	<u>8</u> <u>14</u>	35	<u>39</u> <u>26</u>	35	<u>46</u> <u>60</u>	35	<u>56</u> <u>57</u>	35	<u>75</u> <u>89</u>	35	<u>37</u> <u>66</u>
45	<u>64</u> <u>63</u>	45	<u>86</u> <u>63</u>	45	<u>28</u> <u>62</u>	45	<u>97</u> <u>85</u>	45	<u>98</u> <u>26</u>	45	<u>99</u> <u>20</u>	45	<u>80</u> <u>42</u>	45	<u>85</u> <u>59</u>	45	<u>70</u> <u>15</u>	45	<u>61</u> <u>78</u>
46	<u>17</u> <u>26</u>	46	<u>16</u> <u>72</u>	47	<u>48</u> <u>68</u>	47	<u>22</u> <u>1</u>	47	<u>74</u> <u>94</u>	47	<u>39</u> <u>88</u>	47	<u>44</u> <u>73</u>	47	<u>95</u> <u>13</u>	47	<u>63</u> <u>3</u>	47	<u>53</u> <u>52</u>
57	<u>23</u> <u>39</u>	57	<u>63</u> <u>56</u>	56	<u>89</u> <u>93</u>	56	<u>72</u> <u>9</u>	56	<u>5</u> <u>46</u>	56	<u>20</u> <u>71</u>	58	<u>90</u> <u>94</u>	58	<u>30</u> <u>13</u>	58	<u>17</u> <u>8</u>	58	<u>80</u> <u>77</u>
68	<u>40</u> <u>92</u>	68	<u>32</u> <u>67</u>	58	<u>37</u> <u>75</u>	58	<u>85</u> <u>80</u>	58	<u>2</u> <u>69</u>	58	<u>100</u> <u>76</u>	59	<u>30</u> <u>73</u>	59	<u>51</u> <u>81</u>	59	<u>32</u> <u>89</u>	59	<u>90</u> <u>95</u>
69	<u>18</u> <u>59</u>	69	<u>1</u> <u>25</u>	69	<u>55</u> <u>52</u>	69	<u>21</u> <u>79</u>	69	<u>36</u> <u>97</u>	69	<u>77</u> <u>11</u>	67	<u>84</u> <u>99</u>	67	<u>38</u> <u>87</u>	67	<u>94</u> <u>50</u>	67	<u>73</u> <u>29</u>
7A	<u>57</u> <u>43</u>	7A	<u>75</u> <u>29</u>	7A	<u>24</u> <u>19</u>	7A	<u>12</u> <u>26</u>	7A	<u>61</u> <u>74</u>	7A	<u>22</u> <u>82</u>	6A	<u>17</u> <u>47</u>	6A	<u>90</u> <u>98</u>	6A	<u>87</u> <u>19</u>	6A	<u>78</u> <u>81</u>
7B	<u>41</u> <u>27</u>	7B	<u>11</u> <u>31</u>	7B	<u>24</u> <u>94</u>	7B	<u>9</u> <u>21</u>	7B	<u>92</u> <u>15</u>	7B	<u>56</u> <u>27</u>	7B	<u>74</u> <u>7</u>	7B	<u>16</u> <u>69</u>	7B	<u>77</u> <u>22</u>	7B	<u>58</u> <u>21</u>
8C	<u>30</u> <u>67</u>	8C	<u>68</u> <u>28</u>	8C	<u>56</u> <u>90</u>	8C	<u>66</u> <u>21</u>	8C	<u>2</u> <u>97</u>	8C	<u>16</u> <u>80</u>	8C	<u>60</u> <u>55</u>	8C	<u>44</u> <u>29</u>	8C	<u>48</u> <u>12</u>	8C	<u>74</u> <u>21</u>
8D	<u>40</u> <u>75</u>	8D	<u>14</u> <u>81</u>	8D	<u>40</u> <u>70</u>	8D	<u>59</u> <u>63</u>	8D	<u>33</u> <u>99</u>	8D	<u>59</u> <u>31</u>	8D	<u>87</u> <u>1</u>	8D	<u>12</u> <u>10</u>	8D	<u>84</u> <u>47</u>	8D	<u>13</u> <u>55</u>
9E	<u>73</u> <u>44</u>	9E	<u>90</u> <u>16</u>	9E	<u>26</u> <u>58</u>	9E	<u>71</u> <u>84</u>	9E	<u>47</u> <u>93</u>	9E	<u>52</u> <u>76</u>	9E	<u>34</u> <u>26</u>	9E	<u>47</u> <u>46</u>	9E	<u>17</u> <u>47</u>	9E	<u>98</u> <u>100</u>
9F	<u>32</u> <u>97</u>	9F	<u>11</u> <u>45</u>	9F	<u>35</u> <u>90</u>	9F	<u>13</u> <u>75</u>	9F	<u>17</u> <u>31</u>	9F	<u>87</u> <u>89</u>	9F	<u>62</u> <u>59</u>	9F	<u>10</u> <u>22</u>	9F	<u>70</u> <u>34</u>	9F	<u>59</u> <u>10</u>
AC	<u>82</u> <u>78</u>	AC	<u>97</u> <u>99</u>	AC	<u>39</u> <u>0</u>	AC	<u>3</u> <u>84</u>	AC	<u>27</u> <u>16</u>	AC	<u>36</u> <u>94</u>	AC	<u>7</u> <u>8</u>	AC	<u>93</u> <u>6</u>	AC	<u>18</u> <u>87</u>	AC	<u>93</u> <u>99</u>
AE	<u>100</u> <u>34</u>	AE	<u>26</u> <u>58</u>	AE	<u>5</u> <u>19</u>	AE	<u>40</u> <u>78</u>	AE	<u>5</u> <u>81</u>	AE	<u>51</u> <u>0</u>	AE	<u>51</u> <u>5</u>	AE	<u>36</u> <u>18</u>	AE	<u>10</u> <u>77</u>	AE	<u>91</u> <u>76</u>
BD	<u>28</u> <u>54</u>	BD	<u>96</u> <u>35</u>	BD	<u>32</u> <u>83</u>	BD	<u>67</u> <u>39</u>	BD	<u>69</u> <u>47</u>	BD	<u>20</u> <u>28</u>	BD	<u>81</u> <u>68</u>	BD	<u>48</u> <u>77</u>	BD	<u>81</u> <u>12</u>	BD	<u>36</u> <u>44</u>
BF	<u>12</u> <u>98</u>	BF	<u>24</u> <u>67</u>	BF	<u>39</u> <u>59</u>	BF	<u>34</u> <u>46</u>	BF	<u>64</u> <u>22</u>	BF	<u>17</u> <u>32</u>	BF	<u>38</u> <u>26</u>	BF	<u>96</u> <u>37</u>	BF	<u>40</u> <u>32</u>	BF	<u>18</u> <u>35</u>
CF	<u>77</u> <u>28</u>	CF	<u>82</u> <u>73</u>	CF	<u>19</u> <u>75</u>	CF	<u>93</u> <u>43</u>	CF	<u>85</u> <u>27</u>	CF	<u>60</u> <u>47</u>	CF	<u>68</u> <u>33</u>	CF	<u>67</u> <u>86</u>	CF	<u>65</u> <u>32</u>	CF	<u>18</u> <u>37</u>
DE	<u>16</u> <u>62</u>	DE	<u>55</u> <u>83</u>	DE	<u>34</u> <u>16</u>	DE	<u>35</u> <u>61</u>	DE	<u>33</u> <u>96</u>	DE	<u>99</u> <u>6</u>	DE	<u>25</u> <u>60</u>	DE	<u>74</u> <u>43</u>	DE	<u>83</u> <u>23</u>	DE	<u>59</u> <u>2</u>
211	2016	212	2179	213	2138	214	2117	215	2108	216	2047	217	1966	218	2009	219	2121	220	1939
01	<u>46</u> <u>60</u>	01	<u>38</u> <u>86</u>	01	<u>97</u> <u>32</u>	01	<u>1</u> <u>88</u>	01	<u>22</u> <u>43</u>	01	<u>47</u> <u>38</u>	01	<u>13</u> <u>43</u>	01	<u>45</u> <u>1</u>	01	<u>51</u> <u>64</u>	01	<u>9</u> <u>81</u>
02	<u>32</u> <u>58</u>	02	<u>10</u> <u>24</u>	02	<u>87</u> <u>68</u>	02	<u>42</u> <u>49</u>	02	<u>1</u> <u>75</u>	02	<u>45</u> <u>75</u>	02	<u>22</u> <u>44</u>	02	<u>6</u> <u>54</u>	02	<u>21</u> <u>56</u>	02	<u>76</u> <u>26</u>
03	<u>69</u> <u>17</u>	03	<u>79</u> <u>66</u>	03	<u>70</u> <u>79</u>	03	<u>3</u> <u>50</u>	03	<u>29</u> <u>4</u>	03	<u>33</u> <u>44</u>	03	<u>61</u> <u>78</u>	03	<u>81</u> <u>68</u>	03	<u>1</u> <u>64</u>	03	<u>91</u> <u>5</u>
12	<u>2</u> <u>88</u>	12	<u>56</u> <u>63</u>	12	<u>5</u> <u>13</u>	12	<u>56</u> <u>73</u>	12	<u>48</u> <u>75</u>	12	<u>43</u> <u>43</u>	12	<u>30</u> <u>99</u>	12	<u>72</u> <u>93</u>	12	<u>88</u> <u>22</u>	12	<u>49</u> <u>2</u>
13	<u>89</u> <u>77</u>	13	<u>87</u> <u>60</u>	13	<u>74</u> <u>51</u>	13	<u>46</u> <u>33</u>	13	<u>34</u> <u>24</u>	13	<u>84</u> <u>47</u>	13	<u>21</u> <u>89</u>	13	<u>55</u> <u>35</u>	13	<u>8</u> <u>58</u>	13	<u>50</u> <u>62</u>
24	<u>71</u> <u>19</u>	24	<u>29</u> <u>11</u>	24	<u>48</u> <u>51</u>	24	<u>20</u> <u>17</u>	24	<u>75</u> <u>15</u>	24	<u>6</u> <u>2</u>	24	<u>66</u> <u>11</u>	24	<u>23</u> <u>12</u>	24	<u>56</u> <u>78</u>	24	<u>17</u> <u>81</u>
35	<u>8</u> <u>98</u>	35	<u>87</u> <u>76</u>	35	<u>32</u> <u>29</u>	35	<u>45</u> <u>16</u>	35	<u>97</u> <u>19</u>	35	<u>56</u> <u>88</u>	35	<u>12</u> <u>30</u>	35	<u>9</u> <u>86</u>	35	<u>17</u> <u>87</u>	35	<u>32</u> <u>67</u>
46	<u>92</u> <u>24</u>	46	<u>32</u> <u>48</u>	46	<u>43</u> <u>100</u>	46	<u>5</u> <u>29</u>	46	<u>83</u> <u>99</u>	46	<u>2</u> <u>6</u>	46	<u>86</u> <u>17</u>	46	<u>42</u> <u>24</u>	46	<u>58</u> <u>92</u>	46	<u>65</u> <u>93</u>
47	<u>47</u> <u>41</u>	47	<u>39</u> <u>10</u>	47	<u>83</u> <u>77</u>	47	<u>44</u> <u>96</u>	47	<u>53</u> <u>37</u>	47	<u>12</u> <u>44</u>	47	<u>76</u> <u>4</u>	47	<u>48</u> <u>97</u>	47	<u>97</u> <u>78</u>	47	<u>3</u> <u>64</u>
58	<u>71</u> <u>14</u>	58	<u>27</u> <u>93</u>	58	<u>12</u> <u>29</u>	58	<u>39</u> <u>14</u>	58	<u>46</u> <u>27</u>	58	<u>26</u> <u>36</u>	58	<u>10</u> <u>84</u>	58	<u>34</u> <u>10</u>	58	<u>56</u> <u>62</u>	58	<u>94</u> <u>27</u>
59	<u>31</u> <u>2</u>	59	<u>26</u> <u>61</u>	59	<u>63</u> <u>57</u>	59	<u>24</u> <u>49</u>	59	<u>95</u> <u>46</u>	59	<u>9</u> <u>11</u>	59	<u>18</u> <u>63</u>	59	<u>17</u> <u>29</u>	59	<u>48</u> <u>53</u>	59	<u>39</u> <u>0</u>
67	<u>26</u> <u>56</u>	67	<u>77</u> <u>54</u>	67	<u>72</u> <u>15</u>	67	<u>50</u> <u>61</u>	67	<u>82</u> <u>1</u>	68	<u>72</u> <u>39</u>	68	<u>98</u> <u>17</u>	68	<u>50</u> <u>89</u>	68	<u>9</u> <u>1</u>	68	<u>58</u> <u>44</u>
6A	<u>10</u> <u>17</u>	6A	<u>66</u> <u>42</u>	6A	<u>7</u> <u>3</u>	6A	<u>73</u> <u>42</u>	6A	<u>49</u> <u>24</u>	6A	<u>27</u> <u>16</u>	6A	<u>78</u> <u>77</u>	6A	<u>62</u> <u>98</u>	6A	<u>81</u> <u>4</u>	6A	<u>75</u> <u>18</u>
7B	<u>15</u> <u>14</u>	7B	<u>54</u> <u>3</u>	7B	<u>3</u> <u>70</u>	7B	<u>99</u> <u>7</u>	7B	<u>81</u> <u>14</u>	7B	<u>43</u> <u>44</u>	7B	<u>16</u> <u>93</u>	7B	<u>85</u> <u>19</u>	7B	<u>47</u> <u>32</u>	7B	<u>14</u> <u>3</u>
8C	<u>7</u> <u>79</u>	8C	<u>78</u> <u>19</u>	8C	<u>91</u> <u>10</u>	8C	<u>95</u> <u>64</u>	8C	<u>2</u> <u>73</u>	7B	<u>62</u> <u>80</u>	7B	<u>12</u> <u>3</u>	7B	<u>85</u> <u>98</u>	7B	<u>79</u> <u>72</u>	7B	<u>66</u> <u>13</u>
8D	<u>68</u> <u>37</u>	8D	<u>85</u> <u>4</u>	8D	<u>46</u> <u>9</u>	8D	<u>46</u> <u>17</u>	8D	<u>19</u> <u>17</u>	8B	<u>52</u> <u>58</u>	8B	<u>78</u> <u>21</u>	8B	<u>32</u> <u>42</u>	8B	<u>53</u> <u>83</u>	8B	<u>23</u> <u>27</u>
9E	<u>75</u> <u>26</u>	9E	<u>64</u> <u>36</u>	9E	<u>43</u> <u>48</u>	9E	<u>66</u> <u>77</u>	9E	<u>87</u> <u>69</u>	9A	<u>84</u> <u>74</u>	9A	<u>58</u> <u>25</u>	9A	<u>87</u> <u>15</u>	9A	<u>28</u> <u>15</u>	9A	<u>88</u> <u>0</u>
9F	<u>25</u> <u>3</u>	9F	<u>74</u> <u>34</u>	9F	<u>92</u> <u>83</u>	9F	<u>69</u> <u>97</u>	9F	<u>22</u> <u>22</u>	AC	<u>14</u> <u>92</u>	AC	<u>65</u> <u>79</u>	AC	<u>22</u> <u>33</u>	AC	<u>73</u> <u>63</u>	AC	<u>81</u> <u>10</u>
AC	<u>32</u> <u>81</u>	AC	<u>88</u> <u>30</u>	AC	<u>26</u> <u>64</u>	AC	<u>16</u> <u>67</u>	AC	<u>45</u> <u>25</u>	BD	<u>64</u> <u>67</u>	BD	<u>0</u> <u>40</u>	BD	<u>38</u> <u>91</u>	BD	<u>0</u> <u>10</u>	BD	<u>78</u> <u>23</u>
AE	<u>12</u> <u>79</u>	AE	<u>38</u> <u>30</u>	AE	<u>62</u> <u>69</u>	AE	<u>86</u> <u>63</u>	AE	<u>73</u> <u>96</u>	CE	<u>33</u> <u>11</u>	CE	<u>26</u> <u>97</u>	CE	<u>78</u> <u>10</u>	CE	<u>2</u> <u>76</u>	CE	<u>11</u> <u>3</u>
BD	<u>31</u> <u>89</u>	BD	<u>55</u> <u>77</u>	BD	<u>84</u> <u>85</u>	BD	<u>89</u> <u>8</u>	BD	<u>87</u> <u>87</u>	CF	<u>49</u> <u>16</u>	CF	<u>42</u> <u>63</u>	CF	<u>54</u> <u>8</u>	CF	<u>54</u> <u>44</u>	CF	<u>59</u> <u>7</u>
BF	<u>19</u> <u>25</u>																		

231	2074	232	2183	233	2078	234	2047	235	2157	236	2062	237	2054	238	2039	239	2119	240	2084
01	<u>37</u> 94	01	56 14	01	54 <u>25</u>	01	27 <u>25</u>	01	<u>5</u> 49	01	<u>32</u> 20	01	<u>10</u> 98	01	4 84	01	<u>46</u> 54	01	48 <u>24</u>
02	6 <u>5</u>	02	65 8	02	<u>57</u> 88	02	<u>36</u> 5	02	47 <u>10</u>	02	53 79	02	70 78	02	23 <u>84</u>	02	60 <u>16</u>	02	58 58
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12	28 42	12	31 79	12	64 97	12	67 30	12	84 14	12	<u>7</u> 52	12	<u>32</u> 81	12	<u>10</u> 75	12	61 62	12	78 <u>0</u>
13	<u>2</u> 86	13	64 <u>84</u>	13	49 <u>71</u>	13	70 <u>13</u>	14	68 49	14	9 72	14	22 66	14	81 48	14	<u>1</u> 21	14	79 54
24	28 <u>60</u>	24	11 <u>81</u>	24	69 66	24	<u>3</u> 49	25	<u>1</u> <u>56</u>	25	<u>62</u> 33	25	<u>93</u> 42	25	22 79	25	42 <u>32</u>	25	14 <u>84</u>
35	<u>41</u> 73	35	80 32	35	92 <u>40</u>	35	16 <u>63</u>	34	50 <u>82</u>	34	43 9	34	90 <u>21</u>	34	<u>43</u> 74	34	75 <u>17</u>	34	89 16
46	40 <u>47</u>	46	94 <u>51</u>	46	<u>50</u> 52	46	3 65	35	<u>31</u> 43	36	54 15	36	55 29	36	23 82	36	<u>87</u> 95	36	69 <u>30</u>
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58	<u>37</u> 17	58	<u>51</u> 2	58	36 43	58	80 48	57	14 81	57	49 80	57	<u>63</u> 74	56	81 <u>23</u>	56	23 27	56	99 92
59	25 99	59	31 <u>11</u>	59	74 <u>14</u>	59	71 29	68	97 <u>43</u>	58	<u>16</u> 29	58	47 42	58	<u>58</u> 69	58	35 <u>40</u>	58	69 <u>14</u>
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7C	<u>18</u> 11	7C	37 <u>28</u>	7C	64 37	7C	85 45	7B	<u>77</u> 82	7B	2 <u>46</u>	7B	<u>7</u> 37	7B	6 99	7B	<u>23</u> 99	7B	41 1
7D	83 <u>6</u>	7D	<u>60</u> 78	7D	<u>22</u> 37	7D	<u>31</u> 75	8C	71 <u>56</u>	8C	56 85	8C	10 <u>26</u>	8C	<u>2</u> 1	8C	16 <u>55</u>	8C	70 100
8A	<u>88</u> 43	8A	<u>77</u> 50	8A	68 <u>14</u>	8A	42 85	8D	<u>57</u> 80	8D	69 76	8D	<u>0</u> 44	8D	<u>79</u> 92	8D	91 47	8D	11 3
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9E	74 <u>8</u>	9E	81 54	9E	18 <u>1</u>	9E	<u>0</u> 74	9F	<u>29</u> 47	9F	<u>7</u> 49	9F	92 14	9F	77 77	9F	39 78	9F	74 54
9F	<u>26</u> 13	9F	44 <u>9</u>	9F	44 3	9F	49 <u>59</u>	AC	42 98	AC	<u>18</u> 78	AC	57 90	AC	83 61	AC	24 28	AC	<u>12</u> 77
AD	<u>7</u> 57	AD	75 87	AD	68 71	AD	37 65	AE	31 73	AE	87 35	AE	85 57	AE	<u>6</u> 79	AE	89 <u>25</u>	AE	25 25
BC	18 <u>43</u>	BC	45 48	BC	4 <u>17</u>	BC	54 26	BD	<u>41</u> 79	BD	31 95	BD	32 50	BD	<u>29</u> 57	BD	62 4	BD	<u>14</u> 99
BE	<u>49</u> 86	BE	53 <u>48</u>	BE	<u>20</u> 40	BE	32 <u>28</u>	BF	7 24	BF	85 <u>6</u>	BF	<u>0</u> 92	BF	58 <u>13</u>	BF	<u>25</u> 58	BF	35 <u>49</u>
DF	82 97	DF	<u>13</u> 26	DF	94 <u>25</u>	DF	<u>32</u> 56	CF	72 <u>18</u>	CF	81 14	CF	24 <u>11</u>	CF	5 68	CF	67 <u>21</u>	CF	<u>37</u> 66
EF	23 91	EF	86 49	EF	93 31	EF	39 43	DE	<u>25</u> 43	DE	<u>71</u> 16	DE	<u>46</u> 74	DE	79 63	DE	<u>48</u> 86	DE	9 69
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01	85 8	01	<u>26</u> 50	01	21 <u>22</u>	01	20 69	01	87 51	01	88 8	01	88 33	01	21 81	01	20 84	01	28 48
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03	86 <u>73</u>	03	98 <u>57</u>	03	50 65	03	39 <u>30</u>	03	<u>31</u> 8	03	13 23	03	<u>17</u> 17	03	<u>70</u> 88	03	7 93	03	25 <u>44</u>
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14	<u>5</u> 61	14	86 67	14	42 35	14	91 17	14	58 68	14	12 <u>20</u>	14	64 <u>20</u>	14	19 <u>58</u>	14	37 <u>4</u>	14	<u>42</u> 89
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8D	99 <u>7</u>	8D	<u>54</u> 67	8D	93 <u>36</u>	8D	3 <u>59</u>	8D	74 72	8D	<u>13</u> 5	8D	98 <u>48</u>	8D	<u>28</u> 8	8D	<u>32</u> 53	8D	8 <u>14</u>
9E	18 84	9E	96 61	9E	<u>59</u> 71	9E	<u>12</u> 43	9E	87 <u>68</u>	9E	<u>70</u> 81	9E	78 66	9E	51 70	9E	53 <u>73</u>	9E	<u>10</u> 47
9F	<u>9</u> 24	9F	<u>54</u> 72	9F	84 57	9F	31 31	9F	20 61	9F	92 <u>6</u>	9F	55 <u>37</u>	9F	<u>2</u> <u>42</u>	9F	68 <u>2</u>	9F	99 55
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CF	57 <u>16</u>	CF	63 <u>21</u>	CF	<u>13</u> 16	CF	<u>77</u> 52	CF	<u>1</u> 39	CF	36 23	CF	<u>44</u> 41	CF	<u>51</u> 17	CF	<u>15</u> 90	CF	91 <u>4</u>
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14	50 92	14	<u>95</u> 60	14	11 <u>35</u>	14	<u>73</u> 26	14	15 52	14	36 80	14	<u>7</u> 37	14	13 <u>20</u>	14	<u>28</u> 92	14	89 <u>67</u>
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47	94 <u>75</u>	47	<u>43</u> 38	47	98 86	47	<u>7</u> 81	47	<u>9</u> 98	47	83 <u>20</u>	47	<u>23</u> 73	47	65 <u>12</u>	47	<u>85</u> 83	47	92 92
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67	<u>54</u> 33	67	56 32	67	41 <u>49</u>	67	30 52	67											

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7D	87	24	7D	9	65	7D	4	78	7D	34	96	7D	32	41	7D	97	33	7D	50	15	7D	32	18	7D	96	81	7D	82	41
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8E	52	24	8E	56	93	8E	35	93	8E	35	24	8C	18	83	8C	16	51	8C	89	74	8C	10	20	8C	73	35	8C	80	65
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8E 95 21	9E 39 24	9E 26 73	9E 25 97	9E 77 15	9E 27 65	9E 18 7	9E 10 34	9E 34 69	9E 72 88
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9F 42 78	AC 30 4	AC 22 94	AC 26 60	AC 1 64	AC 31 10	AC 15 60	AC 7 56	AC 14 51	AC 75 32
AF 72 22	AE 98 69	AE 42 96	AE 44 55	AE 20 69	AE 95 2	AE 42 84	AE 54 2	AE 78 30	AE 45 74
BE 92 72	BD 23 4	BD 91 35	BD 48 72	BD 38 42	BD 48 36	BD 59 33	BD 90 3	BD 96 58	BD 98 8
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CE 51 56	CF 10 79	CF 91 77	CF 63 22	CF 43 67	CF 85 38	CF 45 42	CF 71 61	CF 31 89	CF 37 44
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AE 38 1	AE 75 61	AE 27 88	AE 2 63	AE 54 63	AE 68 35	AE 3 41	AE 71 78	AE 85 80	AF 58 43
BD 8 66	BD 66 11	BD 9 41	BD 59 95	BD 48 95	BD 31 15	BD 29 100	BD 6 9	BD 64 94	BE 96 95
BF 28 4	BF 75 73	BF 38 52	BF 70 93	BF 84 23	BF 64 20	BF 37 5	BF 80 88	BF 69 15	BF 8 54
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36 <u>25</u> 90	36 <u>8</u> 85	36 82 <u>14</u>	36 92 <u>64</u>	36 86 <u>3</u>	36 <u>18</u> 37	36 62 66	36 57 <u>47</u>	36 <u>3</u> 10	36 98 <u>1</u>
37 89 <u>17</u>	37 47 <u>47</u>	37 <u>25</u> 73	37 <u>23</u> 41	37 72 11	37 92 <u>45</u>	37 27 <u>32</u>	37 74 66	37 15 <u>26</u>	37 79 76
48 94 <u>26</u>	48 <u>14</u> 4	48 <u>9</u> 6	48 37 81	48 <u>100</u> 35	48 54 <u>69</u>	48 87 <u>36</u>	48 64 <u>12</u>	48 89 80	48 60 93
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5A <u>41</u> 1	5A 89 <u>8</u>	5A 52 72	5A 53 <u>39</u>	5A 54 <u>98</u>	5A 83 55	5A <u>42</u> 99	5A <u>5</u> 87	5A <u>56</u> 92	5A <u>5</u> 53
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6C <u>9</u> 76	6C <u>7</u> 76	6C 70 <u>37</u>	6C 34 <u>13</u>	6C 64 24	6C <u>2</u> 12	6C 81 <u>52</u>	6C 84 <u>45</u>	6C 57 83	6C 39 <u>9</u>
7D 31 <u>41</u>	7D 96 <u>18</u>	7D <u>16</u> 57	7D <u>1</u> 91	7D <u>35</u> 33	7D 78 <u>3</u>	7D 73 89	7D <u>24</u> 26	7D <u>100</u> <u>11</u>	7D 69 <u>10</u>
89 67 10	89 58 <u>0</u>	89 40 <u>29</u>	89 43 63	89 <u>9</u> 60	89 31 67	89 98 31	89 57 40	8A <u>33</u> <u>44</u>	8A 52 <u>55</u>
8E <u>6</u> <u>34</u>	8E <u>30</u> 54	8E <u>28</u> 24	8E <u>42</u> 91	8E <u>3</u> <u>71</u>	8E <u>3</u> <u>72</u>	8E 97 43	8E 22 <u>53</u>	8C <u>21</u> 21	8C <u>73</u> 46
9F <u>32</u> 73	9F 91 <u>10</u>	9F 75 61	9F <u>15</u> 33	9F 26 80	9F <u>8</u> 91	9F <u>13</u> 56	9F 41 <u>4</u>	9D <u>59</u> 56	9D <u>26</u> 45
AC 90 70	AC 70 <u>69</u>	AC <u>43</u> 46	AC 45 24	AC 31 97	AC 50 <u>23</u>	AC 57 90	AC 71 78	9E <u>77</u> <u>24</u>	9E 64 78
AE <u>42</u> 38	AE 47 72	AE 17 <u>50</u>	AE 36 <u>44</u>	AE 12 66	AE <u>25</u> 9	AE <u>40</u> 10	AE <u>67</u> 94	AD 21 52	AD 84 43
BD <u>4</u> 29	BD <u>8</u> 83	BD <u>6</u> <u>20</u>	BD <u>9</u> 4	BD 91 71	BD <u>51</u> 76	BD <u>92</u> 53	BD 78 <u>42</u>	BE 45 29	BE 33 41
BF 20 <u>57</u>	BF <u>40</u> 94	BF <u>6</u> 52	BF 79 81	BF <u>16</u> 22	BF 74 <u>32</u>	BF 81 54	BF <u>24</u> 45	BF 53 <u>37</u>	BF 51 <u>5</u>
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8C <u>12</u> 62	8C <u>4</u> 99	8C 79 <u>59</u>	8C <u>43</u> 50	8C 60 29	8C 31 77	8C 32 <u>3</u>	8D 90 86	8D <u>5</u> 7	8D 89 93
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AD 69 <u>45</u>	AD 99 <u>29</u>	AD <u>24</u> 82	AD 46 <u>12</u>	AD 94 <u>40</u>	AD 76 29	AD 96 <u>8</u>	BF <u>27</u> 87	BF 44 <u>54</u>	BF 67 95
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BF <u>72</u> 49	BF <u>17</u> 30	BF 53 <u>14</u>	BF <u>67</u> 20	BF 53 69	BF 45 66	BF 59 56	CF 36 43	CF 35 73	CF <u>11</u> 80
CF 47 72	CF 53 61	CF 48 75	CF 74 36	CF 56 75	CF 55 <u>33</u>	CF 20 <u>10</u>	DE 87 92	DE 36 15	DE <u>87</u> 25
EF 77 <u>11</u>	EF 41 <u>1</u>	EF <u>11</u> 62	EF 59 79	EF <u>19</u> 61	EF <u>5</u> 9	EF <u>19</u> 33	DF 97 <u>40</u>	DF <u>35</u> 38	DF 84 <u>3</u>
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5B 87 <u>57</u>	5B <u>25</u> 70	5B 47 <u>22</u>	5B <u>18</u> 36	5B <u>7</u> 30	5B 13 57	5B 18 <u>18</u>	5B 20 <u>24</u>	5B <u>7</u> 64	5B 29 61
68 77 41	68 55 <u>12</u>	68 80 20	68 <u>9</u> 39	68 23 <u>4</u>	68 49 <u>66</u>	68 <u>78</u> 31	68 54 65	68 59 <u>16</u>	68 26 61
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BE 86 <u>7</u>	BE <u>35</u> 77	BE 72 54	BE 63 67	BE <u>26</u> 45	BE 58 67	9F 50 <u>2</u>	9F 97 95	9F 38 31	9F 55 <u>27</u>
BF <u>100</u> <u>87</u>	BF 91 <u>5</u>	BF 31 <u>56</u>	BF						

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381 2102	382 1996	383 2143	384 2093	385 2115	386 2083	387 1959	388 2189	389 2079	390 2034
01 <u>57</u> 65	01 82 61	01 99 22	01 86 11	01 61 15	01 84 56	01 0 35	01 <u>15</u> 26	01 <u>2</u> 65	01 6 <u>11</u>
02 <u>61</u> 57	02 83 <u>47</u>	02 48 <u>0</u>	02 <u>28</u> 47	02 <u>31</u> 16	02 30 <u>3</u>	02 98 20	02 23 <u>33</u>	02 93 75	02 <u>17</u> 98
03 <u>77</u> <u>42</u>	03 <u>30</u> 35	03 35 8	03 61 <u>1</u>	03 <u>62</u> 59	03 <u>49</u> 23	03 <u>10</u> 89	03 84 41	03 50 <u>83</u>	03 83 9
14 <u>15</u> 76	14 37 <u>1</u>	14 <u>31</u> 38	14 46 <u>25</u>	14 <u>33</u> 75	14 <u>14</u> 47	14 18 <u>1</u>	14 6 86	14 68 19	14 7 <u>6</u>
15 91 81	15 <u>7</u> 90	15 98 <u>41</u>	15 <u>54</u> 75	15 44 <u>71</u>	15 75 <u>10</u>	15 31 57	15 <u>43</u> 45	15 <u>1</u> 90	15 97 38
24 <u>62</u> 65	24 79 100	24 <u>66</u> <u>57</u>	24 74 49	24 92 81	24 69 53	24 <u>17</u> 74	24 90 <u>44</u>	24 69 <u>52</u>	24 31 54
25 70 <u>46</u>	25 92 <u>26</u>	25 71 21	26 <u>33</u> 78	26 11 <u>37</u>	26 82 <u>73</u>	26 39 <u>38</u>	26 68 76	26 <u>13</u> 4	26 <u>28</u> 42
36 69 13	36 73 95	36 <u>86</u> 82	35 47 <u>18</u>	35 <u>25</u> 43	35 <u>46</u> 36	35 <u>45</u> 36	35 52 <u>16</u>	35 42 71	35 <u>9</u> 55
37 90 <u>44</u>	37 78 54	37 97 <u>12</u>	36 32 59	36 52 43	36 22 74	36 38 65	36 <u>25</u> 57	36 53 83	36 99 <u>46</u>
46 <u>49</u> 82	46 77 <u>22</u>	46 89 19	47 1 <u>8</u>	47 73 35	47 41 25	47 77 77	47 70 <u>80</u>	47 <u>86</u> <u>26</u>	47 89 83
58 <u>57</u> <u>10</u>	58 8 64	58 17 <u>32</u>	58 97 44	58 6 88	58 41 17	58 <u>3</u> 92	58 55 79	58 <u>19</u> 71	58 <u>48</u> 53
69 <u>12</u> 27	69 25 <u>38</u>	69 <u>9</u> 65	69 <u>84</u> 15	69 75 <u>28</u>	69 33 <u>17</u>	69 60 <u>85</u>	69 <u>86</u> 6	69 <u>48</u> 87	69 48 71
7A 47 <u>19</u>	7A 66 <u>13</u>	7A 92 <u>67</u>	7A 35 <u>94</u>	7A 89 <u>12</u>	7A 68 <u>65</u>	7A 39 26	7A 95 50	7A 69 89	7A 71 <u>8</u>
7B 73 94	7B <u>75</u> 63	7B 94 56	7B 65 76	7B <u>0</u> 76	7B <u>23</u> 65	7B 85 <u>24</u>	7B 81 <u>2</u>	7B 80 <u>32</u>	7B <u>54</u> 66
8C 81 <u>27</u>	8C 23 <u>2</u>	8C 78 <u>55</u>	8C 87 <u>4</u>	8C <u>34</u> 73	8C 5 <u>47</u>	8C <u>1</u> 17	8C <u>10</u> 55	8C 53 54	8C 37 37
8D 5 48	8D <u>11</u> 8	8D 84 78	8D <u>7</u> 45	8D <u>86</u> <u>27</u>	8D <u>3</u> 70	8D 95 16	8D 74 <u>45</u>	8D <u>2</u> 37	8D <u>5</u> 27
9E <u>59</u> 89	9E 62 <u>0</u>	9E 42 8	9E 63 64	9E 96 89	9E 56 99	9E 90 19	9E <u>86</u> 97	9E 29 53	9E 83 <u>47</u>
9F 14 51	9F 23 3	9F <u>32</u> 85	9F <u>10</u> 80	9F 14 <u>80</u>	9F 85 <u>9</u>	9F 27 <u>13</u>	9F 45 85	9F <u>41</u> 44	9F <u>69</u> 46
AC 48 98	AC 62 86	AC 69 89	AC 87 22	AC 35 <u>2</u>	AC 79 70	AC 89 <u>26</u>	AC 47 81	AC 16 <u>34</u>	AC 55 <u>25</u>
AE 34 53	AE 96 83	AE 44 <u>24</u>	AE 51 <u>43</u>	AE 66 6	AE 58 <u>81</u>	AE <u>13</u> 57	AE 96 <u>53</u>	AE <u>37</u> <u>54</u>	AE 55 10
BD 28 <u>17</u>	BD 38 33	BD <u>72</u> 39	BD 28 57	BD 99 59	BD 62 97	BD 1 <u>43</u>	BD 68 96	BD 11 89	BD 50 29
BF <u>23</u> 90	BF <u>63</u> 30	BF 73 35	BF 31 <u>16</u>	BF <u>65</u> 88	BF <u>25</u> 76	BF 35 73	BF 16 <u>17</u>	BF 74 14	BF 57 45
CF <u>2</u> <u>37</u>	CF 43 <u>38</u>	CF 47 <u>4</u>	CF 36 95	CF 3 71	CF 73 35	CF 93 27	CF <u>34</u> 75	CF 90 <u>0</u>	CF 96 <u>29</u>
DE 50 <u>45</u>	DE <u>23</u> 16	DE <u>21</u> 67	DE <u>68</u> 83	DE 97 <u>23</u>	DE <u>18</u> 57	DE 38 <u>5</u>	DE 36 76	DE 73 16	DE <u>32</u> 52
391 2128	392 2033	393 2087	394 2126	395 2037	396 2053	397 2115	398 2118	399 2167	400 2167
01 46 <u>29</u>	01 28 90	01 83 88	01 <u>12</u> 99	01 91 55	01 71 <u>37</u>	01 <u>26</u> 66	01 <u>1</u> 70	01 58 62	01 2 <u>42</u>
02 78 98	02 <u>3</u> 86	02 51 <u>47</u>	02 80 <u>67</u>	02 <u>20</u> 49	02 <u>38</u> 75	02 82 94	02 80 70	02 42 18	02 12 61
03 <u>50</u> 57	03 46 <u>13</u>	03 <u>23</u> 43	03 76 76	03 63 <u>35</u>	03 7 56	03 22 <u>35</u>	03 79 <u>82</u>	03 38 <u>16</u>	03 <u>12</u> 58
14 38 59	14 95 <u>40</u>	14 <u>24</u> 73	14 <u>14</u> 97	14 <u>51</u> 31	14 69 52	14 <u>6</u> 27	14 <u>34</u> 9	14 57 88	14 15 91
15 98 <u>16</u>	15 <u>63</u> 72	15 58 <u>1</u>	15 30 11	15 94 <u>28</u>	15 77 <u>42</u>	15 39 59	15 65 62	15 <u>59</u> 74	15 70 <u>78</u>
24 54 <u>25</u>	24 <u>5</u> 35	24 89 <u>36</u>	24 77 58	24 22 91	24 <u>14</u> 49	24 86 72	24 34 59	24 <u>23</u> 35	24 38 <u>30</u>
26 <u>73</u> 22	26 53 99	26 5 87	26 85 <u>42</u>	26 <u>13</u> 31	26 35 54	26 45 <u>14</u>	26 2 86	26 21 <u>27</u>	26 <u>50</u> 69
35 10 52	35 74 67	35 50 35	35 <u>8</u> 38	35 92 93	35 81 53	35 36 <u>20</u>	35 <u>15</u> 66	35 47 76	35 96 66
37 <u>41</u> 42	37 60 <u>35</u>	37 <u>1</u> 88	37 13 <u>65</u>	37 37 <u>18</u>	37 42 <u>12</u>	37 55 96	37 92 <u>62</u>	37 73 <u>55</u>	37 <u>16</u> 35
47 47 <u>58</u>	47 19 24	47 63 30	47 <u>37</u> 76	47 50 64	47 <u>56</u> 90	47 <u>0</u> 58	47 <u>42</u> 30	47 <u>20</u> 48	47 52 <u>40</u>
58 7 <u>44</u>	58 <u>48</u> 17	58 89 <u>65</u>	58 <u>52</u> 82	58 73 <u>62</u>	58 7 <u>10</u>	58 96 <u>61</u>	58 <u>48</u> 47	58 <u>28</u> 81	58 50 <u>39</u>
69 96 25	69 96 <u>34</u>	69 18 <u>82</u>	69 6 <u>49</u>	69 <u>89</u> 7	69 <u>16</u> 43	69 33 <u>97</u>	69 <u>15</u> 98	69 96 84	69 <u>56</u> 94
6A <u>2</u> 66	6A <u>42</u> 26	6A <u>77</u> 71	6A 79 63	6A 20 44	6A 49 <u>16</u>	6A 44 56	6A 29 <u>10</u>	6A 28 <u>40</u>	6A 91 65
7B 40 37	7B 70 <u>11</u>	7B <u>22</u> 68	7B 5 25	7B 87 <u>2</u>	7B 93 30	7B <u>53</u> 89	7B 48 69	7B 84 55	7B 40 38
8C 94 53	8C 96 88	8C 49 76	8C 51 79	8C 37 <u>42</u>	8C 51 <u>16</u>	8C 50 8	8C 39 65	8C 68 66	8C 3 <u>11</u>
8D 89 <u>55</u>	8D <u>24</u> 40	8D 49 <u>81</u>	8D 52 94	8D 43 49	8D 39 37	8D 70 60	8D <u>25</u> 64	8D <u>81</u> 62	8D 50 52
9C <u>16</u> 30	9C 94 10	9C 30 <u>10</u>	9C 66 <u>16</u>	9C <u>6</u> 90	9C 72 76	9C 94 40	9C 92 74	9C 17 <u>46</u>	9C 99 81
9E 5 54	9E 75 <u>47</u>	9E 69 84	9E 76 48	9E 34 32	9E <u>5</u> 71	9E 85 <u>28</u>	9E <u>61</u> 25	9E 87 98	9E 29 39
AD 93 35	AD 51 43	AD <u>5</u> 82	AD <u>22</u> 36	AD 56 <u>0</u>	AD 34 <u>22</u>	AD 23 <u>51</u>	AD 49 <u>24</u>	AD 76 34	AD <u>49</u> 72
AF 81 33	AF <u>9</u> 59	AF 72 96	AF 28 85	AF <u>28</u> 66	AF 70 23	AF <u>59</u> 51	AF 87 60	AF 78 41	AF 94 88
BE <u>27</u> 5	BE 95 89	BE <u>12</u> 97	BE 94 <u>23</u>	BE 69 1	BE 57 <u>80</u>	BE <u>37</u> 79	BE 70 <u>67</u>	BE 73 <u>21</u>	BE 95 <u>22</u>
BF 35 <u>37</u>	BF 93 60	BF 92 91	BF <u>53</u> 93	BF 29 <u>34</u>	BF <u>16</u> 37	BF 98 61	BF <u>13</u> 85	BF <u>49</u> 98	BF <u>16</u> 23
CF <u>36</u> 80	CF 58 <u>23</u>	CF 31 <u>1</u>	CF <u>67</u> <u>39</u>	CF 54 82	CF 50 <u>73</u>	CF 74 <u>20</u>	CF 17 <u>31</u>	CF <u>100</u> <u>17</u>	CF 78 <u>68</u>
DE 39 <u>19</u>	DE <u>36</u> 62	DE 89 63	DE <u>27</u> 60	DE 80 <u>9</u>	DE 44 15	DE 34 31	DE 2 39	DE <u>27</u> 11	DE <u>38</u> 91

Appendix C

Implementation of graph reduction algorithm

This appendix gives a complete implementation of Algorithms 3.1 to 3.4 for GNU Octave / MATLAB. All graph inputs should be adjacency matrices. The function `graph_reduction` returns a cell vector of function handles, which may be passed as the first argument to `apply_reduction`. The function handles in this vector may be one or more of `red_cut`, `red_cycle`, `red_diamond`, `red_forced`, `red_hcycle`, `red_H`, `red_I`, `red_NH`, `red_path`, `red_pinwheel`, `red_radial` and `red_triangle`. The functions `eorbits`, `config` and `nauty_write` are used to calculate the edge orbits as necessary by executing `dreadnaut` from the `nauty` software package [55].

For convenience, the source code is distributed under the GNU General Public License and may be downloaded from the *FHCP Dissertations* page on the Flinders Hamiltonian Cycle Project website: <http://fhcp.edu.au>. To use the implementation it is necessary that a correct path to `dreadnaut` be set in `config.m`. The current URL for `nauty` is <http://pallini.di.uniroma1.it/>.

Before listings of the code we give a short example of usage:

```
>> petersen = [0 1 0 0 1 1 0 0 0 0
               1 0 1 0 0 0 1 0 0 0
               0 1 0 1 0 0 0 1 0 0
               0 0 1 0 1 0 0 0 1 0
               1 0 0 1 0 0 0 0 0 1
               1 0 0 0 0 0 0 1 1 0
               0 1 0 0 0 0 0 0 1 1
               0 0 1 0 0 1 0 0 0 1
               0 0 0 1 0 1 1 0 0 0
               0 0 0 0 1 0 1 1 0 0];
```

```

>> P = graph_reduction(petersen)
P =
{
  [1,1] = @red_NH
  [1,2] = @(g) red_forced (g, 9, 4)
  [1,3] = @(g) red_pinwheel (g, 2, 3, 7)
  [1,4] = @(g) red_radial (g, 1, 2, 5, 6)
}
>> reduced = apply_reduction(P, petersen)
reduced =
  0  1
  1  0

```

Code listings are now given in the order they are referenced, starting with the two functions comprising the main interface; `graph_reduction` and `apply_reduction`. An index to the files is shown below:

C.1	<code>graph_reduction.m</code>	206
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C.3	<code>red_H.m</code>	212
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C.6	<code>red_forced.m</code>	212
C.7	<code>red_path.m</code>	213
C.8	<code>red_cycle.m</code>	213
C.9	<code>red_triangle.m</code>	214
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C.17	<code>nauty_write.m</code>	219

Listing C.1: graph_reduction.m

```

% p = graph_reduction(g)
%
% Find a Hamiltonicity-preserving graph reduction
% g should be an adjacency matrix of a simple undirected graph
% degree 0 vertices will be treated as absent from the graph
% P is a cell vector of function handles which should be applied to g
% P will be empty if no applicable graph reduction was found
%
% Use apply_reduction(P, g) to produce the resulting graph

function P = graph_reduction(g)
if (~issimple(g))
    error('g is not a simple graph')
end
P = {};
while true
    if (length(P) > 1 && isequal(P{1}, @red_NH))
        return
    end
    if (~is2connected(g))
        P = {@red_NH, P{:}};
        return
    end
    n = nvertices(g);
    if (2*nedges(g) == n*(n-1))
        % g is complete (and 2-connected as above)
        P = {@red_H, P{:}};
        return
    end
    if (min_nonadjacent_deg_sum(g) >= n)
        % satisfies necessary condition in Ore's theorem
        P = {@red_H, P{:}};
        return
    end
    F = forced_edges(g);
    p = forced_edge_reduction(g, F);
    if (~isequal(p, @red_I))
        P = {p P{:}};
        g = p(g);
        continue
    end
    p = subgraph_reduction(g);
    if (~isequal(p, @red_I))
        P = {p P{:}};
        g = p(g);
        continue
    end
    p = edge_orbit_reduction(g, F);
    if (~isequal(p, @red_I))
        P = {p P{:}};
        g = p(g);
        continue
    end
    % no more reductions found
    return
end

function p = forced_edge_reduction(g, F)
n = nvertices(g);
if (max(sum(F)) > 2)
    % too many forced edges at a vertex
    p = @red_NH;
    return
end
for u = find(sum(F) == 2 & sum(g) > 2, 1)
    p = eval(['@g red_forced(g' sprintf(',%d', u, find(g(u,:)-F(u,:))) ')]);
    return
end
H = vsubgraph(g, sum(g)==2);
for c=components(H, sum(g)~=2)
    if (sum(c) > 1)
        if (n == 3)
            p = @red_I;
            return
        end
    end
end

```

```

    end
    V = trace_path(vsubgraph(H,c));
    if (length(V) > n-2)
        V = V(1:n-2);
    end
    p = eval(['@(g) red_path(g' sprintf(',%d', V) ')']);
    return
else
    v = find(c);
    V = adjacent(g,v);
    if (g(V(1),V(2)))
        p = eval(['@(g) red_cycle(g' sprintf(',%d', V(1), v, V(2)) ')']);
        return
    end
end
end
end
p = @red_I;

function p = subgraph_reduction(g)
if (nvertices(g) <= 4)
    p = @red_I;
    return
end
deg = sum(g);
for t=triangles(g)
    if (all(deg(t) == 3) && length(adjacent(g,t')) == 6)
        p = eval(['@(g) red_triangle(g' sprintf(',%d', t) ')']);
        return
    end
end
end
for d=diamonds(g)
    % d is already ordered as returned by diamonds
    if (all(deg(d)==3) && length(intersect(adjacent(g,d(1)),adjacent(g,d(4))))==2)
        p = eval(['@(g) red_diamond(g' sprintf(',%d', d) ')']);
        return
    end
end
end
p = @red_I;

function p = edge_orbit_reduction(g, F)
O = edge_orbits(g);
[C, K] = classify_orbits(O);
n = nvertices(g);
for i=find(C == 'C' & K == 1)
    if (nvertices(O{i}) == n && any(sum(g) > 2))
        % found Hamiltonian cycle
        p = eval(['@(g) red_hcycle(g' sprintf(',%d', trace_path(O{i})) ')']);
        return
    end
end
end
for i=find(C == 'K' | C == 'P')
    % find_cycle uses degree 2 vertices only so isn't doing any special processing
    cycle = find_cycle(O{i} | F);
    if (length(cycle) == n)
        % found Hamiltonian cycle
        p = eval(['@(g) red_hcycle(g' sprintf(',%d', cycle) ')']);
        return
    end
end
end
for i=find((C == 'K' | C == 'P') & log2(K) ~= fix(log2(K)))
    % number of disjoint edges or 2-paths with odd divisor
    comps = components(g & ~O{i}, sum(g)==0);
    if (size(comps,2) > 1)
        E = edges(O{i});
        Ecomp = arrayfun(@(v) find(comps(v,:), E), E);
        [E, Ecomp] = reorder_edges_by_components(E, Ecomp);
        c1 = Ecomp(end,1);
        c2 = Ecomp(end,2);
        if (mod(nnz(Ecomp == c1),2) == 1)
            E = E(any(Ecomp == c1, 2),:);
        elseif (mod(nnz(Ecomp == c2),2) == 1)
            E = E(any(Ecomp == c2, 2),:);
        else
            continue
        end
    end
    % odd number of edges connecting a component to the rest of the graph

```

```

        p = eval(['@(g) red_cut(g' sprintf(',%d', E) ')']);
        return
    end
end
for i=find(C == 'S' | C == 'X', 1)
    centre = find(sum(O{i}) >= 3, 1);
    p=eval(['@(g) red_radial(g' sprintf(',%d',centre,adjacent(O{i},centre) ')']);
    return
end
for i=find(C == 'K' | C == 'P')
    cycle = find_cycle(O{i} | F);
    if (~isempty(cycle) && length(cycle) ~= n && ~is_cycle_in(cycle, F))
        cycle = reorder_cycle_break_on_nonforced(cycle, F);
        p = eval(['@(g) red_cycle(g' sprintf(',%d', cycle) ')']);
        return
    end
end
% search for a vertex with a forced edge and two or more edges from the same orbit
for v=find(sum(F)==1)
    Fv = adjacent(F, v);
    for j=find(C ~= 'K')
        Ov = adjacent(O{j}, v);
        A = setdiff(Ov, Fv);
        if (length(A) >= 2)
            p = eval(['@(g) red_pinwheel(g' sprintf(',%d', v, A) ')']);
            return
        end
    end
end
for i=find(C == 'C')
    if (K(i) ~= 1 || nvertices(O{i}) ~= n)
        p = eval(['@(g) red_cycle(g' sprintf(',%d', trace_path(O{i})) ')']);
        return
    end
end
p = @red_I;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function b = issimple(g)
b = issymmetric(g) && size(g,1) && nnz(g) && ~any(diag(g)) && isequal(g,logical(g));

function b = is2connected(g)
if (ncomponents(g) ~= 1)
    b = false;
    return
end
if (any(sum(g) == 1))
    b = false;
    return
end
n = size(g,1);
for v=find(sum(g) >= 2)
    adj = adjacent(g,v);
    % temporarily remove edges
    g(v,adj) = 0;
    g(adj,v) = 0;
    if (ncomponents(g) ~= 1)
        b = false;
        return
    end
    % restore edges
    g(v,adj) = 1;
    g(adj,v) = 1;
end
b = true;

function n = nvertices(g)
n = nnz(sum(g)); % ignores degree 0 vertices

function n = nedges(g)
n = nnz(triu(g));

function c = ncomponents(varargin)
c = size(components(varargin{:}), 2);

```

```

function C = components(g, ignore)
n = size(g,1);
c = zeros(1,n);
if (nargin < 2)
    ignore = (sum(g) == 0); % ignore degree 0 vertices
end
c(ignore) = -1;
while nnz(c) < n
    % vector for next component
    v = double(1:n == find(c == 0, 1));
    vnz = 0;
    while nnz(v) > vnz
        vnz = nnz(v);
        v = v + v*g;
    end
    c(v>0) = max(c)+1;
end
nc = max(max(c),0);
C = false(n, nc);
for i=1:nc
    C(:,i) = (c == i)';
end

```

```

function s = min_nonadjacent_deg_sum(g)
s = Inf;
n = size(g,1);
for i=1:n
    if (sum(g(i,:)) == 0)
        % ignore degree 0 vertices
        continue
    end
    for j=i+1:n
        if (sum(g(j,:)) == 0)
            % ignore degree 0 vertices
            continue
        end
        if (~g(i,j))
            s = min(s, sum(g(i,:))+sum(g(j,:)));
        end
    end
end
end

```

```

function F = forced_edges(g)
n = size(g,1); % include degree 0 vertices
F = zeros(n);
for i=1:n
    for j=i+1:n
        if (~g(i,j))
            continue
        end
        % temporarily remove edge
        g(i,j) = 0;
        g(j,i) = 0;
        if (~is2connected(g))
            F(i,j) = 1;
            F(j,i) = 1;
        end
        % restore edge
        g(i,j) = 1;
        g(j,i) = 1;
    end
end
end

```

```

function H = vsubgraph(G, vertices)
H = zeros(size(G,1));
H(vertices,vertices) = G(vertices,vertices);

```

```

function V = trace_path(g)
V = [];
if (nnz(g) == 0)
    return
end
[i,j] = find(g, 1);
V = [j, i]; % j < i
g(:,i) = 0;
g(j,:) = 0;

```

```

g(i,V) = 0;
g(V,j) = 0;
while (nnz(g(V(end),:)))
    k = find(g(V(end),:), 1);
    g(:,k) = 0;
    g(k, V) = 0;
    V = [V, k];
end
while (nnz(g(:,V(1))))
    k = find(g(:,V(1)), 1);
    g(k,:) = 0;
    g(V,k) = 0;
    V = [k, V];
end
if (V(1) > V(end))
    V = fliplr(V);
end

function T = triangles(g)
n = size(g,1);
T = zeros(3,0);
for i=1:n
    if (sum(g(i,:)) == 0)
        continue
    end
    for j=i+1:n
        if (~g(i,j))
            continue
        end
        for k=j+1:n
            if (~g(i,k) || ~g(j,k))
                continue
            end
            T(:,end+1) = [i j k]';
        end
    end
end

function A = adjacent(g, vertices)
n = size(g,1);
A = zeros(1,n);
for i=1:length(vertices)
    A = A + g(vertices(i),:);
end
A = find(A);

function D = diamonds(g)
n = size(g,1);
D = zeros(4,0);
for t=triangles(g)
    i=t(1);
    j=t(2);
    k=t(3);
    for l=i+1:n
        if (l == i || l == j || l == k || sum(g([i, j, k], l)) ~= 2)
            continue
        end
        if (g(i,l) && g(j,l) && l > k)
            D(:,end+1) = [k i j l]';
        elseif (g(i,l) && g(k,l) && l > j)
            D(:,end+1) = [j i k l]';
        elseif (g(j,l) && g(k,l))
            D(:,end+1) = [i j k l]';
        end
    end
end

function O = edge_orbits(g)
n = size(g,1);
[g, vmap] = compact(g);
[orbits, E] = eorbits(g);
norbits = max(orbits);
E = vertex_map(E, vmap);
O = cell(1, norbits);
for i=1:norbits
    H = zeros(n);

```

```

    for edge = E(orbits == i,:)
        H(edge(1),edge(2)) = 1;
        H(edge(2),edge(1)) = 1;
    end
    O{i} = H;
end

function [g, vmap] = compact(g)
vmap = find(sum(g));
g = g(vmap, vmap);

function E = edges(g)
[i,j] = find(tril(g));
E = [j i];

function M = vertex_map(M, vmap)
f = @(x) scalar_map(x, vmap);
M = arrayfun(f, M);

function x = scalar_map(x, vmap)
x = vmap(x);

function [c, k] = classify_orbits(O)
c = '';
k = zeros(1,length(O));
for i=1:length(O)
    H = O{i};
    degrees = unique(sum(H));
    if (degrees(1) == 0)
        degrees = degrees(2:end);
    end
    a = degrees(1);
    if (length(degrees) == 1)
        b = a;
    elseif (length(degrees) == 2)
        b = degrees(2);
    end
    k(i) = ncomponents(H);
    if (a == 1 && b == 1)
        c(i) = 'K'; % K_2
    elseif (a == 1 && b == 2)
        c(i) = 'P'; % P_2
    elseif (a == 1 && b > 2)
        c(i) = 'S'; % S_n
    elseif (a == 2 && b == 2)
        c(i) = 'C'; % C_n
    elseif (a == b)
        c(i) = 'X'; % X_n
    elseif (a < b)
        c(i) = 'X'; % X_m,n
    end
end

function C = find_cycle(g)
% cycles must be on degree 2 vertices
g = vsubgraph(g, sum(g)==2);
if (nnz(g))
    for c = components(g)
        if (sum(c) >= 3)
            h = vsubgraph(g,c);
            C = trace_path(h);
            if (h(C(end),C(1)))
                return
            end
        end
    end
end
% no cycle found
C = [];

function C = reorder_cycle_break_on_nonforced(C, F)
n=length(C);
shifts=0;
while (F(C(n),C(1)))
    C = circshift(C, [0 -1]);
    shifts = shifts+1;
end

```

```

end

function [E, C] = reorder_edges_by_components(E, C)
c1 = min(C(end,:));
c2 = max(C(end,:));
for i=1:size(E,1)
    if (C(i,1) == c2 || C(i,2) == c1)
        % swap
        tmp = C(i,1);
        C(i,1) = C(i,2);
        C(i,2) = tmp;
        tmp = E(i,1);
        E(i,1) = E(i,2);
        E(i,2) = tmp;
    end
end

function b = is_cycle_in(cycle, g)
if (length(cycle) < 3)
    b = false;
    return
end
n = length(cycle);
cycle(n+1) = cycle(1);
for i=1:n
    if (~g(cycle(i),cycle(i+1)))
        b = false;
        return
    end
end
end
b = true;

```

Listing C.2: apply_reduction.m

```

% g = apply_reduction(P, g)
%
% P should be a cell of function handles to be applied to g from last to first
% g should be an adjacency matrix

function g = apply_reduction(P, g)
for i=numel(P):-1:1
    p = P{i};
    g = p(g);
end
g = g(sum(g)>0,sum(g)>0);

```

Listing C.3: red_H.m

```

% g = red_H(g)
% returns a small Hamiltonian graph K_3
function g = red_H(g)
g = 1-eye(3);

```

Listing C.4: red_I.m

```

% g = red_I(g)
% identity "reduction" - returns g unmodified
function g = red_I(g)

```

Listing C.5: red_NH.m

```

% g = red_NH(g)
% returns a small non-Hamiltonian graph K_2
function g = red_NH(g)
g = 1-eye(2);

```

Listing C.6: red_forced.m

```

% g = red_forced(g, u, v1, ...)
% unusable edge reduction
function g = red_forced(varargin)
if (nargin < 3)
    error('too few arguments')

```

```

end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
u = varargin{2};
V = [varargin{3:end}];
if (u < 1 || u > size(g,1) || min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
for v=V
    if (~g(u,v))
        error('edge (%d, %d) not in graph', u, v)
    end
end

g(u,V) = 0;
g(V,u) = 0;

```

Listing C.7: red_path.m

```

% g = red_path(g, v1, v2, ...)
% path reduction
function g = red_path(varargin)
if (nargin < 3)
    error('too few arguments')
end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
V = [varargin{2:end}];
if (min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
if (length(V) ~= length(unique(V)))
    error('repeated arguments')
end
if (any(sum(g(:,V)) ~= 2))
    error('vertices must be degree 2')
end
if (length(V) > nvertices(g)-2)
    error('too many vertices in path')
end
for i=1:length(V)-1
    if (~g(V(i),V(i+1)))
        error('edge (%d, %d) not in graph', V(i), V(i+1))
    end
end

endpoint = find(g(V(end),:).*(1:size(g,1) ~= V(end-1)));

% remove all but first vertex
dv = V(2:end);
g(dv,:)=0;
g(:,dv)=0;

% connect first vertex to endpoint (if not already)
g(V(1),endpoint) = 1;
g(endpoint,V(1)) = 1;

function n = nvertices(g)
n = nnz(sum(g)); % ignores degree 0 vertices

```

Listing C.8: red_cycle.m

```

% g = red_cycle(g, v1, v2, v3, ...)
% remove an edge from a short cycle of redundant edges
function g = red_cycle(varargin)
if (nargin < 4)
    error('too few arguments')
end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')

```

```

end
V = [varargin{2:end}];
if (min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
n = length(V);
if (n ~= length(unique(V)))
    error('repeated arguments')
end
if (n == nvertices(g))
    error('cycle is not short')
end
% make loop
V(end+1) = V(1);
for i=1:n
    if (~g(V(i),V(i+1)))
        error('edge (%d, %d) not in graph', V(i), V(i+1))
    end
end
% remove edge
g(V(1),V(n)) = 0;
g(V(n),V(1)) = 0;

function n = nvertices(g)
n = nnz(sum(g)); % ignores degree 0 vertices

```

Listing C.9: red_triangle.m

```

% g = red_triangle(g, u, v, w)
% contract degree 3 triangle into single vertex
function g = red_triangle(g, u, v, w)
if (nargin ~= 4)
    error('wrong number of arguments')
end
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
if (min([u v w]) < 1 || max([u v w]) > size(g,1))
    error('arguments out of bounds')
end
if (any(sum(g(:,[u,v,w])) ~= 3))
    error('vertices are not degree 3')
end
if (~g(u,v) || ~g(u,w) || ~g(v,w))
    error('not triangle')
end
% find other vertices
gu = g(u,:);
gu([v w]) = 0;
ou = find(gu);
gv = g(v,:);
gv([u w]) = 0;
ov = find(gv);
gw = g(w,:);
gw([u v]) = 0;
ow = find(gw);
if (ou == ov || ou == ow || ov == ow)
    error('triangle does not connect to 3 distinct outside vertices')
end

% remove v and w
g([v w],:) = 0;
g(:,[v w]) = 0;

% connect u to other vertices
g(u,[ov ow]) = 1;
g([ov ow],u) = 1;

```

Listing C.10: red_diamond.m

```

% g = red_diamond(g, u, v, w, x)
% contract cubic diamond into a single vertex
function g = red_diamond(g, u, v, w, x)
if (nargin ~= 5)
    error('wrong number of arguments')

```

```

end
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
if (min([u v w x]) < 1 || max([u v w x]) > size(g,1))
    error('arguments out of bound')
end
if (any(sum(g(:, [u v w x])) ~= 3))
    error('vertices of diamond are not degree 3')
end
if (~g(u,v) || ~g(u,w) || ~g(v,w) || ~g(v,x) || ~g(w,x) || g(u,x))
    error('not diamond')
end

xn = setdiff(find(g(x,:)), [v w]);
assert(isscalar(xn));

if (g(u,xn))
    error('endpoints of diamond have a common neighbour')
end

% remove v w x
g([v w x], :) = 0;
g(:, [v w x]) = 0;

% connect u to xn
g(u,xn) = 1;
g(xn,u) = 1;

```

Listing C.11: red_hcycle.m

```

% g = red_hcycle(g, v1, v2, ..., vn)
% remove all edges but those in a given Hamiltonian cycle
% v1 ... vn should trace out a Hamiltonian cycle
% n must be the number of vertices in g
function g = red_hcycle(varargin)
if (nargin < 1)
    error('too few arguments')
end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
n = nvertices(g);
if (nargin ~= 1 + n)
    error('wrong number of arguments')
end
V = [varargin{2:end}];
if (min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
if (length(unique(V)) ~= n)
    error('repeated arguments')
end
% make loop
V(end+1) = V(1);
for i=1:n
    if (~g(V(i),V(i+1)))
        error('edge (%d, %d) not in graph', V(i), V(i+1))
    end
end

% remove all edges
g(:, :) = 0;
for i=1:n
    % restore Hamiltonian cycle
    g(V(i),V(i+1)) = 1;
    g(V(i+1),V(i)) = 1;
end

function n = nvertices(g)
n = nnz(sum(g)); % ignores degree 0 vertices

```

Listing C.12: red_cut.m

```

% g = red_cut(g, u1, v1, u2, v2, u3, v3, ...)
% remove an edge from an odd edge cut
function g = red_cut(varargin)
if (nargin < 3 || mod(nargin,2) ~= 1)
    error('wrong number of arguments')
end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
U = [varargin{2:2:end-1}];
V = [varargin{3:2:end}];
if (min(U) < 1 || max(U) > size(g,1) || min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
n = length(U);
if (size(unique(sort([U V'], 2), 'rows'),1) ~= n)
    error('repeated edges in arguments')
end
h = g;
for i=1:n
    if (~g(U(i),V(i)))
        error('edge (%d,%d) not in graph', U(i), V(i));
    end
    h(U(i),V(i)) = 0;
    h(V(i),U(i)) = 0;
end
C = components(h, sum(g) == 0);
nc = size(C, 2);
if (nc < 2)
    error('not edge cut');
end
for i=1:n
    h(U(i),V(i)) = 1;
    h(V(i),U(i)) = 1;
    if (size(components(h, sum(g) == 0), 2) == nc)
        error('edge cut not minimal');
    end
    h(U(i),V(i)) = 0;
    h(V(i),U(i)) = 0;
end

% remove last edge from cut
g(U(end),V(end)) = 0;
g(V(end),U(end)) = 0;

function C = components(g, ignore)
N = size(g,1);
c = zeros(1,N);
if (nargin < 2)
    ignore = (sum(g) == 0); % ignore degree 0 vertices
end
c(ignore) = -1;
while nnz(c) < N
    % vector for next component
    v = double(1:N == find(c == 0, 1));
    vnz = 0;
    while nnz(v) > vnz
        vnz = nnz(v);
        v = v + v*g;
    end
    c(v>0) = max(c)+1;
end
nc = max(max(c),0);
C = false(N, nc);
for i=1:nc
    C(:,i) = (c == i)';
end

```

Listing C.13: red_radial.m

```

% g = red_radial(g, u, v1, v2, v3, ...)
% remove an edge from a star where all the edges are redundant
function g = red_radial(varargin)
if (nargin < 5)
    error('too few arguments')

```

```

end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
u = varargin{2};
V = [varargin{3:end}];
if (u < 1 || u > size(g,1) || min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
if (length(V) ~= length(unique(V)))
    error('repeated arguments')
end
for v=V
    if (~g(u,v))
        error('edge (%d, %d) not in graph', u, v)
    end
end
end

g(u,V(end)) = 0;
g(V(end),u) = 0;

```

Listing C.14: red_pinwheel.m

```

% g = red_pinwheel(g, u, v1, v2, ...)
% remove all but one redundant edge where a Hamiltonian edge was found adjacent
function g = red_pinwheel(varargin)
if (nargin < 4)
    error('too few arguments')
end
g = varargin{1};
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
u = varargin{2};
V = [varargin{3:end}];
if (u < 1 || u > size(g,1) || min(V) < 1 || max(V) > size(g,1))
    error('arguments out of bound')
end
if (length(V) ~= length(unique(V)))
    error('repeated arguments')
end
for v=V
    if (~g(u,v))
        error('edge (%d, %d) not in graph', u, v)
    end
end
end
for v=V(2:end)
    g(u,v) = 0;
    g(v,u) = 0;
end
end

```

Listing C.15: eorbits.m

```

% [orbits, edges] = eorbits(g)
%
% label edges according to their edge orbits
%
% g should be a simple graph
%
% edges is an Mx2 matrix where M is the number of edges in the graph
% orbits is an Mx1 matrix assigning an integer from 1:N_EDGE_ORBITS to each edge
function [orbits, edges] = eorbits(g)
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
[i,j] = find(tril(g));
edges = [j i];
m = size(edges, 1);
if (m < 1)
    orbits = [];
    return;
end
orbits = [1:m]';
gorders = [];

```

```

generators = autgen(g);
for g=1:length(generators)
    gen = generators{g};
    orders = cellfun(@length, gen);
    order = 1;
    for o=orders
        order = lcm(order, o);
    end
    gorders(g) = order;
end

for i=1:m
    edge = edges(i,:);
    for g=1:length(generators)
        perm = generators{g};
        for j=1:gorders(g)-1
            edge = apply_cycles(edge, perm);
            edgei = find(edges(:,1) == edge(1) & edges(:,2) == edge(2));
            if (orbits(edgei) == orbits(i))
                continue;
            end
            oidx = orbits == orbits(edgei) | orbits == orbits(i);
            orbits(oidx) = min(orbits(edgei), orbits(i));
        end
    end
end

uniq = unique(orbits);
norbits = length(uniq);
for i=1:norbits
    orbits(orbits == uniq(i)) = i;
end

function edge = apply_cycles(edge, perm)
for i=length(perm):-1:1
    cycle = perm{i};
    order = length(cycle);
    if (order < 2)
        continue;
    end
    ind = find(cycle == edge(1));
    if (length(ind) == 1)
        ind = ind + 1;
        if (ind > order)
            ind = 1;
        end
        edge(1) = cycle(ind);
    end
    ind = find(cycle == edge(2));
    if (length(ind) == 1)
        ind = ind + 1;
        if ind > order
            ind = 1;
        end
        edge(2) = cycle(ind);
    end
end
edge = sort(edge, 2);

function generators = autgen(g)
config();
tmp = tempname;
nauty_write(g, tmp);
fid = fopen(tmp, 'a');
fprintf(fid, 'x\n');
fclose(fid);

[status, output] = system(['dreadnaut ' < ' ' tmp '']);
delete(tmp);
if (status ~= 0)
    error('dreadnaut failed to run. Output:\n\n%s', output);
end

output = strrep(output, sprintf('\n  '), ''); % join split output lines
output = regexprep(output, '\n$', ''); % remove trailing newline
lines = strsplit(output, sprintf('\n'));

```

```

generators = {};
for i=1:length(lines)
    line = lines{i};
    if (line(1) == '(')
        gen = {};
        cycles = strsplit(regexprep(line, '^(\\|\\)', '\\|'), '(');
        for j=1:length(cycles)
            gen{end+1} = str2num([' ' cycles{j} '']);
        end
        generators{end+1} = gen;
    else
        grpssize = strfind(line, 'grpssize=');
        if grpssize
            line = line(grpssize+8:end);
            line = line(1:strfind(line, ';')-1);
        end
    end
end
end

```

Listing C.16: config.m

```

% edit the options here to configure the algorithm
function config()

% path for dreadnaut
% download and compile from http://pallini.di.uniroma1.it/
% or from http://cs.anu.edu.au/~bdm/nauty/
if (isunix)
    dreadnaut = 'nauty/dreadnaut';
else % Windows
    dreadnaut = 'nauty/dreadnaut.exe';
end

% don't edit below this line
if (~(exist(dreadnaut, 'file')))
    error('%s: not found. Please edit dreadnaut path in config.m', dreadnaut);
end
assignin('caller', 'dreadnaut', dreadnaut);

```

Listing C.17: nauty_write.m

```

% nauty_write(g, filename)
%
% save a graph in nauty format
%
% g is the adjacency matrix of a simple undirected graph
% filename is a string, recommended to end in ".dre"
%
% nauty is a program for computing automorphisms of graphs. It can be
% downloaded from http://cs.anu.edu.au/~bdm/nauty/
function nauty_write(g, filename)
if (~(issymmetric(g) && size(g,1) && ~any(diag(g)) && isequal(g,logical(g))))
    error('bad input graph')
end
n = size(g,1);
fid = fopen(filename,'w');
fprintf(fid,'% $ 1\n'); % sets nauty to start number vertices from 1
fprintf(fid,'n=%d\n', n); % write the number of vertices
fprintf(fid,'g\n'); % begin the graph
for v=1:n-1
    Nv = find(g(v,v+1:end)) + v;
    if isempty(Nv)
        continue
    end
    fprintf(fid,'%d:', v);
    fprintf(fid,' %d', Nv);
    fprintf(fid,';\n');
end
fprintf(fid,'.\n'); % end writing the graph
fclose(fid);

```

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