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Extremal Directed and Mixed Graphs

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Abstract

We consider three problems in extremal graph theory, namely the degree/diameter problem, the degree/geodecity problem and Turán problems, in the context of directed and partially directed graphs.

A directed graph or mixed graph G is k-geodetic if there is no pair of vertices u, v of G such that there exist distinct non-backtracking walks with length $\leq k$ in G from u to v. The order of a k-geodetic digraph with minimum out-degree d is bounded below by the *directed Moore bound* $M(d,k) = 1 + d + d^2 + \cdots + d^k$; similarly the order of a k-geodetic mixed graph with minimum undirected degree r and minimum directed out-degree z is bounded below by the *mixed Moore bound*. We will be interested in networks with order exceeding the Moore bound by some small *excess* ϵ.

The *degree/geodecity problem* asks for the smallest possible order of a k-geodetic digraph or mixed graph with given degree parameters. We prove the existence of extremal graphs, which we call *geodetic cages*, and provide some bounds on their order and information on their structure.

We discuss the structure of digraphs with excess one and rule out the existence of certain digraphs with excess one. We then classify all digraphs with out-degree two and excess two, as well as all diregular digraphs with out-degree two and excess three. We also present the first known non-trivial examples of geodetic cages.

We then generalise this work to the setting of mixed graphs. First we address the question of the total regularity of mixed graphs with order close to the Moore bound and prove bounds on the order of mixed graphs that are not totally regular. In particular using spectral methods we prove a conjecture of López and Miret that mixed graphs with diameter two and order one less than the Moore bound are totally regular.

Using counting arguments we then provide strong bounds on the order of totally regular k-geodetic mixed graphs and use these results to derive new extremal mixed graphs.

Finally we change our focus and study the Turán problem of the largest possible size of a k-geodetic digraph with given order. We solve this problem and also prove an exact expression for the restricted problem of the largest possible size of strongly connected 2-geodetic digraphs, as well as providing constructions of strongly connected k-geodetic digraphs that we conjecture to be extremal for larger k. We close with a discussion of some related generalised Turán problems for k-geodetic digraphs.

Preface

Acknowledgements

I would like to dedicate this thesis to my wife Irina, whom I met, courted and married during the course of my PhD. In fact we were introduced by the degree/diameter problem and a vain attempt to explain in my limited Russian what it has to do with bridges in her nearby town of Kaliningrad. May she continue to distract me from mathematics for many years to come.

Thank you also to my parents and grandparents for their unflagging love and support, not merely during my PhD, but the entire course of my life.

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A big thank you to my coauthors Grahame Erskine, Nika Salia, Elias John Thomas and Ullas Chandran. I look forward to working on new problems with all of you in the future! I am very grateful also to my 'academic siblings' Rob Lewis, Jay Fraser, Olivia Jeans, Kirstie Asciak and again Grahame Erskine, as well as my 'academic cousins' David Marchant, Jakub Sliačan and Margaret Stanier, in addition to (if I may strain a metaphor to the limits) my 'academic uncle' Terry Griggs, for many fruitful discussions over the years. I am particularly grateful to the intersection of these two sets of mathematicians, Grahame Erskine, who always manages to prove something interesting from any crazy idea thrown at him in a Friday evening email.

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Declaration

Unless stated otherwise, all results in this thesis are the original work of the author. In the case of results from joint papers all significant contributions of co-authors are acknowledged in the text.

This thesis contains material from the following seven papers, with the corresponding chapters of the thesis in brackets:

- Tuite, J., *Digraphs with degree two and excess two are diregular,* Discrete Mathematics 342 (5) (2019), 1233-1244 (Chapter 5).
- Tuite, J., *On diregular digraphs with degree two and excess three,* Discrete Applied Mathematics 266 (2019), 331-339 (Chapter 6).
- Tuite, J., *On diregular digraphs with degree two and excess two,* Discrete Applied Mathematics 238 (2018), 167-174 (Chapter 6).
- Tuite, J. and Erskine, G., *On total regularity of mixed graphs with order close to the Moore bound,* Graphs and Combinatorics (35) (2019), 1253-1272 (Chapter 8).
- Tuite, J., Erskine, G. and Salia, N., *Turán problems for k-geodetic digraphs,* arXiv preprint arXiv:2102.04957 (2021) (Chapter 10).
- Tuite, J. and Erskine, G., *On networks with order close to the Moore bound,* arXiv preprint arXiv:2108.05820 (2021) (Chapter 9).
- Tuite, J., *The structure of digraphs with excess one,* arXiv preprint arXiv:2109.14488 (2021) (Chapter 4).

Other publications arising from my PhD but not contained in this thesis include:

- Erskine, G. and Tuite, J., *Large Cayley graphs of small diameter,* Discrete Applied Mathematics 250 (2018), 202-214.
- Thomas, E., Chandran, U. and Tuite, J., *On monophonic position sets in graphs,* arXiv preprint arXiv:2012.10330 (2020).
- Tuite, J., Thomas, E. and Chandran, U., *On some extremal position problems for graphs,* arXiv preprint arXiv:2106.06827 (2021).

- Erskine, G. and Tuite, J., *Small graphs and hypergraphs of given degree and girth,* arXiv preprint arXiv:2201.07117 (2022).
- Thomas, E., Chandran, U. and Tuite, J., *On the general position number of Mycielskian graphs,* arXiv preprint arXiv:2203.08170 (2022).

Contents

1 Introduction **11**

1.1 Terminology 12

1.2 Outline 22

2 Background **25**

2.1 The undirected degree/diameter problem 25

2.2 The undirected degree/girth problem 28

2.3 The degree/diameter problem for directed graphs 31

2.4 Turán problems 37

3 The degree/geodecity problem **39**

3.1 Motivation 39

3.2 Existence of cages 44

3.3 Monotonicity of geodetic cages 48

3.4 Connectivity of geodetic cages 49

4 Digraphs with excess one **53**

4.1 Vertex-transitive digraphs with excess one 54

4.2 Diregular digraphs with excess one and degree three 59

4.3 Automorphisms of digraphs with excess one 63

4.4 Structure of the outlier function 66

4.5 Spectral results 70

4.6 2-geodetic digraphs with excess one 73

5 Diregularity of digraphs with small excess **81**

5.1 Background 81

5.2 Basic structural results 82

5.3 Digraphs with out-degree two and excess two 84

5.4 Digraphs with degree two and excess three 101

6 Diregular digraphs with small excess 103

6.1 The Neighbourhood Lemma 103

6.2 Diregular digraphs with degree two and excess two 104

6.3 Classification of $(2, 2; +2)$-digraphs 109

6.4 Diregular digraphs with degree two and excess three 116

6.5 Classification of $(2, 3; +3)$-digraphs 122

7 The degree/geodecity problem for mixed graphs 127

7.1 Mixed Moore graphs 127

7.2 Mixed graphs with positive defect 132

7.3 The mixed degree/geodecity problem: cages and monotonicity 134

8 Total regularity of mixed graphs with order close to the Moore bound 139

8.1 Introduction 139

8.2 $(r, z, 2; -1)$-graphs are totally regular 141

8.3 Total regularity of $(1, 1, k; -1)$-graphs for $k \geq 3$ 145

8.4 Total regularity of 2-geodetic mixed graphs with excess one 148

8.5 Total regularity of $(r, 1, k; +1)$-graphs for $k \geq 3$ 150

9 Bounds on the order of mixed graphs 155

9.1 Bounds on totally regular mixed graphs with small excess 155

9.2 Excess of mixed graphs that are not totally regular 163

9.3 The unique $(2, 1, 2; +1)$-graph 170

9.4 Bounds on totally regular mixed graphs with small defect 174

9.5 Mixed geodetic cages and record graphs 179

10 Turán problems for k-geodetic directed graphs 185

10.1 Introduction 185

10.2 The largest size of a strongly connected 2-geodetic digraph 190

10.3 Classification of extremal 2-geodetic digraphs without sources and sinks 197

10.4 Extremal strongly connected k-geodetic digraphs for $k \geq 3$ 203

10.5 Generalised Turán problems for k-geodetic digraphs 207

11 Conclusion **211**

11.1 Bounds for directed graphs 211

11.2 Bounds for mixed graphs 217

Chapter 1

Introduction

Networks permeate every aspect of our lives. Whilst reading these words electrical signals pass through the network of neurons in our brains. Our transportation consists of interconnected networks of roads, railways, streets, cycleways, air routes and bus lines. We communicate by complicated networks of telephone lines and linked computers.

Our relationships with other people can be described by networks of friendship, collaboration and cooperation; this includes online social networks such as Facebook and Twitter. Plants communicate and obtain nutrients through networks of roots; slime moulds for example are well known for their ability to create efficient and reliable networks [7]. Relationships between animals can be described by networks of predation (the *food chain* or the *food web*) or genetic relatedness (such as the *tree of life*).

Networks are described mathematically by means of *graphs*, which are collections of *vertices* or *nodes* that are joined by *edges*. When designing an interconnection network, or analysing a naturally occurring network, there are many useful graph-theoretic parameters that describe desirable properties of the network. For example

- *order*: the number of nodes in the network,
- *size*: the number of connections in the network,
- *degree* or *valency*: the number of connections per node,
- *diameter*: the largest number of connections that must be traversed from one node to another,
- *girth*: this describes the 'local efficiency' of communication, or the smallest length of two internally disjoint paths between a pair of nodes,
- *connectivity*: the smallest number of nodes that must be deleted in order to split the network up into several parts, and
- *symmetry*: if the network has a high degree of symmetry, then parts of the network can be mass-produced and the same routing algorithms can be used for many nodes.

Frequently we need to find a network that has the largest possible value of one or more of these parameters subject to restrictions on the others. Such problems belong to the field of *extremal graph theory*. For example, when designing an integrated circuit a large number of transistors must be fitted onto each circuit board, which makes computation faster, subject to having relatively few connections per transistor for ease of layout and fast connections between each transistor. Similarly, when constructing a communication network it is desirable to connect a large number of users or switches, whilst each switch has a relatively low number of connections and the maximum number of connections needed for communication between any pair of switches is small.

If we model these situations by means of a graph in which the vertices represent transistors or switches, then we require the graph to have large order, subject to low diameter and small degrees for all of the nodes. This mathematical question is known as the *degree/diameter problem*. In this thesis we will discuss this problem and some of its relatives for graphs containing both directed and undirected connections.

1.1 Terminology

We shall begin by establishing the terminology and notation that we shall use; for any graph-theoretical concepts not defined here we refer to [28] as our standard. A *graph* G consists of a set $V(G)$ of *vertices* together with a set $E(G)$ of unordered pairs of vertices called *edges*. We will often denote an edge $\{u, v\}$ simply by uv. If there is an edge $\{u, v\}$ between vertices u and v, then we say that u and v are *adjacent* and we write $u \sim v$, whereas if u and v are not adjacent we write $u \not\sim v$. If $u \sim v$, then u and v are *neighbours*. The edge uv is *incident* with its endpoints u and v. This definition is quite abstract; it is often more useful to portray a graph by a drawing, in which vertices are represented by nodes and edges by lines between nodes that do not pass through nodes other than its endpoints. One famous graph is displayed in Figure 1.1.

An edge uu from a vertex to itself is called a *loop*. If a network G contains two edges that are incident with the same pair of vertices u and v, then there are *multiple edges* in G. Our definition of 'graph' tacitly rules out both of these scenarios; therefore, unless stated otherwise, all graphs are assumed to be *simple*. All graphs considered here will also be finite, that is $V(G)$ and $E(G)$ will always be finite sets.

The *order* of a graph G is the cardinality of its vertex set and is typically denoted by n. The *size* of a graph G is the number of edges in G and we will often represent the

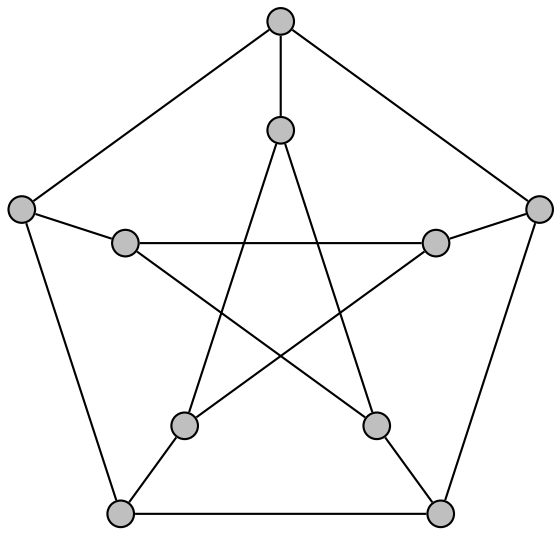

Figure 1.1: The Petersen graph

size by m. The number of edges incident to a vertex u is the *degree* of u, denoted by $d(u)$. The set $N(u) = \{v \in V(G) : u \sim v\}$ of all neighbours of a vertex u is the *neighbourhood* of u. Therefore for all $u \in V(G)$ we have $d(u) = |N(u)|$. The smallest value of the degree in a graph G is the *minimum degree* of G and is typically denoted by δ; similarly the *maximum degree* of G is $\Delta = \max\{d(u) : u \in V(G)\}$ (note however that the letter δ is also traditionally used for the defect of a graph, although this should cause no confusion). If there is some d such that $d(u) = d$ for every vertex u of G then G is *d-regular*, or just *regular*. A 3-regular graph is called *cubic*. For disjoint subsets $U_1, U_2 \subseteq V(G)$ we will denote the set of all edges between U_1 and U_2 by $E(U_1, U_2)$.

In the sum $\sum_{u \in V(G)} d(u)$ every edge is counted twice; this yields the 'first theorem' of graph theory (frequently called the *Handshaking Lemma*), which is due to Euler.

Theorem 1.1. *If a graph G has size m, then the sum of its vertex degrees satisfies*

$$\sum_{u \in V(G)} d(u) = 2m.$$

A *walk* W of length ℓ in a graph G is a sequence of vertices $u_0, u_1, \ldots, u_{l-1}, u_\ell$ such that $u_i \sim u_{i+1}$ for $0 \leq i \leq \ell - 1$. If the edges $u_i u_{i+1}$ are distinct for $0 \leq i \leq \ell - 1$ then the walk W is a *trail*. A *path* P_ℓ of length ℓ is a walk $u_0, u_1, \ldots, u_\ell$ such that all of the vertices $u_0, u_1, \ldots, u_\ell$ are distinct. The *initial* and *terminal* vertices of W are u_0 and u_ℓ respectively and W is a u_0, u_ℓ-walk (or trail/path as appropriate). W is *closed* if its initial and terminal vertices coincide. We will also say that W is *non-backtracking* if W does not include three consecutive vertices u, v, u, i.e. if the walk does not

traverse an edge $e = uv$ and then immediately retrace it in the opposite direction. If the length of a walk is $\leq k$, then we will speak of a $\leq k$-*walk*, $\leq k$-*path*, etc. The graph G is *connected* if for all $u, v \in V(G)$ there is a walk in G from u to v; otherwise G is *disconnected*.

The *distance* $d(u, v)$ between two vertices u and v is the length of a shortest path from u to v, when such a path exists. The *diameter* of G is defined to be $\max\{d(u, v) : u, v \in V(G)\}$.

A graph H is a *subgraph* of a graph G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. For any set U of vertices of G the subgraph $\langle U \rangle$ of G induced by U is the graph with vertex set U in which two vertices of $\langle U \rangle$ are adjacent if and only if they are adjacent in G. A subgraph H of G is an *induced subgraph* if $H = \langle V(H) \rangle$.

The *complete graph* K_n is the unique graph with n vertices such that all pairs of distinct vertices are adjacent to each other. Hence the size of K_n is $\binom{n}{2}$. The graph with n vertices and no edges is the *empty graph* E_n. A complete subgraph of a graph G is a *clique*, whereas an induced empty subgraph of G is an *independent set*; the size of the largest clique and independent set are the *clique number* and *independence number* of G respectively. A *cycle* C_ℓ of length ℓ is a walk $u_1, u_2, \ldots, u_\ell$ such that $u_1 \sim u_\ell$ and all of the vertices $u_1, \ldots, u_\ell$ are distinct. The *girth* of G is the length of the shortest cycle contained in G. At the other extreme, the longest cycle of G could pass through every vertex of G; in this case G is *Hamiltonian*.

The graph $G - S$ formed by deleting a set of vertices $S \subseteq V(G)$ is the subgraph of G induced by $V(G) - S$. We can also delete a set $E' \subseteq E(G)$ of edges: the graph $G - E'$ is the graph with vertex set $V(G)$ and edge set $E(G) - E'$. A *cutset* is a set of vertices such that $G - S$ is disconnected and an *edge cut* is a set of edges such that $G - E$ is disconnected. The *connectivity* $\kappa(G)$ of a connected graph G is defined to be the size of the smallest cutset of G (or $n - 1$ in the case $G = K_n$). G is k-connected if $\kappa(G) \geq k$. The *edge connectivity* $\lambda(G)$ is the size of the smallest edge cut of G and G is k-edge-connected if $\lambda(G) \geq k$. For any vertex u the set of edges incident with u forms an edge cut, so that $\lambda(G) \leq \delta(G)$. In fact we have the following inequality due to Whitney (a proof can be found in [28]):

$$\kappa(G) \leq \lambda(G) \leq \delta(G). \tag{1.1}$$

If equality holds throughout Inequality 1.1 then G is *maximally connected*. If the edge-connectivity satisfies $\lambda(G) = \delta(G)$ then G is *maximally edge-connected*. For some

maximally edge-connected graphs we can make a stronger statement about the structure of the edge cuts; in [24, 25] a graph G is defined to be *edge super-connected* or *super-λ* if all minimal edge cuts of G are of the form $E(\{u\}, V(G) - \{u\})$ for some vertex u of G. A super-λ graph is maximally edge-connected, but the converse does not hold.

1.1.1 Directed graphs

Often a real-life network that we wish to model will contain links that are one-way; for example during the pandemic one-way systems are enforced in many shops. We can describe this situation mathematically by allowing our network to contain directed *arcs*, which are ordered pairs of distinct vertices. A *directed graph* G, or *digraph* for short, consists of a set of vertices $V(G)$ and a set $A(G)$ of directed arcs. If there is an arc from a vertex u to a vertex v then we will write $u \to v$ and say that v is an *out-neighbour* of u and u is an *in-neighbour* of v. If $U_1, U_2 \subseteq V(G)$, then the set of arcs from U_1 to U_2 will be written as (U_1, U_2).

Let G be a digraph. The *out-neighbourhood* $N^+(u)$ of a vertex u of G is the set of all out-neighbours of u, i.e. $N^+(u) = \{v \in V(G) : u \to v\}$. Similarly, the *in-neighbourhood* $N^-(u)$ of u is the set $\{v \in V(G) : v \to u\}$ of all in-neighbours of u. The *out-degree* $d^+(u)$ of u is the number of out-neighbours of u and the *in-degree* $d^-(u)$ of u is the number of in-neighbours of u; thus $d^+(u) = |N^+(u)|$ and $d^-(u) = |N^-(u)|$. A vertex with out-degree zero is called a *sink* and a vertex with in-degree zero is a *source*.

The *in-degree sequence* of G is the sequence of values of $d^-(u)$ for all $u \in V(G)$, arranged in non-decreasing order. If there exists a value of d such that $d^+(u) = d$ for all vertices u of G, then G is *out-regular*. If furthermore we have $d^-(u) = d^+(u) = d$ for all vertices u, then G is *diregular*. For a diregular digraph we will often shorten 'out-degree' to 'degree'.

We will continue to use many of the definitions introduced for undirected graphs in the context of directed graphs, with suitable changes made to respect the direction of arcs. For example, a *directed walk* W of length ℓ is a sequence of vertices such that $u_i \to u_{i+1}$ for $0 \leq i \leq \ell - 1$; if all of the vertices in W are distinct, then W is a *directed path*. A *directed cycle* of length ℓ is a sequence $u_1, u_2, \ldots, u_\ell$ of distinct vertices such that $u_i \to u_{i+1}$ for $1 \leq i \leq \ell - 1$ and $u_\ell \to u_1$. It will be convenient to refer to a walk of length ℓ as a $\leq \ell$*-walk* and similarly a path of length $\leq \ell$ as a $\leq \ell$*-path*.

The *distance* $d(u,v)$ from vertex u to vertex v in a digraph is the length of the shortest directed path from u to v. In particular note that, in contrast to the undirected case, we may have $d(u,v) \neq d(v,u)$. The *diameter* of G is the largest value of $d(u,v)$ over all pairs of vertices u,v of G. For all $\ell \geq 1$ we define $N^{+\ell}(u) = \{v \in V(G) : d(u,v) = \ell\}$ and $N^{-\ell}(u) = \{v \in V(G) : d(v,u) = \ell\}$, so that $N^{+1}(u) = N^{+}(u)$ and $N^{-1}(u) = N^{-}(u)$. Putting $\ell = 0$ gives $N^0(u) = \{u\}$. For $0 \leq \ell \leq k$ we set $T_\ell(u) = \bigcup_{0 \leq r \leq \ell} N^{+r}(u)$ and $T_{-\ell}(u) = \bigcup_{0 \leq r \leq \ell} N^{-r}(u)$. Equivalently, $T_\ell(u)$ is the set of vertices of G that can be reached from u by paths of length $\leq \ell$ and $T_{-\ell}(u)$ is the set of vertices that can reach u by paths of length $\leq \ell$.

The *girth* of G is the length of the shortest directed cycle contained in G (if such a cycle exists). A digraph without directed cycles is *acyclic*. If clear from the context we will frequently dispose of the adjective 'directed' for such subgraphs.

In a digraph we may have arcs between the same pair of vertices, but in opposite directions, $u \to v$ and $v \to u$. This forms a 2-cycle or *digon*. A digraph without 2-cycles is an *oriented graph*; an oriented graph can be obtained by assigning a direction to every edge of a simple undirected graph. Conversely from any digraph G we can form the *underlying graph* of G by removing the directions from the arcs of G and removing all 2-cycles, i.e. in the underlying graph of G we set $u \sim v$ if and only if $u \to v$ or $v \to u$.

An orientation of a complete graph K_n is called a *tournament*. For every value of n there exists an acyclic tournament with order n. The *complete digraph* with order n is the unique digraph with an arc between each pair of distinct vertices in its vertex set. The *converse* of a digraph G is the digraph G' formed by reversing the direction of every arc in G. Given a digraph G we can also define a new digraph on the arc set of G: the *line digraph* G' of G is the digraph with vertex set $V(G')$ equal to the arc set $A(G)$ of G, with an arc in G' from an arc (x,y) of G to every arc of G of the form (y,z).

If the underlying undirected graph of a digraph G is connected then G is *weakly connected*; otherwise we can divide G into *weak components*, the vertex sets of which coincide with the connected components of the underlying graph of G. If G has the stronger property that for all pairs of vertices u,v of G there is a directed path from u to v then G is *strongly connected* or simply *strong*. An induced subdigraph of G that is maximal subject to strong-connectivity is a *strong component* of G; the relation of being 'mutually reachable' in G is an equivalence relation, so the strong components partition the vertex set of G.

(a) This digraph is not 2-geodetic

(b) This digraph is 2-geodetic but is not 3-geodetic

Figure 1.2: Digraphs with low geodetic girth

The size of the smallest set of vertices S such that $G - S$ is not strongly connected is the *strong connectivity* of G, which we will continue to denote by $\kappa(G)$; if $\kappa(G) \geq k$, then G is *k-connected*. We also define the *weak connectivity* of G to be the size of the smallest set $S \subset V(G)$ such that $G - S$ is not weakly connected; if a digraph G has weak connectivity at least k, then G is *k-weakly-connected*.

Similarly the *arc-connectivity* $\lambda(G)$ is the size of the smallest set A' of arcs such that $G - A'$ is not strongly connected; such a set is an *arc cut* and a digraph G is *k-arc-connected* if $\lambda(G) \geq k$. The nice inequality $\kappa(G) \leq \lambda(G) \leq \delta(G)$ continues to hold for directed graphs if $\delta(G)$ is interpreted to be $\min(\{d^-(u) : u \in V(G)\} \cup \{d^+(u) : u \in V(G)\})$ [77]. If equality holds, we will, as for undirected graphs, say that G is *maximally connected*. If all minimal arc cuts of G consist of all the arcs from a vertex u or the arcs to u, then G is *arc-superconnected* or super-λ.

A digraph G is *k-geodetic* if for each pair u, v of vertices of G there is at most one walk of length $\leq k$ from u to v. For every vertex u there is a trivial walk of length zero from u to u, so in particular the girth of a k-geodetic digraph is at least $k + 1$.

We shall refer several times to a family of digraphs called the *permutation digraphs*. These digraphs were introduced in [71] and more of their properties were derived in [36]. For $d, k \geq 2$ the permutation digraph $P(d, k)$ is defined as follows. The vertices of $P(d, k)$ are all permutations $x_0x_1 \ldots x_{k-1}$ of length k of symbols from the set $[d + k] = \{0, 1, \ldots, d + k - 1\}$. A vertex $x_0x_1 \ldots x_{k-1}$ has an arc to all permutations of the form $x_1x_2 \ldots x_{k-1}x_k$ for any $x_k \notin \{x_0, x_1, \ldots, x_{k-1}\}$. An example, $P(2, 2)$, is shown in Figure 3.2. It is simple to verify that $P(d, k)$ is diregular with out-degree d and is k-geodetic. The order of $P(d, k)$ is $n = (d + k)(d + k - 1) \cdots (d + 1)$ and has size $m = nd \sim n^{\frac{k+1}{k}}$.

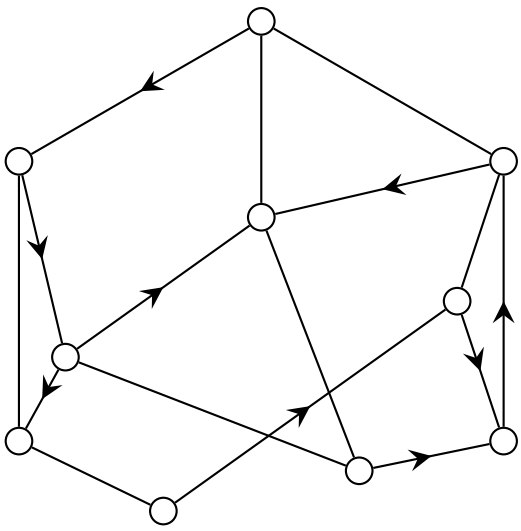

Figure 1.3: A mixed graph

1.1.2 Mixed graphs

More generally, a network may include both undirected links and directed arcs. A good example is the network of streets in a city, which will typically contain both two-way and one-way streets. A *mixed graph* G consists of a set $V(G)$ of vertices, a set $E(G)$ of undirected edges as well as a set of directed arcs $A(G)$. An example is shown in Figure 1.3. If for any pairs of vertices u, v there is an undirected edge between u and v or a directed arc from u to v then we will continue to write $u \sim v$ and $u \to v$ respectively. We will require all of our mixed graphs to be *simple*: we do not allow multiple arcs in the same direction (i.e. the arc (u, v) cannot occur more than once) or multiple edges between a pair of vertices, and we also will not admit mixed graphs in which there is both an edge and an arc between a pair of vertices, i.e. we do not allow both $u \sim v$ and $u \to v$. However digons are permissible; we can have $u \to v$ and $v \to u$ in G.

We can view a mixed graph as the union of two parts:

- The *undirected subgraph* of a mixed graph G is the undirected graph with vertex set $V(G)$ and edge set $E(G)$ and will be denoted by G^U.
- The *directed subgraph* of G is the directed graph with vertex set $V(G)$ and arc set $A(G)$ and will be denoted by G^Z.

Occasionally it will be helpful to work with these two subgraphs separately. To indicate the distance between two vertices u and v in the undirected subgraph and the directed subgraph we will write $d_U(u, v)$ and $d_Z(u, v)$ respectively.

As in the case of directed graphs, all definitions related to walks in mixed graphs must respect the direction of the arcs. In particular, a walk W of length ℓ in a mixed graph is a sequence $u_0, u_1, u_2, \ldots, u_\ell$ such that for each i in the range $0 \leq i \leq \ell - 1$ we have either $u_i \sim u_{i+1}$ or $u_i \to u_{i+1}$. As for undirected graphs, W is *non-backtracking* if W does not contain three consecutive vertices u, v, u such that there is an undirected edge $u \sim v$ (i.e. an undirected edge cannot be crossed and then immediately retraced in the opposite direction). We will abuse notation slightly for the sake of convenience and call a non-backtracking mixed walk a *mixed path*. The *distance* $d(u, v)$ from u to v is the length of the shortest mixed walk in G from u to v and the *diameter* of G is the maximum value of $d(u, v)$ over all pairs u, v of vertices. A mixed graph G is *k-geodetic* if for any pair u, v of vertices there is at most one mixed path (i.e. non-backtracking mixed walk) in G of length $\leq k$ from u to v. In accordance with our abuse of notation, a k-geodetic mixed graph cannot contain any non-trivial closed mixed walks of length $\leq k$.

The *undirected degree* of a vertex of G is the number of undirected edges of G that are incident with u. The undirected degree of u will be written simply as $d(u)$ and the collection of all undirected neighbours of u is $U(u)$; thus $U(u)$ is the neighbourhood of u in the undirected subgraph of G. The *directed out-degree* $d^+(u)$ of u is the number of directed arcs with u as initial vertex and the in-degree $d^-(u)$ of u is the number of arcs with u as terminal vertex. When bounding the vertex degrees of G we will tend to denote the undirected degree by the letter r and the directed out-degree by the letter z.

If there exist r and z such that every vertex of G has $d(u) = r$ and $d^+(u) = z$, then G is *out-regular*. If we have the stronger property that $d(u) = r$ and $d^-(u) = d^+(u) = z$ for every vertex u, then G is *totally regular*. Equivalently, G is totally regular if and only if G^U is regular and G^Z is diregular.

The *directed out-neighbourhood* $Z^+(u)$ of u in G is the out-neighbourhood of u in the directed subgraph of G and the *directed in-neighbourhood* $Z^-(u)$ of u in G is the in-neighbourhood of u in the directed subgraph. Therefore

$$U(u) = \{v \in V(G) : u \sim v\}, Z^+(u) = \{v \in V(G) : u \to v\}, Z^-(u) = \{v \in V(G) : v \to u\}.$$

For convenience, we also set

$$N^+(u) = U(u) \cup Z^+(u), N^-(u) = U(u) \cup Z^-(u).$$

Thus $N^+(u)$ is the set of vertices that can be reached by a mixed path of length one

from u and $N^-(u)$ is the set of vertices that can reach u by a mixed path of length one. If u is not contained in any digons then we will have $N^+(u) \cap N^-(u) = U(u)$.

1.1.3 Automorphisms

An *isomorphism* of a (directed, undirected or mixed) graph G to a graph H is a bijection $\phi : V(G) \to V(H)$ such that for all $u, v \in V(G)$ we have $u \sim v$ if and only if $\phi(u) \sim \phi(v)$ and $u \to v$ if and only if $\phi(u) \to \phi(v)$; in this case G and H are *isomorphic*. We will typically not distinguish between isomorphic graphs, except, for example, when counting the number of subgraphs of a graph G that are isomorphic to a graph H. An isomorphism from G to itself is an *automorphism* of G. The collection $\mathrm{Aut}(G)$ of automorphisms of a graph G forms a group under composition.

A graph G is *vertex-transitive* if for any two vertices u, v of G there exists an automorphism ϕ of G such that $\phi(u) = v$. In particular, a vertex-transitive undirected graph is regular, a vertex-transitive digraph is diregular and a vertex-transitive mixed graph is totally regular; the converse however does not hold. A digraph is *arc-transitive* if the automorphism group $\mathrm{Aut}(G)$ of G acts transitively on the arcs of G, i.e. for any two arcs $(u, v), (u', v') \in A(G)$ there is an automorphism ϕ of G such that $\phi(u) = u'$ and $\phi(v) = v'$. Every arc-transitive digraph without sinks must be vertex-transitive. More generally, a digraph is r-arc-transitive if for any two directed walks $u_0 \to u_1 \to u_2 \to \cdots \to u_r$ and $v_0 \to v_1 \to v_2 \to \cdots \to v_r$ of length r there exists an automorphism ϕ that maps u_i to v_i for $0 \leq i \leq r$.

A convenient way to construct vertex-transitive graphs is to define a graph using a group. Given a group H and any identity-free subset $S \subseteq H$ that generates the group, we define the Cayley digraph $\mathrm{Cay}(H, S)$ to be the digraph with vertex set H with an arc from $h \in H$ to $h' \in H$ if and only if $h' = hs$ for some $s \in S$. If S contains an element s as well as its inverse s^{-1} (for example, s could be an involution) then $\mathrm{Cay}(H, S)$ will contain the digon $h \to hs \to h$. Invertible elements in S allow us to introduce undirected edges. In the context of Cayley mixed graphs we will not allow digons, instead regarding any such digon as an edge. More formally, a Cayley mixed graph $\mathrm{Cay}(H, A, B)$ consists of a group H, which also constitutes the vertex set, an inverse-closed set A (i.e. $a \in A$ implies $a^{-1} \in A$) and an inverse-free set B ($b \in B$ implies that $b^{-1} \notin B$), such that the union $A \cup B$ generates H and does not contain the group identity; then we define the edge and arc sets of $\mathrm{Cay}(H, A, B)$ by inserting an edge $u \sim ua$ for each $u \in H$ and $a \in A$ and an arc $u \to ub$ for each $u \in H$ and $b \in B$. A Cayley graph of a cyclic group is called a *circulant*.

1.1.4 The adjacency matrix

It often happens that listing the vertices and edges of a graph, or alternatively presenting a drawing, is not the most efficient way of specifying a network. We can also uniquely determine a graph up to isomorphism by means of a single matrix, the *adjacency matrix*. For maximum generality, let G be a mixed graph; the definition of the adjacency matrix of undirected and directed graphs is a special case.

Definition 1.2. If a mixed graph G has order n, then the adjacency matrix $A(G)$ is the $n \times n$ matrix with rows and columns indexed (in the same order) by the vertices of G, with (u, v)-entry A_{uv} defined to be one if there is an edge $u \sim v$ or an arc $u \to v$, and zero otherwise.

Observe that if A is an undirected graph, then its adjacency matrix is symmetric; if G contains directed arcs this will typically not be the case. Representing graphs by matrices will also allow us to bring to bear the powerful methods of matrix algebra to the study of extremal graphs; this is possible thanks to the following theorem that connects the existence of walks of specified lengths with the entries of powers of the adjacency matrix.

Theorem 1.3. *If a mixed graph G (possibly purely undirected or directed) has adjacency matrix A, then the number of walks of length r from a vertex u to a vertex v of G is given by the (u, v)-entry of the matrix A^r.*

A proof for undirected graphs is given in [41] and this is not difficult to extend to directed and mixed graphs.

The adjacency matrix A of a graph G has an associated spectrum of n eigenvalues; we will refer to these as the *eigenvalues* of G (their value is evidently independent of the labelling of the vertices of G). The *characteristic polynomial* of G is the degree n polynomial $\det(xI - A)$. As the trace of a matrix is the sum of its eigenvalues, we have the following useful relation.

Lemma 1.4. *If G is a graph with order n and spectrum λ_i, $1 \leq i \leq n$, then if we let $W(u, \ell)$ be the number of closed u, u-walks of length ℓ in G, then*

$$\sum_{u \in V(G)} W(u, \ell) = \sum_{i=1}^{n} \lambda_i^{\ell}.$$

Proof. By Theorem 1.3 the (u, u)-entry of A^{ℓ} is $W(u, \ell)$. The spectrum of A^{ℓ} is λ_i^{ℓ},

$1 \leq i \leq n$, so the trace of A^ℓ is equal to the sum of $W(u, \ell)$ over all vertices u of G and the sum of the ℓ-th powers of the eigenvalues of G. □

1.2 Outline

In Chapter 2 we review the fundamental results of the three extremal problems that serve as the foundation and inspiration for this research: the degree/diameter problem, the degree/girth problem and Turán problems.

In Chapter 3 we motivate the degree/geodecity problem for directed graphs as an extension of the degree/girth problem for undirected graphs. We prove the existence of extremal digraphs, which we call *geodetic cages*, provide elementary upper and lower bounds on their order and discuss the problem of monotonicity of geodetic cages.

In Chapter 4 we study the natural first question for k-geodetic digraphs: do there exist k-geodetic digraphs with order one more than the directed Moore bound? We prove results on the structure of such digraphs and their automorphism groups and use this information to prove the non-existence of certain digraphs with excess one. We also provide strong divisibility conditions for the existence of a vertex-transitive digraph with excess one and conclude the classification of 2-geodetic digraphs with excess one.

Chapter 5 discusses the issue of regularity of extremal networks. It is easier to analyse the structure of k-geodetic digraphs that are diregular; therefore we use relatively complex counting arguments to show that all digraphs with out-degree two and excess two must be diregular to set the stage for our classification of such digraphs in the following chapter.

Chapter 6 begins with the proof of a connection between out-neighbourhoods and outlier sets in digraphs with small excess called the *Neighbourhood Lemma*. We use this result to complete the classification of digraphs with out-degree two and excess two that we began in Chapter 5 and as a result present the first non-trivial examples of geodetic cages. We then stretch our methods further to prove the non-existence of diregular digraphs with out-degree two and excess three.

We then generalise our discussion to mixed graphs in Chapter 7; these are networks containing both undirected links and directed arcs. We give a review of the degree/diameter problem for mixed graphs and thereby motivate our definition of the

degree/geodecity problem for mixed graphs. As in Chapter 3, we prove the existence of mixed geodetic cages and prove some monotonicity relations.

Chapter 8 deals with the question of total regularity of mixed graphs with order close to the Moore bound. We answer an open question of López and Miret by showing that any mixed graph with diameter two and defect one must be totally regular and, as a by-product, prove the same result for 2-geodetic mixed graphs with excess one. We also discuss total regularity of mixed graphs with defect or excess one for some values of the degree parameters for larger values of the diameter or geodecity.

In Chapter 9 we introduce a powerful counting argument that yields a strong lower bound on the excess of totally regular k-geodetic mixed graphs. This also allows us to extend the result that the outlier function of a digraph with excess one is an automorphism to mixed graphs with excess one. We then generalise our counting argument to give a slightly weaker bound that does not assume total regularity. We make practical application of these results by classifying some 2-geodetic mixed graphs with excess one. We also build on a result of Dalfó et al. by deriving a new lower bound on the defect of mixed graphs with undirected degree one, directed out-degree one and diameter $k \geq 3$. Finally we present the results of a computer search that identifies new mixed geodetic cages and gives upper bounds for some values of the degree parameters and geodetic girth for which geodetic cages have not yet been identified.

We change direction in Chapter 10 and take a different approach to studying geodetic girth in digraphs. Instead of bounding the out-degree and geodetic girth of a digraph, we ask the following Turán-type problem: what is the largest possible number of arcs in a k-geodetic digraph with given order n? We solve this problem completely. It turns out that the restriction of the problem to strongly-connected k-geodetic digraphs is much more complex; we offer a conjecture on the maximum size of such digraphs and prove it for $k = 2$. Finally we discuss some generalised Turán problems for k-geodetic digraphs.

We conclude our discussion in Chapter 11 by summarising the main results of the thesis, gathering together the main open problems that have arisen and suggesting some directions for future research.

Chapter 2

Background

In this chapter we provide some background material on the three problems that are the foundation for this research: the degree/diameter problem, the degree/girth problem and Turán problems. As three of the cornerstones of modern extremal graph theory, each of these problems has an extremely large and rapidly growing literature. Therefore we make no attempt at an exhaustive survey of any of these fields, but refer the reader to survey papers for each problem. For an introduction to all three questions see also the classic work [26] of Bollobás.

2.1 The undirected degree/diameter problem

The problem now known as the degree/diameter problem was first raised by Edward Forrest Moore. It was inspired by the design of efficient interconnection networks. A survey of the degree/diameter problem for both undirected and directed graphs is given in [119], which lists more than 350 references in the 2013 edition.

Problem 2.1 (Degree/diameter problem for undirected graphs)**.** *What is the largest possible order of a graph with maximum degree d and diameter k?*

Moore pointed out the following simple upper bound for the order of a graph G with given maximum degree d and diameter k. Fix a vertex u of G; we are going to grow a tree (the *Moore tree*) of depth k rooted at u. Call the root vertex Level 0 of the tree. Below u at Level 1 draw the $\leq d$ neighbours $u_1, u_2, \ldots, u_{d(u)}$ of u. For each of these neighbours u_i draw their other neighbours (i.e. apart from u) below them at Level 2 of the tree. In general for $1 \leq t \leq k-1$ each vertex v at Level t will have an edge to a vertex v' at Level $t-1$ and we draw edges from v to Level $t+1$ to every neighbour of v apart from v'. As G has diameter k, every vertex of G is contained at least once in this tree. The Moore tree for a 3-regular graph with diameter $k = 3$ is shown in Figure 2.1.

Observe that the root vertex u has at most d neighbours in Level 1 and every vertex at Level t (where $1 \leq t \leq k-1$) has an edge to Level $t-1$ and hence has at most $d-1$ edges to Level $t+1$. In general there are at most $d(d-1)^{t-1}$ vertices at distance

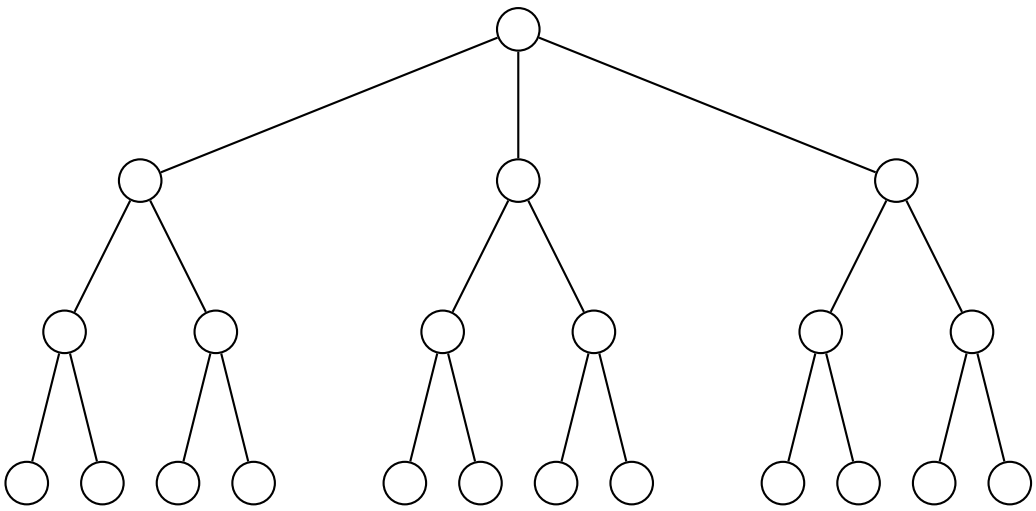

Figure 2.1: The Moore tree for $d = 3$ and diameter $k = 3$.

t from the root u for $1 \leq t \leq k$. It follows that the order of the graph is bounded above by

$$1 + d + d(d-1) + d(d-1)^2 + \cdots + d(d-1)^{k-1}.$$

This upper bound is named the *Moore bound* (for undirected graphs). In particular the Moore bound for a graph with maximum degree d and diameter two is given by $d^2 + 1$. We will not introduce special notation for this bound, as we will make more use of the analogous Moore bound for directed graphs (see Section 2.3).

A graph that meets this bound is called a *Moore graph*. It is easily seen that a graph G meets the Moore bound if and only if i) it is d-regular, ii) G has diameter k and iii) all of the vertices in the Moore tree are distinct. Condition iii) will be met if and only if the girth of G is at least $2k + 1$.

The first paper that appeared on the subject of Moore graphs was [91] by Hoffman and Singleton. They used elegant spectral methods to show that the only possible values of the degree d for which a Moore graph with diameter two can exist are $d = 2, 3, 7$ or 57. Moore graphs with diameter two and degrees $d = 2, 3$ and 7 do exist; these graphs are given by the 5-cycle C_5 for $d = 2$, the Petersen graph (shown in Figure 1.1) with order 10 for $d = 3$ and the Hoffman-Singleton graph with order 50 for $d = 7$. The existence of a Moore graph with diameter two, degree 57 and order 3250 is a famous open problem in graph theory; this hypothetical graph is known as the *missing Moore graph*. The three Moore graphs with diameter two and degrees $d = 2, 3$ and 7 are all vertex-transitive. By contrast, it is known that if the missing Moore graph does exist, then it has at most 375 automorphisms [109], which is a very small number compared with the order of the graph.

In [91] the authors also showed that the unique Moore graph with diameter $k = 3$ is the 7-cycle C_7. This result was extended to show that the only Moore graphs with diameter $k \geq 3$ are the cycles with length $2k + 1$. This was proven independently by Damerell [52] using results on distance-regularity and by Bannai and Ito [11] using spectral methods.

As Moore graphs are so scarce, we are forced to consider graphs with order less than the Moore bound by some *defect* δ. Erdős et al. proved that apart from C_4 there are no graphs with diameter two and defect one, i.e. order one less than the Moore bound [61]. This non-existence result was later extended by Bannai and Ito [12] and Kurosawa and Tsujii [94], showing that graphs with defect one exist only trivially in the form of cycles. There is a large literature on the existence of graphs with small defect $\delta \geq 2$, for which we refer the reader to [119]. Notable highlights include the following theorems.

Theorem 2.2.

- *There are exactly two cubic graphs with diameter $k = 2$ and defect $\delta = 2$ and a unique cubic graph with defect $\delta = 2$ and diameter $k = 3$, but there are no such cubic graphs with diameter $k \geq 4$ ([96]).*
- *There is a unique graph with degree $d = 4$, diameter $k = 2$ and defect $\delta = 2$ ([34]), but no graphs with degree $d = 4$, defect $\delta = 2$ and larger diameter $k \geq 3$ ([69]).*
- *There are no cubic graphs with defect $\delta \leq 4$ and diameter $k \geq 5$ ([117]).*
- *There are no graphs with diameter $k = 2$, defect $\delta = 2$ and degree d in the range $6 \leq d \leq 49$ ([44]).*

An alternative approach to searching for graphs with small defect is to try to construct families of graphs with large order. The family of *de Bruijn graphs* have degree d, diameter k and order asymptotically equal to $(\frac{d}{2})^k$ (see [54]). For odd diameter, this can be improved to order approximately $2(\frac{d}{2})^k$ using graphs on alphabets [81]. Canale and Gómez provide an asymptotic improvement to this bound in [40] by constructing graphs of order approximately $(\frac{d}{1.6})^k$ for infinitely many pairs d, k. It is also known that the Moore bound for diameters $k = 2, 3$ and 5 can be approached asymptotically as d tends to infinity [55]. For example, in [135] graphs with diameter $k = 2$, suitably large degree d and order at least $d^2 - 2d^{1.525}$ are constructed by making suitable modifications to the Brown graphs.

As noted in Chapter 1, it is frequently desirable for a network to have a large degree of symmetry; it is therefore significant that the preceding result can be strengthened

to show that the Moore bounds for diameters two and three can be approached asymptotically by Cayley graphs [8, 130]. Other families of large Cayley graphs are given in [67]; however, these typically have order only a small fraction of the Moore bound.

2.2 The undirected degree/girth problem

As we saw in Section 2.1, there are very few Moore graphs. In the degree/diameter problem we widened our view to include graphs in which the Moore tree contains some repeated vertices, or equivalently, in which the girth is $\leq 2k$. It is easily seen that a graph is Moore if and only if it is d-regular, has diameter k and girth $2k+1$. We can also take the 'converse' approach to studying graphs with a 'Moore-like' structure: instead of keeping the diameter condition and relaxing the requirement on the girth, we can demand that the girth of the graph be $2k+1$, but allow the diameter to be $\geq k+1$; this corresponds to requiring all of the vertices in an arbitrary Moore tree of depth k for the graph to be distinct, but without the condition that the tree should contain all vertices of the graph. This gives rise to the *undirected degree/girth problem.*

Problem 2.3 (Degree/girth problem for undirected graphs)**.** *What is the smallest possible order of a graph with minimum degree d and girth $g = 2k+1$?*

By the same counting argument that we used to obtain an upper bound on the order of a graph with given degree and diameter, we see that the undirected Moore bound $1 + d + d(d-1) + \cdots + d(d-1)^{k-1}$ also serves as a lower bound on the order of a graph with minimum degree d and girth $2k+1$. With the exception of the rare cases in which there exists a Moore graph, the order of the graph will exceed the Moore bound by some (hopefully small) *excess* ϵ. We are particularly interested in the extremal graphs.

Definition 2.4. A smallest possible graph with minimum degree d and girth g is a (d, g)-*cage*; if the degree and girth are clear from the context, then we call such a graph simply a *cage*.

The classic survey of the degree/girth problem is [68]; see also [23] for the definitive paper on the degree/girth problem for cubic graphs. The degree/girth problem is traditionally defined for regular graphs, but in the context of graphs with small excess this is not a significant restriction. It must also be pointed out that smallest graphs with given degree and even girth $g = 2k$ are also of interest in the degree/girth

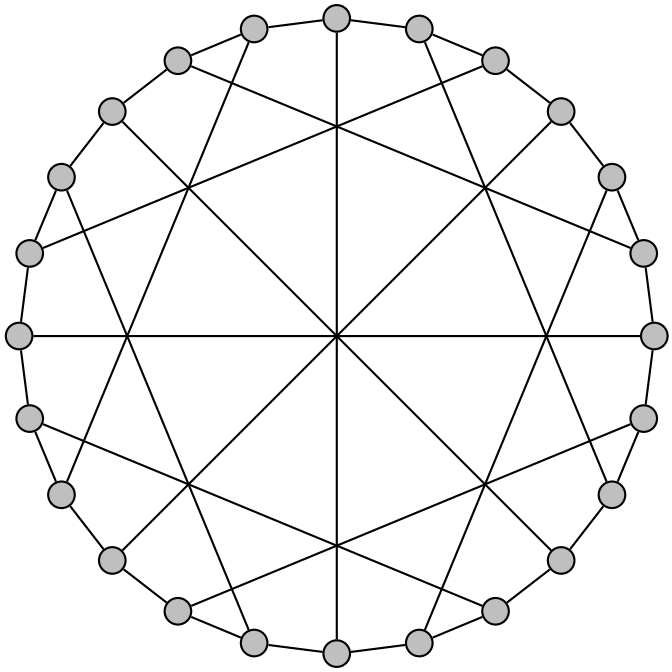

Figure 2.2: The McGee graph, the unique $(3, 7)$-cage

problem (in which case the lower bound is derived by hanging a Moore tree from an edge rather than a vertex), but we will not touch further on this case here, except to say that the existence of a Moore graph with even girth is connected with the existence of *generalised n-gons*. The smallest cubic cage that is not also a Moore graph is the unique $(3, 7)$-cage called the McGee graph, which is displayed in Figure 2.2. The Moore bound for degree $d = 3$ and girth $g = 7$ is $n = 22$, whereas the McGee graph has order 24 and hence excess $\epsilon = 2$.

Using quite involved spectral techniques Bannai and Ito demonstrated that there are no graphs with excess one and girth $g \geq 5$ apart from cycles. Therefore if $g \geq 6$ or $g = 5$ and $d \notin \{2, 3, 7, 57\}$, then the smallest possible order of a d-regular graph with girth g is at least two more than the Moore bound. In fact this remains the only completely general lower bound.

Theorem 2.5 ([12])**.** *For $d \geq 3$ and $g \geq 5$ there are no regular graphs with excess one.*

One subtle point that does not arise in the degree/diameter problem is that it is not immediately clear that cages exist for all values of d and g; therefore it is necessary to prove that for any $d \geq 2$ and $g \geq 3$ there exists a graph with degree d and girth g. This result was first shown in 1963 by Sachs in [126] by a recursive construction. The upper bound in [126] was subsequently improved in a joint paper by Sachs and Erdős [62]. An approachable presentation of these proofs is given in an appendix of [68]. These upper bounds were further improved in 1967 by Sauer; we present his

result only for odd girth.

Theorem 2.6 ([127]). *For all $d \geq 2$ and odd $g \geq 3$, the order of a (d, g)-cage does not exceed $2(d-2)^{g-2}$.*

Thus we have the unfortunate situation that the best known general constructions are orders of magnitude away from the Moore bound. The best known general upper bound on the order of cages is due to a construction of Lazebnik, Ustimenko and Woldar.

Theorem 2.7 ([101]). *Let $d \geq 2$ and $g \geq 5$ and let q be the smallest odd prime power such that $d \leq q$. Then the order of a (d, g)-cage does not exceed $2dq^{\frac{3g}{4}-a}$, where $a = 4, \frac{11}{4}, \frac{7}{2}$ and $\frac{13}{4}$ for $g \equiv 0, 1, 2, 3 \pmod 4$ respectively.*

2.2.1 Properties of cages

It is intuitively obvious that the order of (d, g)-cage should grow with increasing d and g; however, this is surprisingly non-trivial to prove. Monotonicity in g was proven by Fu, Huang and Rodger in [73]; we will generalise their approach to mixed graphs in Chapter 7. Monotonicity in the degree remains an open question, but a partial result is contained in [150]. For the statement of the following theorems let $f(d, g)$ be the order of (d, g)-cage.

Theorem 2.8 ([73]). *For $d \geq 2$ and $g \geq 3$ the function $f(d, g)$ is strictly increasing in g, i.e. $f(d, g) < f(d, g+1)$.*

Theorem 2.9 ([150]). *For $d \geq 2$ and $g \geq 3$ we have $f(d, g) \leq f(d+2, g)$. Also $f(2, g) < f(3, g)$.*

It also follows from a result of Tashkinov on 3-factors in [140] that $f(3, g) \leq f(4, g)$.

Another structural property of cages that has received a great deal of attention is connectivity. The following conjecture was made by Fu, Huang and Rodger.

Conjecture 2.10 ([73]). *All (d, g)-cages are d-connected.*

In their paper [73], the authors of this conjecture proved that all cages are at least 2-connected. It was shown independently in [53, 95] that cages are 3-connected. Whilst we are more concerned with the case of odd girth, it is known that the (d, g)-cages with girth six and eight are d-connected [112]. A major step towards Conjecture 2.10 was taken in [10], which showed that (d, g)-cages are at least

$\lceil \frac{d}{2} \rceil$-connected for odd girth $g \geq 3$. However a complete proof of Conjecture 2.10 remains elusive.

By contrast, the edge connectivity of cages is completely understood. In [151] Wang et al. showed that cages with odd girth are maximally edge-connected, i.e. if G is a (d, g)-cage for odd $g \geq 3$, then $\lambda(G) = d$. This result was extended to even girths in [103]. The edge-connectivity of any cage is thus equal to its degree. However in [111] Marcote and Balbuena showed the much stronger property that cages with odd girth are edge-superconnected, i.e. all minimal edge cuts of a (d, g)-cage G for odd $g \geq 3$ are of the form $E(\{u\}, V(G) - \{u\})$ for some vertex u of G. The even-girth version of this result was proven in [102]. For the many papers on connectivity of cages that we have not had space to mention here we again refer the reader to the survey [68].

2.3 The degree/diameter problem for directed graphs

2.3.1 Moore digraphs

The degree/diameter problem has also been studied extensively in the setting of directed graphs in the following form (see the second section of the survey [119]).

Problem 2.11 (Degree/diameter problem for directed graphs)**.** *What is the largest possible order of a directed graph with maximum out-degree d and diameter k?*

We can derive a Moore bound for directed graphs using a directed Moore tree. Let G be a digraph with maximum out-degree d and diameter k. Fix a root vertex u at Level 0 and for each t in the range $0 \leq t \leq k-1$ draw below each vertex v at Level t an arc to each out-neighbour of v at Level $t+1$. As each vertex of G has $\leq d$ out-neighbours, it can be shown by induction that for $0 \leq t \leq k$ there are at most d^t vertices at distance t from u. The directed Moore tree for out-degree $d = 3$ and diameter $k = 2$ is shown in Figure 2.3.

This shows that the order of such a digraph is bounded above by the *directed Moore bound* $M(d, k) = 1 + d + d^2 + \cdots + d^k$. Due to its importance we include this expression as a separate definition.

Definition 2.12. For $d, k \geq 2$ the directed Moore bound is

$$M(d, k) = 1 + d + d^2 + \cdots + d^k = \frac{d^{k+1} - 1}{d - 1}.$$

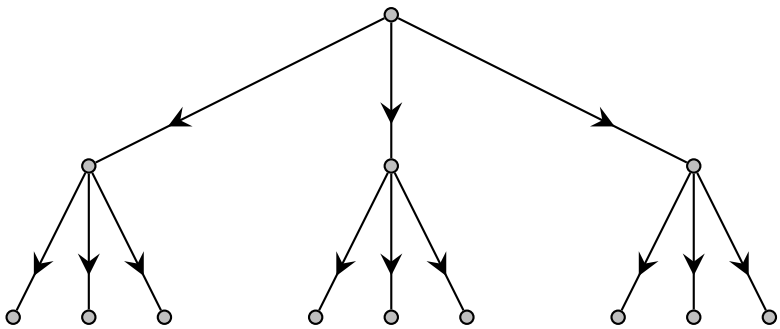

Figure 2.3: The Moore tree for out-degree $d = 3$ and diameter $k = 2$

One feature of the directed degree/diameter problem that distinguishes it from the undirected version of the problem is the fact that there are no *Moore digraphs*, except for directed $(k+1)$-cycles with $d = 1$ and complete digraphs with diameter $k = 1$, which we will refer to as trivial Moore digraphs. This was first proven in 1974 by Plesník and Znám in [123]. A very elegant independent proof using spectral theory was presented by Bridges and Toueg in 1980 [33]. As we will later make use of such spectral arguments we reproduce their proof as an introduction to the method. Again observe that a digraph is Moore if and only if it is diregular with degree d, has diameter k and is k-geodetic.

Theorem 2.13 ([33])**.** *There are no non-trivial Moore digraphs.*

Proof. Let G be a Moore digraph with out-degree $d \geq 2$ and diameter $k \geq 2$. Let A be the adjacency matrix of G. For any two vertices u, v of G there is a unique directed walk of length $\leq k$ from u to v. It follows from Theorem 1.3 that

$$I + A + A^2 + \cdots + A^k = J,$$

where I is the $n \times n$ identity matrix and J is the $n \times n$ all-one matrix. The eigenvalues of J are n and 0 with multiplicity $n - 1$. It follows that the eigenvalues of G are d together with $n - 1$ other eigenvalues λ_i, $1 \leq i \leq n - 1$, each of which satisfies $1 + \lambda_i + \lambda_i^2 + \cdots + \lambda_i^k = 0$. Hence each λ_i is a $(k+1)$-th root of unity, $\lambda_i^{k+1} = 1$.

The trace of any matrix is the sum of its eigenvalues. Furthermore, by Theorem 1.3 for $0 \leq j \leq k$ the trace of A^j is the sum over all vertices $u \in V(G)$ of the number $W(u, j)$ of closed u, u-walks of length j; as G is k-geodetic, there can be no such walks, so that

$$\mathrm{Tr}(A^j) = d^j + \sum_{i=1}^{n-1} \lambda_i^j = 0.$$

For each λ_i, $1 \leq i \leq n-1$, we have $\overline{\lambda_i} = \lambda_i^{-1} = \lambda_i^k$, so, as d is a real number, it follows that

$$-d = \sum_{i=1}^{n-1} \lambda_i = \sum_{i=1}^{n-1} \overline{\lambda_i} = \sum_{i=1}^{n-1} \lambda_i^k = -d^k.$$

Thus $d = d^k$, which implies that either $d = 1$ or $k = 1$. □

2.3.2 Almost Moore digraphs

Given this embarrassing lack of Moore digraphs, we ask instead for digraphs with out-degree d, diameter k and order $M(d,k) - \delta$, where δ is the defect of the digraph. We will call such a digraph a $(d,k;-\delta)$-*digraph*. The obvious question is whether there exist any non-trivial digraphs with defect one? Such a digraph is called an *almost Moore digraph*. Any almost Moore digraph G must be out-regular and so for any vertex u of G there is exactly one vertex $r(u)$ of G (called the *repeat* of u) that occurs twice in the Moore tree rooted at u.

Definition 2.14. The *repeat function* of a digraph G with maximum out-degree d, diameter k and order $M(d,k) - 1$ is the function $r : V(G) \to V(G)$ defined by the following condition: for any vertex u of G, $r(u)$ is the unique vertex of G such that there are two distinct $u, r(u)$-walks in G with length not exceeding k.

It was proven in [15] that the repeat function is actually an automorphism of any almost Moore digraph. This connection between the existence of short paths in G and the global symmetries of G has proven to be extremely fruitful. If we represent the repeat function of G by a permutation matrix P, then Theorem 1.3 shows that the adjacency matrix A of G satisfies

$$I + A + A^2 + \cdots + A^k = J + P.$$

It turns out that there are infinitely many almost Moore digraphs. Up to isomorphism there are three $(2,2;-1)$-digraphs [114], which are displayed in Figure 2.4. In [72] Fiol et al. constructed an almost Moore digraph with diameter $k = 2$ and any degree $d \geq 3$ by iterating the line digraph operation. The classification of almost Moore digraphs with diameter two was completed by Gimbert using the spectral technique; it transpires that the almost Moore digraphs identified in [72] are the unique digraphs with defect one with these parameters. Interestingly then in the undirected degree/diameter problem there exist non-trivial Moore graphs, but no

non-trivial almost Moore graphs, whereas in the directed problem there are no non-trivial Moore digraphs, but infinitely many digraphs with defect one.

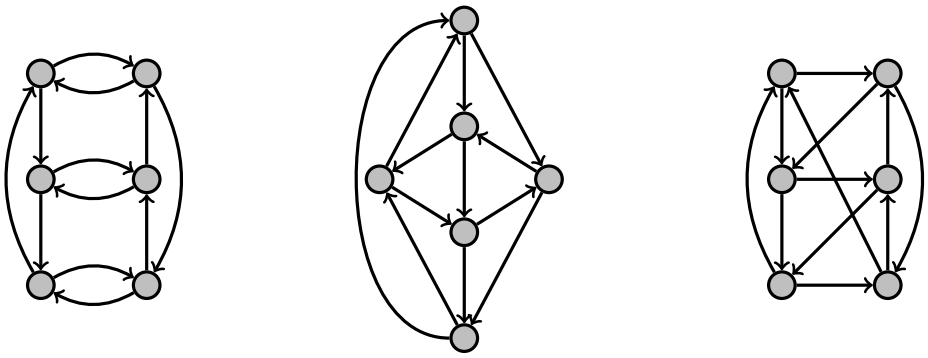

Figure 2.4: The three $(2, 2; -1)$-digraphs

The picture for larger diameters $k \geq 3$ is much less clear. Conde, Gimbert et al. extended the use of the spectral method to demonstrate a link between the existence of almost Moore digraphs with diameter k and the irreducibility of the polynomial $\Phi_n(1 + x + x^2 + \cdots + x^k)$, where Φ_n is the n-th cyclotomic polynomial [47]. Using this relationship and some algebraic number theory they proved in [46, 47] that there are no almost Moore digraphs with diameters $k = 3$ or 4 and out-degree $d \geq 2$. More generally, it is shown in [45] that the non-existence of almost Moore digraphs with diameter $k \geq 3$ follows from a conjecture concerning the irreducibility of the aforementioned polynomials; the authors use this to show the non-existence of almost Moore digraphs with diameter $k = 5$ and degree $d \leq 6$.

Another approach to the existence of almost Moore digraphs is to restrict attention to a fixed value of the out-degree d. Using counting arguments Miller and Friš showed that there are no almost Moore digraphs with out-degree $d = 2$ and diameter $k \geq 3$.

The next case to consider is the existence of $(3, k; -1)$-digraphs. The same paper [15] that showed that the repeat function r is an automorphism gave a strong divisibility condition for the existence of a $(3, k; -1)$-digraph, specifically that if such a digraph exists, then $(k + 1)$ divides $\frac{9}{2}(3^k - 1)$; this rules out the existence of such digraphs for infinitely many k. A later paper [16] ruled out the existence of almost Moore digraphs with degree three lying in a certain class of Cayley digraphs. These efforts culminated in a complete proof of the non-existence of $(3, k; -1)$-digraphs in [17]. For larger d, some inroads were made into the problem of the existence of $(4, k; -1)$- and $(5, k; -1)$-digraphs in [48] using the spectral method.

These results were in large measure facilitated by investigations into the permutation structure of the repeat function of a digraph G with defect one. Viewed as a

permutation, the repeat function r can contain cycles of length one if a vertex u of G lies in a directed k-cycle; such a vertex is called a *self-repeat*. Baskoro et al. showed in [14] that a $(d, k; -1)$-digraph contains at most one k-cycle, so that there are either no self-repeats, or exactly k self-repeats. Choliliy, Baskoro et al. also derived a great deal of information on the possible cycle structure of r in papers including [13] and [42], in which these results are again used to produce divisibility conditions for the existence of an almost Moore digraph.

2.3.3 Digraphs with larger defect

In general, we are forced to consider the possibility of there being many repeated vertices in the Moore tree; a complicating factor is that one vertex could appear several times in the tree. For a vertex u of a $(d, k; -\delta)$-digraph G we therefore consider the *repeat multiset* $R(u)$ of u (which, by a common abuse of notation, we will always call the *repeat set*); we define $R(u)$ by specifying that any vertex v that appears $t \geq 2$ times in the Moore tree of depth k rooted at u appears $t - 1$ times in $R(u)$. Thus if G is out-regular, then $R(u)$ has δ elements for any $u \in V(G)$.

The first study of digraphs with defect $\delta \geq 2$ is found in [113], in which Miller uses quite complex counting arguments to derive an extremely strong divisibility condition on the possible values of the diameter k of a diregular $(2, k; -2)$-digraph, i.e. if there exists such a digraph, then $(k + 1)$ must divide $2(2^{k+1} - 3)$. In fact, there are only two values of k in the range $3 \leq k \leq 10^7$ that satisfy this condition [113]. This line of enquiry was completed in [118], which showed that there are no diregular $(2, k; -2)$-digraphs with diameter $k \geq 3$; this paper is the inspiration for the research contained in Chapter 6.

For larger defect δ, we no longer have the nice properties of the repeat automorphism to work with; however, we do have the next best thing. For any subset U of vertices of a $(d, k; -\delta)$-digraph, we define $N^+(U)$ to be the multiset $\bigcup_{u \in U} N^+(u)$ (so that a vertex v appears r times in $N^+(U)$ if it is an out-neighbour of r vertices in U). Similarly for a set U of vertices we define $R(U)$ to be the multiset union $\bigcup_{u \in U} R(u)$. It was proved by Sillasen in her thesis that these multisets obey the following relation, called the *Neighbourhood Lemma*, which is an extension of the concept of an automorphism.

Lemma 2.15 ([131]). *If G is a diregular $(d, k; -\delta)$-digraph, then*

$$N^+(R(u)) = R(N^+(u))$$

for all vertices $u \in V(G)$.

Sillasen used this powerful result in [131] to give the first result for digraphs with defect three, namely that the girth of any diregular $(2, k; -3)$-digraph is at least k.

Experience suggests that it is harder to come close to the Moore bound for increasing values of the out-degree d and diameter k. However, as we have seen, proving even a lower bound of two for the defect of digraphs with diameter $k \geq 3$ is a difficult problem. The only progress in providing a larger general bound is due to a recent result by Filipovski and Jajcay [70], which answers a question of Bermond and Bollobás by showing that for any positive integer c there is a degree/diameter pair (d, k) such that any $(d, k; -\delta)$-digraph has defect $\delta \geq c$.

Rather than looking for digraphs with order very close to the directed Moore bound, an alternative approach to the directed degree/diameter problem is to ask for families of large digraphs. Recall that for the undirected degree/diameter problem the largest known graphs for general d and k have asymptotic order significantly smaller than the Moore bound. By contrast, in the directed version of the problem we have a family of digraphs, the *Kautz digraphs*, with order asymptotically equal to the Moore bound for fixed diameter.

The Kautz digraph $K(d, k)$ defined in [98] has out-degree d, diameter k and order $d^k + d^{k-1}$. They can be constructed as follows. Let Ω be an alphabet of size $d+1$. The vertex set of $K(d, k)$ consists of all strings $x_0x_1 \ldots x_{k-1}$ of length k of symbols drawn from Ω, with the sole condition that for $0 \leq i \leq k-2$ we have $x_i \neq x_{i+1}$. We define the arcs by the relation $x_0x_1x_2 \ldots x_{k-1} \to x_1x_2 \ldots x_{k-1}x_k$ for any $x_k \in \Omega - \{x_{k-1}\}$. Kautz digraphs are essentially iterated line digraphs of complete digraphs and as such are a generalisation of the almost Moore digraphs considered in [72].

2.3.4 Diregularity of digraphs with small defect

It is easily shown that a $(d, k; -\delta)$-digraph with defect $\delta < M(d, k-1)$ must be out-regular. However, one major issue that we did not draw attention to in the preceding subsections is the problem of diregularity: must a $(d, k; -\delta)$-digraph with small defect δ be diregular? The analysis in Subsections 2.3.2 and 2.3.3 holds only for diregular digraphs, so it is conceivable that there could be digraphs with small defect and a more elusive, less 'balanced' structure that are not covered by the above reasoning.

The first paper to address this problem was [115], in which Miller et al. deduced relations between the set $S = \{u \in V(G) : d^-(u) < d\}$ of vertices with 'too small' in-degree and the set $S' = \{u \in V(G) : d^-(u) > d\}$ of vertices with 'too large' in-degree to show that any almost Moore digraph must be diregular.

Results on the diregularity of digraphs with defect two are mainly due to Slamin. In [137] Slamin and Miller prove that $(2, k; -2)$-digraphs are diregular, so that, combined with the result of [118], it follows that there are no $(2, k; -2)$-digraphs with $k \geq 3$. The paper [136] also gives some information on the structure of a non-diregular $(3, k; -2)$-digraph, although the existence of non-diregular $(3, k; -2)$-digraphs is still an open question. Some more general results on non-diregular $(d, k; -2)$-digraphs can be found in [50], which shows that such digraphs must be 'nearly diregular' in a certain precise sense.

In [138] the same authors found a method to derive from a diregular $(d, k; -\delta)$-digraph a non-diregular $(d, k; -(\delta + 1))$-digraph. A natural conjecture is that largest $(d, k; -\delta)$-digraphs are all diregular; however, this result shows that the order of the largest non-diregular digraph with given out-degree and diameter lags behind the order of the largest diregular digraph by at most one (and could potentially exceed it). In [131] Sillasen also derives some structural information on non-diregular $(2, k; -3)$-digraphs. To the author's knowledge, the aforementioned conjecture has not been spelt out explicitly in the literature, so we record it here specially.

Conjecture 2.16. *If G is a largest possible digraph with out-degree d and diameter k, then G is diregular.*

2.4 Turán problems

Turán-type problems constitute one of the most investigated areas of extremal graph theory; these problems are discussed in detail in [26] and a survey is given in [74]. A Turán problem typically asks for the largest possible size of a graph G with a family $\mathcal{F}$ of forbidden subgraphs. The first Turán-type problem to be solved was published in 1907 by Mantel. In [110], Mantel proved that the largest possible number of edges in a triangle-free graph with order n is given by $\lfloor \frac{n^2}{4} \rfloor$ and this bound is achieved by the complete bipartite graph $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. This was later generalised by Turán in 1941 to the largest possible size of a graph with clique number $\leq r$.

Theorem 2.17 ([147])**.** *The number of edges of a K_{r+1}-free graph H is at most $(1 - \frac{1}{r})\frac{n^2}{2}$.*

Surprisingly, the more general asymptotic problem for families of non-complete forbidden subgraphs is not significantly more complicated; Erdős, Stone and Simonovits showed in [63, 65] that if we set $r = \min\{\chi(F) : F \in \mathcal{F}\}$ and $r \geq 2$, then the largest possible size of a graph with order n and no subgraphs belonging to $\mathcal{F}$ is asymptotic to $(1 - \frac{1}{r})\frac{n^2}{2}$. However, if $\mathcal{F}$ contains a bipartite graph the problem is much more difficult.

One such question was investigated by Erdős, who asked in 1975 for the largest possible size of a graph with order n containing no C_3 or C_4 [60]. If this extremal size for given order n is denoted by $f(n)$, then his conjecture can be written as $f(n) = (\frac{1}{2} + o(1))^{3/2} n^{3/2}$. It is shown in [75] that

$$\frac{1}{2\sqrt{2}} \leq \liminf_{n\to\infty} \frac{f(n)}{n^{\frac{3}{2}}} \leq \limsup_{n\to\infty} \frac{f(n)}{n^{\frac{3}{2}}} \leq \frac{1}{2}. \tag{2.1}$$

The article [75] finds exact values of $f(n)$ for $n \leq 24$ and gives constructive lower bounds for larger n. The latest results on the problem are given in [29]. However, no significant progress has been made on reducing the gap between the coefficients in the upper and lower bounds in Equation 2.1. More generally, one can ask for the largest size of a graph with order n and girth $\geq g$ for $g \geq 4$; for $g \geq 6$ the bounds on this problem are not well understood. Examples of some of the many papers dealing with $g \geq 6$ are [1, 2, 139].

2.4.1 Looking forward

One of the main goals of this thesis is to investigate a problem, called the *degree/geodecity problem*, that is a generalisation of the degree/girth problem to directed graphs, in which we search for k-geodetic digraphs with order slightly exceeding the Moore bound. The analogue of the repeat function (or repeat set) for the degree/geodecity problem is the *outlier function* (resp. *outlier set*). We will see that there is a strong analogy between the notions of repeat and outlier and that we can learn a great deal about k-geodetic digraphs with order close to the Moore bound by combining spectral techniques, counting arguments, neighbourhood relations and permutation structures. In Chapter 10, we will also discuss a directed version of the Turán problem for graphs with prescribed girth.

Chapter 3

The degree/geodecity problem

3.1 Motivation

The undirected degree/girth problem asks for the smallest order of a graph with minimum degree d and girth g. It is of great interest to ask how this problem can be adapted to the setting of directed graphs. The directed degree/girth problem is a natural extension of the undirected degree/girth problem.

Question 3.1 (Directed degree/girth problem)**.** *What is the smallest possible order of a digraph with minimum out-degree d and girth g?*

Let us denote the order of the smallest digraph with out-degree d and girth g by $f(d, g)$. In [19] Behzad, Chartrand and Wall proved the upper bound $f(d, g) \leq d(g-1)+1$ for all $d \geq 1$ and $g \geq 2$. This bound is attained by the circulant digraph on $\mathbb{Z}_{d(g-1)+1}$ with connection set $\{1, 2, \ldots, d\}$. In the same paper [19] the authors conjecture that equality holds for diregular digraphs.

Conjecture 3.2. *For all $d \geq 1$ and $g \geq 2$ the smallest order of a diregular digraph with degree d and girth g is $d(g-1)+1$.*

This conjecture was proven for all digraphs with degree $d = 2$ in [18], digraphs with degree $d = 3$ in [20] and digraphs with degree $d = 4$ as well as all vertex-transitive digraphs in [85, 86]. Conjecture 3.2 was later extended to all digraphs, diregular or not, by Caccetta and Häggkvist.

Conjecture 3.3 (Caccetta-Häggkvist Conjecture [39])**.** *Any digraph with order n and minimum out-degree d contains a directed cycle of length $\leq \lceil \frac{n}{d} \rceil$.*

The fact that it is by no means obvious that Conjecture 3.2 implies Conjecture 3.3 gives us our first taste of the complications involved with working with digraphs that are not diregular, a theme that we will take up in greater detail in Chapter 5. However it is easily seen that the Caccetta-Häggkvist Conjecture, combined with the construction of [19], implies that $f(d, g) = d(g-1)+1$.

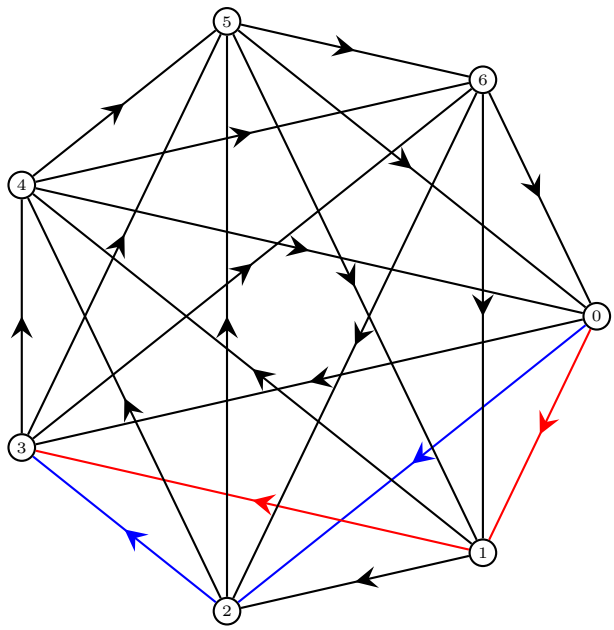

Figure 3.1: An extremal digraph for $d = 3, g = 3$

Conjecture 3.3 was proven for digraphs with minimum out-degree $d = 2$ by Caccetta and Häggkvist in [39], for $d = 3$ in [84] and for all $d \leq 5$ in [90]. Whilst Conjecture 3.3 remains an open question, it is known to be 'nearly true'. In [43] it is shown that any digraph with order n and minimum out-degree d contains a cycle of length $\leq \lceil \frac{n}{d} \rceil + 2500$ and in [122] this estimate is improved to $\frac{n}{d} + 304$. Furthermore Shen has shown in [129] that for any given d there are at most a finite number of counterexamples to Conjecture 3.3.

In many ways the directed degree/girth problem lacks the flavour of the original undirected degree/girth problem; there is no analogue of the Moore bound and no unique path property. The reason for this is that the connection between the girth of an undirected graph and its geodecity breaks down when directions are assigned to the edges. In fact, if the Caccetta-Häggkvist Conjecture is true, then the digraphs on the cyclic group $\mathbb{Z}_{d(g-1)+1}$ with connection set $\{1, 2, \ldots, d\}$ are smallest possible digraphs with given out-degree d and girth g, but these digraphs are not even 2-geodetic by the commutativity of addition, i.e. the directed Moore tree of depth two for these digraphs does not have the unique path property. An example of an extremal digraph for $d = 3$ and $g = 3$ is shown in Figure 3.1; there are two distinct paths (shown in red and blue) from the vertex 0 to the vertex 3, the red path corresponding to addition of the generator 1 followed by the generator 2 and the blue path corresponding to addition of 2 followed by addition of 1.

Therefore it is desirable to ask for small digraphs that preserve the unique path property. This motivates the following definition.

Definition 3.4. A digraph G is *k-geodetic* if and only if for any pair u, v of vertices of G there is at most one directed walk in G from u to v of length not exceeding k. The *geodetic girth* (or *geodecity* for short) of G is the largest value of k such that G is k-geodetic.

We pose the following problem, which we call the directed degree/geodecity problem. This problem was first raised in the seminal paper 'On k-geodetic digraphs with excess one' [132] by Sillasen.

Problem 3.5 (Directed degree/geodecity problem)**.** *For $d \geq 1$ and $k \geq 1$ what is the smallest possible order of a digraph with minimum out-degree d and geodetic girth k?*

We shall denote the order of the smallest k-geodetic digraph with minimum out-degree d by $N(d, k)$. The directed Moore tree of depth k and out-degree d contains at least $M(d, k) = 1 + d + d^2 + \cdots + d^k$ vertices. For a k-geodetic digraph all of the vertices in this Moore tree must be distinct; therefore we see that the directed Moore bound is a lower bound for the order of a k-geodetic digraph with minimum out-degree d. A digraph will meet this lower bound if and only if it is out-regular with degree d, is k-geodetic and has diameter k; hence this lower bound is met if and only if there exists a Moore digraph with out-degree d and diameter k. By Theorem 2.13 this occurs only in the trivial cases $d = 1$ and $k = 1$. We record this result as a lemma.

Lemma 3.6 (Moore bound)**.** *For all $d, k \geq 1$ we have*

$$N(d, k) \geq 1 + d + d^2 + \cdots + d^k = M(d, k).$$

Strict inequality holds for $d, k \geq 2$.

As there exist Moore digraphs for $d = 1$ (directed cycles) and $k = 1$ (complete digraphs), for the remainder of this work we restrict our attention to the cases $d, k \geq 2$. To quantify the amount by which a digraph exceeds the Moore bound we define the *excess* of a digraph.

Definition 3.7. The *excess* of a digraph with order n, minimum out-degree d and geodetic girth k is

$$\epsilon = n - M(d, k).$$

A k-geodetic digraph with minimum out-degree d and excess ϵ is a $(d, k; +\epsilon)$*-digraph*. We define $\epsilon(d, k)$ to be the smallest possible excess of a $(d, k; +\epsilon)$-digraph, i.e. for all

$d, k \geq 2$

$$N(d,k) = M(d,k) + \epsilon(d,k).$$

Hence Problem 3.5 is equivalent to finding $\epsilon(d,k)$. We are particularly interested in the structure of the extremal digraphs for the degree/geodecity problem.

Definition 3.8. A smallest possible k-geodetic digraph with minimum out-degree d is a (d,k)-*geodetic cage*.

The adjective 'geodetic' is inserted to distinguish these extremal digraphs from the extremal digraphs for the directed degree/girth problem; however, as we will not be discussing the directed degree/girth problem further in this work it should cause no confusion if we drop the 'geodetic' and refer to geodetic cages merely as 'cages'.

Let G be a $(d,k;+\epsilon)$-digraph. Recall from Subsection 1.1.1 that for all $\ell \geq 1$ we set $N^{+\ell}(u) = \{v \in V(G) : d(u,v) = \ell\}$ and $N^{-\ell}(u) = \{v \in V(G) : d(v,u) = \ell\}$, so that $N^{+1}(u) = N^{+}(u)$ and $N^{-1}(u) = N^{-}(u)$. Also we define $N^0(u) = \{u\}$. As G is k-geodetic for all i, j in the range $-k \leq i < j \leq k$ such that $j - i \leq k$ we have $N^i(u) \cap N^j(u) = \emptyset$.

For $0 \leq \ell \leq k$ we set $T_\ell(u) = \bigcup_{0 \leq r \leq \ell} N^{+r}(u)$ and $T_{-\ell}(u) = \bigcup_{0 \leq r \leq \ell} N^{-r}(u)$, so that for $\ell \geq 0$ $T_\ell(u)$ is the set of vertices of G that can be reached from u by paths of length $\leq \ell$ and $T_{-\ell}(u)$ is the set of vertices that can reach u by paths of length $\leq \ell$. In particular we introduce the abbreviation $T(u)$ for $T_{k-1}(u)$ and $T^-(u)$ for $T_{-(k-1)}(u)$. In diagrams the sets $T(u)$ and $T^-(u)$ will be indicated by triangles (facing downwards and upwards respectively) - for examples see Figures 5.2 and 6.1.

For each vertex u of a $(d,k;+\epsilon)$-digraph there will be a set $O(u)$ of vertices that lie at distance $\geq k+1$ from u in G. This is called the *outlier set* of the vertex u. Hence $O(u) = V(G) - T_k(u)$. In particular note that unlike the repeat sets discussed in Section 2.3.3 the outlier sets are sets, not multisets.

Definition 3.9. Let G be a $(d,k;+\epsilon)$-digraph. For every vertex u of G and integer ℓ in the range $0 \leq \ell \leq k$ we set $T_\ell(u) = \bigcup_{0 \leq r \leq \ell} N^{+r}(u)$ and $T_{-\ell}(u) = \bigcup_{0 \leq r \leq \ell} N^{-r}(u)$. The *outlier set* $O(u)$ and the *inverse outlier set* of a vertex u are $O(u) = \{v \in V(G) : d(u,v) \geq k+1\}$ and $O^-(u) = \{v \in V(G) : d(v,u) \geq k+1\}$ respectively.

If G is out-regular, then by elementary counting we can assume that each outlier set

contains exactly ϵ vertices. Similarly if G is in-regular (in particular if G is diregular) then we will also have $|O^-(u)| = \epsilon$ for all $u \in V(G)$. In fact in almost all situations of interest here out-regularity is a safe assumption (Theorem 9.9 in Chapter 9 requires a little more care); the proof of the following lemma is an adaption of results from [131] and [132].

Lemma 3.10. *If $\epsilon < M(d, k-1)$, then G is out-regular with degree d.*

Proof. If G is not out-regular, it must contain a vertex u with out-degree at least $d+1$. By k-geodecity, it follows that

$$|V(G)| \geq |T_k(u)| \geq 1 + (d+1) + (d+1)d + \cdots + (d+1)d^{k-1} = M(d,k) + M(d,k-1).$$

As G has order $M(d,k) + \epsilon < M(d,k) + M(d,k-1)$, this is a contradiction. □

Corollary 3.11 ([132])**.** *For $d, k \geq 2$ all $(d, k; +1)$-digraphs are out-regular and have diameter $k+1$.*

If G has excess $\epsilon = 1$, then instead of an outlier set we can (by Corollary 3.11) think of an *outlier function* $o : V(G) \to V(G)$.

Definition 3.12. The *outlier function* of a k-geodetic digraph G with minimum out-degree d and order $M(d,k)+1$ is the function $o : V(G) \to V(G)$ that satisfies the following condition: for any vertex of u of G, $o(u)$ is the unique vertex of G such that there is no $u, o(u)$-walk with length not exceeding k.

The outlier function is the analogue for the degree/geodecity problem of the repeat function for $(d, k; -1)$-digraphs. If we represent the outlier function of a $(d, k; +1)$-digraph G with order $n = M(d,k)+1$ by the $n \times n$ matrix P, which has (u, v)-entry equal to one if $o(u) = v$ and zero otherwise, then Theorem 1.3 shows that the adjacency matrix A of G satisfies

$$I + A + A^2 + \cdots + A^k = J - P. \tag{3.1}$$

Recall from Section 2.3.2 that the repeat function r of a diregular $(d, k; -1)$-digraph has the extremely useful property of being a digraph automorphism. It turns out that its 'mirror image', the outlier function of a digraph with excess one, shares this property. The following short proof of this fact was given in [132].

Theorem 3.13 ([132])**.** *The outlier function o of a diregular $(d, k; +1)$-digraph G is an automorphism of G.*

Proof. As G is diregular the all-one matrix J commutes with the adjacency matrix A, i.e. $AJ = JA$. As A commutes with every term on the left-hand side of Equation 3.1 as well as with J, it must commute with P, so that $PA = AP$. This is equivalent to o being an automorphism of G. □

Making use of this result in [132] Sillasen uses a counting argument somewhat similar to that of [114] to prove the non-existence of diregular $(2, k; +1)$-digraphs.

Theorem 3.14 ([132])**.** *There are no diregular* $(2, k; +1)$*-digraphs for* $k \geq 2$*.*

In the same paper [132] Sillasen provides some information on the structure of a hypothetical non-diregular digraph with excess one. The question of diregularity for digraphs with excess one was completed in a later paper [116] by Miller, Miret and Sillasen, which used the approach taken by Miller, Gimbert, Širáň and Slamin in [115] for digraphs with defect one. We will pick up the topic of diregularity of digraphs with small excess in Chapter 5.

Theorem 3.15 ([116])**.** *For* $d, k \geq 2$ *all* $(d, k; +1)$*-digraphs are diregular.*

The spectral method is also applied to great effect in [116] to k-geodetic digraphs with excess one for small k.

Theorem 3.16 ([116])**.** *There are no* $(d, 2; +1)$*-digraphs for* $d \geq 8$ *and no* $(d, 3; +1)$*- or* $(d, 4; +1)$*-digraphs for* $d \geq 2$*.*

We will address some of the gaps in Theorem 3.16 in Chapter 4.

3.2 Existence of cages

In posing the directed degree/geodecity problem, we have sidestepped one subtle issue: we have not yet established the existence of a digraph with minimum out-degree d and geodetic girth k for all $d, k \geq 2$, so that $N(d, k)$ is not necessarily defined for all values of d and k. Recall from Section 2.2 that the existence of cages in the undirected degree/girth problem was proven in [62, 126].

In the directed degree/geodecity problem we obtain the existence of geodetic cages and a good estimate of their order almost for free from a nice family of digraphs called the *permutation digraphs*. These digraphs were first mentioned in [71] and their properties further developed in [36]. The vertices of the permutation digraph $P(d, k)$

are all permutations of length k of symbols from an alphabet of size $d+k$ and we draw an arc from one permutation $x_0x_1\dots x_{k-1}$ to any other permutation formed from this permutation by deleting the first term x_0 and appending a term x_k at the right that is different from all of the symbols $x_0, x_1, \dots, x_{k-1}$. The smallest non-trivial permutation digraph $P(2,2)$ is displayed in Figure 3.2. We now define this formally.

Definition 3.17. For $d, k \geq 2$ the vertex set of the permutation digraph $P(d,k)$ consists of all sequences $x_0x_1\dots x_{k-1}$ of length k drawn from an alphabet $[d+k] = \{0, 1, 2, \dots, d+k-1\}$ such that for $0 \leq i < j \leq k-1$ we have $x_i \neq x_j$.

The adjacencies of $P(d,k)$ are defined by

$$x_0x_1\dots x_{k-1} \to x_1x_2\dots x_{k-1}x_k,$$

where $x_k \in ([d+k] - \{x_0, x_1, \dots, x_{k-1}\})$.

It is shown in [36] that permutation digraphs are highly symmetric. The symmetric group on $d+k$ symbols acts on $P(d,k)$ in a natural way by permuting the symbols of the underlying alphabet, meaning that they are arc-transitive, although not 2-arc-transitive. The symmetry groups of the permutation digraphs are derived and the Cayley permutation digraphs classified in [36].

Theorem 3.18 ([36])**.** *The permutation digraphs $P(d,k)$ are arc-transitive.*

The important property of the permutation digraphs from our point of view is that $P(d,k)$ is k-geodetic and for fixed $k \geq 2$ the digraphs $P(d,k)$ have order approaching the directed Moore bound $M(d,k)$ asymptotically from above.

Lemma 3.19. *For $d, k \geq 2$ the permutation digraph $P(d,k)$ is diregular with degree d, has geodetic girth k and has order*

$${}^{d+k}P_k = (d+k)(d+k-1)\dots(d+1).$$

Hence for fixed $k \geq 2$ the excess of $P(d,k)$ is

$$((d+k)(d+k-1)\dots(d+1)) - (d^k + d^{k-1} + \dots + d + 1) \sim \left(\frac{k(k+1)}{2} - 1\right) d^{k-1}$$

as $d \to \infty$.

Proof. For all $d, k \geq 2$ the digraph $P(d,k)$ contains directed cycles of length $k+1$, for

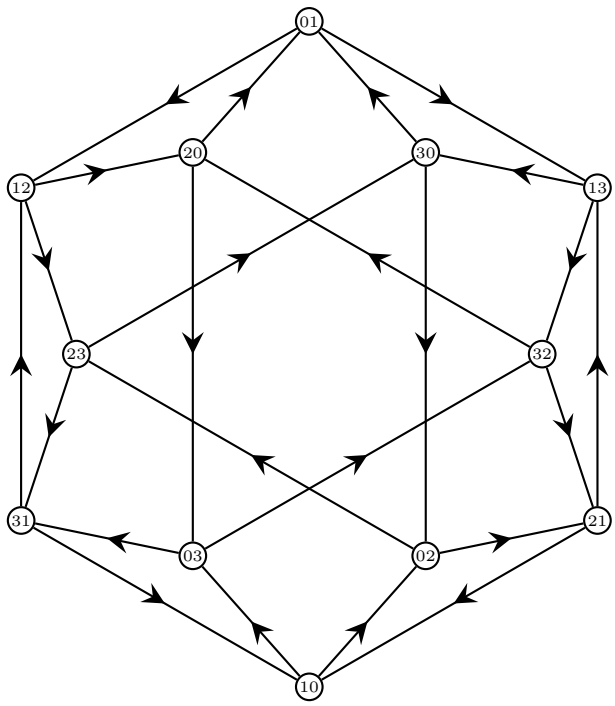

Figure 3.2: $P(2,2)$

example

$$012\ldots(k-1) \to 12\ldots(k-1)k \to 23\ldots(k-1)k0 \to \cdots \to k01\ldots(k-2) \to 012\ldots(k-1),$$

so the geodetic girth of $P(d,k)$ is certainly $\leq k$.

By vertex-transitivity of $P(d,k)$, to prove k-geodecity it is sufficient to demonstrate that if P and Q are $\leq k$-paths in $P(d,k)$ from the vertex $012\ldots(k-1)$ to a vertex $x_0x_1\ldots x_{k-1}$, then $P = Q$. All vertices at distance $r \leq k-1$ from $012\ldots(k-1)$ have first symbol r, whereas all vertices at distance k from $012\ldots(k-1)$ have a first symbol that does not lie in $\{0,1,\ldots,k-1\}$. As $d(01\ldots(k-1), x_0x_1\ldots x_{k-1}) \leq k$ by assumption, it follows that if $x_0 \in \{0,1,\ldots,k-1\}$ then both P and Q have length x_0, whereas if $x_0 \notin \{0,1,\ldots,k-1\}$ then both P and Q must have length k; in either case $l(P) = l(Q)$.

If $x_0 = r \in \{0,1,\ldots,k-1\}$ then the only path with length r from $01\ldots(k-1)$ to $x_0x_1\ldots x_{k-1}$ is the path with initial vertex $01\ldots(k-1)$ obtained by successively deleting the symbol i on the left-hand side and adding the symbol x_{k-r+i} on the right for $i = 0,1,\ldots,r-1$. If $x_0 \notin \{0,1,\ldots,k-1\}$, then the first arc e of both P and Q must be $012\ldots(k-1) \to 12\ldots(k-1)x_0$. Deleting the arc e from P and Q leaves two paths P' and Q' of length $k-1$ from $12\ldots(k-1)x_0$ to $x_0x_1\ldots x_{k-1}$; by the above reasoning $P' = Q'$ and hence $P = Q$. $\square$

The existence of (d, k)-geodetic cages follows immediately from the properties of permutation digraphs given in Lemma 3.19.

Corollary 3.20. *For all $d, k \geq 1$ there exists a (d, k)-geodetic cage.*

Corollary 3.21. *For $d \geq 2$ the excess of a $(d, 2)$-geodetic cage satisfies*

$$1 \leq \epsilon(d, 2) \leq 2d + 1, \tag{3.2}$$

where the lower bound can be increased to 2 for $d \geq 8$ by Theorem 3.16.

We thus have the incredible situation that for fixed k we can approach the directed Moore bound asymptotically from above by arc-transitive digraphs! Therefore, it follows that the directed degree/geodecity problem is already solved in an asymptotic sense; the difficulty lies in finding exact values. This is analogous to the situation in the directed degree/diameter problem, in which the Kautz digraphs provide us with a lower bound that matches the directed Moore bound asymptotically. This is one feature that strongly distinguishes the directed degree/diameter and degree/geodecity problems from the undirected degree/diameter and degree/girth problems.

Another useful property of the permutation digraphs from the point of view of the design of interconnection networks is that for fixed k the diameter does not 'blow up'.

Theorem 3.22 ([36])**.** *For $d \geq k \geq 2$ the permutation digraph $P(d, k)$ has diameter $2k$.*

On the other hand if we fix the value of the degree and let k tend to infinity the diameter seems to behave quite badly; for degree two it is known to grow quadratically in k. The exact diameter of $P(d, k)$ when $3 \leq d \leq k - 1$ is unknown.

Theorem 3.23 ([36])**.** *For $k \geq 2$ the diameter of the permutation digraph $P(2, k)$ is $1 + \binom{k+1}{2}$.*

By the arc-transitive property of the permutation digraphs for all $d, k \geq 2$ we can also ask for the smallest arc-transitive k-geodetic digraph with degree d. We will discuss vertex- and arc-transitive digraphs with excess one in Chapter 4. In general the permutation digraphs are not the smallest arc-transitive k-geodetic digraphs with given degree. Using the census of arc-transitive digraphs with degree two contained in [124] we see that the smallest arc-transitive 2-geodetic digraph with degree two has order 10, whereas the smallest arc-transitive 3-geodetic digraph with degree two has order 27; by contrast, the digraphs $P(2, 2)$ and $P(2, 3)$ have orders 12 and 60

respectively. However, it becomes increasingly difficult to construct arc-transitive k-geodetic digraphs for larger values of the degree d; we therefore hazard the following conjecture.

Conjecture 3.24. *For fixed k and sufficiently large d, the permutation digraph $P(d,k)$ is the smallest arc-transitive k-geodetic digraph with degree d.*

We revisit this conjecture in Section 4.1. A fortiori the permutation digraphs are diregular, so we can also define the smallest diregular k-geodetic digraphs with degree d. The term 'balanced' is often used in place of 'diregular'.

Definition 3.25. A smallest diregular k-geodetic digraph with out-degree d is a (d,k)*-balanced cage.*

3.3 Monotonicity of geodetic cages

Recall from Section 2.2.1 that it was proven by Fu, Huang and Rodger in [73] that the order of undirected cages is strictly monotonic in the value of the girth. The proof in [73] works by taking a cage G with degree d and girth $g+1$, deleting one vertex of G and introducing new edges in such a way that the resulting graph G' still has minimum degree d and girth not less than g.

Theorem 3.26. *For all $d,k \geq 2$ we have*

$$N(d,k) < N(d,k+1).$$

Proof. Let G be a $(d,k+1)$-geodetic cage. Fix a vertex u of G. Delete the vertex u and from each vertex in $N^-(u)$ draw one arc to any vertex of $N^+(u)$ to form a new digraph G' with order $N(d,k+1)-1$; we will call the arcs added at this step *new*. G' has minimum out-degree d. We now show that G' is k-geodetic.

Suppose that there are vertices x and y of G' such that there exist distinct directed paths P and Q with length $\leq k$ in G' from x to y. As G is $(k+1)$-geodetic at least one of these paths, say P, must use a new arc. Each new arc in G' can be replaced by a 2-path through u in G; therefore if both P and Q contain at most one new arc we can extend them to distinct walks P' and Q' with length $\leq k+1$ from x to y in G. It follows that we can assume that P contains at least two new arcs. However, looking at a section of P between consecutive new arcs, this implies that there is a path of length $\leq k-2$ in G from an out-neighbour of u to an in-neighbour of u, so that there is a k-cycle in G, which is impossible. □

The question of monotonicity of the order of cages in the value of the degree turns out to be a highly non-trivial question which remains largely open [150]. We can derive the analogous result for the directed degree/geodecity problem quite easily and furthermore give a relatively strong bound.

Theorem 3.27. *For $d, k \geq 2$ we have $N(d,k) < N(d+1,k)$. More precisely, if $h(d+1,k)$ is the maximum size of the set $T^-(u)$ over all vertices of all $(d+1,k)$-geodetic cages, then $N(d,k) \leq N(d+1,k) - h(d+1,k)$.*

Proof. Let G be a $(d+1,k)$-geodetic cage. If we delete a single out-going arc from every vertex of G, then we obtain a digraph G' with minimum out-degree d, which, being a subdigraph of G, is k-geodetic. In fact, picking any vertex u of G, we can choose these arcs so that every vertex in $T^-(u)$ has in-degree zero in G'. Deletion of these vertices does not affect the geodetic girth or out-degree of G'; therefore there must exist a $(d,k;+\epsilon)$-digraph with order $\max\{|T^-(u)| : u \in V(G)\}$ less than $N(d+1,k)$. □

As the permutation digraphs are diregular, we know that balanced cages, i.e. smallest diregular $(d,k;+\epsilon)$-digraphs, exist for any $d, k \geq 2$. Interestingly, the proofs of both Theorems 3.26 and 3.27 can be adapted in a straightforward way to show strict monotonicity in the order of balanced cages for both the degree and geodecity (in the construction of Theorem 3.26 the arcs from $N^-(u)$ to $N^+(u)$ need to be assigned in a one-to-one manner and in the second construction we delete $M(d+1,k-1)$ vertices).

Corollary 3.28. *Let $N'(d,k)$ be the order of a (d,k)-balanced cage. Then for $d, k \geq 2$ we have $N'(d,k) < N'(d,k+1)$ and $N'(d,k) + M(d+1,k-1) \leq N'(d+1,k)$.*

3.4 Connectivity of geodetic cages

As in the undirected degree/girth problem, it is generally extremely difficult to find geodetic cages except for quite small values of d and k. Nevertheless, even without explicitly determining geodetic cages, it is possible to give some results on their structure. Section 2.2.1 suggests that we should look at the connectivity of geodetic cages.

Recall from Section 1.1.1 that a digraph G is k-arc-connected if the deletion of $\leq k-1$ arcs from G leaves a strongly-connected digraph and that G is maximally

connected if it satisfies $\kappa(G) = \lambda(G) = \delta(G)$, where

$$\delta(G) = \min(\{d^-(u) : u \in V(G)\} \cup \{d^+(u) : u \in V(G)\}).$$

If all minimal arc cuts are of the form $(\{u\}, V(G) - \{u\})$ or $(V(G) - \{u\}, \{u\})$ then G is super-arc-connected or super-λ. By analogy with Conjecture 2.10 it seems reasonable to make the following conjecture.

Conjecture 3.29. *All geodetic cages are maximally connected and super-arc-connected.*

To begin with, we need to confirm that geodetic cages are indeed strongly connected. Weak connectivity is entirely trivial; strong connectivity slightly less so.

Lemma 3.30. *Directed geodetic cages are weakly connected.*

Proof. Let G be a (d, k)-geodetic cage. If G is not weakly connected, then any of its weak components is a k-geodetic digraph with minimum out-degree $\geq d$ and with smaller order than G, which is impossible. □

Theorem 3.31. *All directed geodetic cages are strongly connected.*

Proof. Let G be a (d, k)-geodetic cage. If G is not strongly connected, we can define an equivalence relation by $u \equiv v$ if and only if G contains both a directed path from u to v and a directed path from v to u (see [28]). The equivalence classes V_i, $1 \leq i \leq r$, are the strong components of G.

Form the *condensation* G^* of G as follows: the vertices of G^* are the strong components V_i of G, with an arc from V_i to V_j, $i \neq j$, if and only if there is an arc from a vertex of V_i to a vertex of V_j in G. It is easily seen that the condensation is acyclic. Therefore consider a longest path P in G^* and let V_r be the terminal vertex of P. It follows that vertices in the strong component V_r have arcs only to other vertices in V_r, so the subdigraph induced by V_r is k-geodetic with minimum out-degree $\geq d$, but with order smaller than G, a contradiction. □

We can easily extend these results to balanced cages.

Theorem 3.32. *All (d, k)-balanced cages are strongly connected.*

Proof. Let G be a balanced cage. That G is weakly connected follows from the same reasoning as Lemma 3.30. A diregular digraph is strongly connected if and only if it is weakly connected (see Lemma 2.6.1 of [80]), so G is also strongly connected. □

Pushing this reasoning a little further we can obtain a result analogous to the fact that undirected cages are 2-connected [73].

Theorem 3.33. *For $d, k \geq 2$, all geodetic cages are 2-weakly-connected.*

Proof. Suppose that a (d, k)-geodetic cage G has a 1-cut $\{x\}$. Deleting x gives at least two weak components C_1 and C_2 in $G - x$. Assume that $|C_1| \leq |C_2|$. Let A be the set of vertices in C_1 that have arcs to x and B be the set of vertices with arcs from x. By Theorem 3.31, A and B are non-empty.

Take an isomorphic copy C^* of C_1, with the set A^* in C^* corresponding to A and the set B^* corresponding to B. Form a new digraph G' from the disjoint union $C_1 \cup C^*$ by joining each vertex in A to a vertex of B^* by an arc and each vertex of A^* to a vertex of B by an arc. G' is a k-geodetic digraph with minimum degree $\geq d$, but smaller order than G, a contradiction. □

Some good evidence for the truth of Conjecture 3.29 is that for any fixed k there are at most a finite number of (d, k)-balanced cages that are not maximally connected.

Theorem 3.34. *All (d, k)-balanced cages are maximally connected for sufficiently large d. In particular all $(d, 2)$-balanced cages are maximally connected.*

Proof. By Theorem 2.5 of [9], if $n \leq 2M(d, k) - d$ then G is maximally connected. It follows by the bound in Lemma 3.19 (from the permutation digraphs) that for sufficiently large d any (d, k)-balanced cage is maximally connected. In particular, putting $k = 2$, a $(d, 2)$-balanced cage will be 2-strongly-connected if $(d + 2)(d + 1) \leq 2(1 + d + d^2) - d$, which is true for $d \geq 2$. □

Chapter 4

Digraphs with excess one

As there are no Moore digraphs [33] the obvious first question to address in the directed degree/geodecity problem is the existence of digraphs with excess one. Throughout this section G will stand for a $(d, k; +1)$-digraph. Recall from Section 3.1 that we can make the following assumptions about the structure of G.

Lemma 4.1 ([116, 132])**.** *If G is a $(d, k; +1)$-digraph, then*

- *G is diregular.*
- *Either G is a $(d, 2; +1)$-digraph, where d lies in the range $3 \leq d \leq 7$, or a $(d, k; +1)$-digraph with $d \geq 3$ and $k \geq 5$, or a directed $(k + 2)$-cycle.*
- *The outlier function o of G is an automorphism.*

Our conjecture is that, with the trivial exception of directed $(k + 2)$-cycles, there are no $(d, k; +1)$-digraphs for $k \geq 2$. This chapter represents a step towards this conjecture.

Conjecture 4.2. *There are no $(d, k; +1)$-digraphs with $d, k \geq 2$.*

The fact that a $(d, k; +1)$-digraph G must be diregular leads to a 'duality principle'. This phenomenon has been observed for almost Moore digraphs; in [17] it is shown that taking the converse of a $(d, k; -1)$-digraph yields another $(d, k; -1)$-digraph. The Duality Principle will allow us to interchange out-neighbourhoods and in-neighbourhoods in our results. First we define the inverse of the outlier function of a $(d, k; +1)$-digraph.

Definition 4.3. Let G be a $(d, k; +1)$-digraph with outlier function o. Then the *inverse outlier function* of G is the function $o^- : V(G) \to V(G)$ such that for all $u, v \in V(G)$ we have $o^-(v) = u$ if and only if $v = o(u)$.

As the outlier function o is an automorphism, it follows that for a $(d, k; +1)$-digraph G the inverse outlier function o^- is the group-theoretic inverse of o in $\mathrm{Aut}(G)$.

Lemma 4.4 (Duality Principle)**.** *Let G be a $(d, k; +1)$-digraph with outlier function*

o. Taking the converse of G yields another $(d,k;+1)$-digraph G^-. If o' is the outlier function of G^-, then as a function of $V(G)$ we have $o' = o^-$.

Proof. Let G be a $(d,k;+1)$-digraph. By Lemma 4.1 G is diregular, so G^- is also diregular with degree d. Suppose that there are vertices u, v of G^- such that there are two distinct u,v-walks $u, u_1, u_2, \ldots, u_s, v$ and $u, v_1, v_2, \ldots, v_t, v$ in G^- with length at most k; then by reversing each of the arcs in these walks, we see that $v, u_s, \ldots, u_2, u_1, u$ and $v, v_t, \ldots, v_2, v_1, u$ would be distinct v,u-walks in G with length $\leq k$, contradicting the fact that G is k-geodetic. As G^- also has order $M(d,k)+1$, it follows that G^- is also a $(d,k;+1)$-digraph.

Let o' be the outlier function of G' and fix an arbitrary vertex u of G'. The outlier $o'(u)$ of u in G^- is the unique vertex of G^- such that there is no $u, o'(u)$-walk in G^- of length $\leq k$. Reversing all arcs of G', it follows that there is no $o'(u), u$-walk in G with length $\leq k$. Thus in G we have $o(o'(u)) = u$. Applying the automorphism o^- of G to both sides of this identity, we have $o'(u) = o^-(u)$. □

The plan of this chapter is as follows. Firstly in Section 4.1 we use counting arguments to deduce some strong conditions on digraphs with excess one and a high level of symmetry. In Section 4.2 we investigate the structure of digraphs with degree three and excess one. Then in Section 4.3 we use the approach of Sillasen in [133] to analyse the set of vertices fixed by an automorphism of a $(d,k;+1)$-digraph. As the outlier function o is an automorphism of G these results tell us quite a lot about the structure of o as a permutation. In the final part of this chapter, Section 4.4, we use a spectral approach to exploit the results of Section 4.3 to prove the non-existence of certain $(d,k;+1)$-digraphs.

4.1 Vertex-transitive digraphs with excess one

All of the known Moore graphs are vertex-transitive. This suggests that it is of interest to look for digraphs with order close to the directed Moore bound that have a high degree of symmetry. In her thesis [131] Sillasen uses this approach on digraphs with defect one; we now emulate this approach for digraphs with excess one. Recall that here G will stand for any $(d,k;+1)$-digraph.

In [131] as a basis for her counting arguments Sillasen divides the vertices of an almost Moore digraph into two types, Type I and Type II. Adapting this notation, we make the following definition.

Definition 4.5. A vertex u of a $(d, k; +1)$-digraph is Type II if $o(u) \to u$; otherwise u is Type I.

The type of a vertex is preserved by any automorphism of G. This leads us to the following observation.

Observation 4.6. *If a $(d, k; +1)$-digraph G is vertex-transitive, then either every vertex of G is Type I or every vertex of G is Type II.*

If every vertex of G is Type I, then we can obtain a strong divisibility condition on d and k. The reason for this is that all directed $(k+1)$-cycles of G are arc-disjoint.

Lemma 4.7. *No arc of G is contained in more than one directed $(k+1)$-cycle.*

Proof. Suppose that an arc (u, v) is contained in two $(k+1)$-cycles. Then there are two distinct k-paths from v to u, which contradicts k-geodecity. □

Lemma 4.8. *Any arc (u, v) of G such that $u \neq o(v)$ lies in a unique $(k+1)$-cycle.*

Proof. Let (u, v) be such an arc. As $u \neq o(v)$ there is a path of length k in G from v to u, so the arc (u, v) is contained in a $(k+1)$-cycle, which is unique by Lemma 4.7. □

Corollary 4.9. *Suppose that every vertex of G is Type I. Then $(k+1)$ divides $d(M(d, k) + 1) = 2d + d^2 + d^3 + \cdots + d^{k+1}$.*

Proof. As all vertices of G are Type I, by Lemma 4.7 we can partition the arcs of G into disjoint $(k+1)$-cycles. Therefore the size $m = d(M(d, k) + 1)$ of G is divisible by $k + 1$. □

Computer search shows that for $3 \leq d \leq 12$ and $2 \leq k \leq 10000$ the following values of d and k satisfy this condition:

$d = 3$: $k = 2, 20, 146, 902, 1028, 6320, 7202,$

$d = 4$: $k = 3, 7, 87, 171, 472, 2647,$

$d = 5$: $k = 4, 84, 114,$

$d = 6$: $k = 2, 3, 5, 7, 11, 23, 32, 51, 203, 347, 1095, 3323, 3767, 4903, 9563,$

$d = 7$: $k = 6, 76, 118, 2568,$

$d = 8$: $k = 3, 7, 9, 15, 87, 463, 1171,$

$d = 9$: $k = 2, 8, 68,$

$d = 10$: $k = 3, 4, 7, 9, 15, 19, 39, 79, 555, 1069, 2314, 2986, 4659,$

$d = 11$: $k = 10$,
$d = 12$: $k = 2, 3, 5, 7, 11, 13, 23, 55, 91, 163, 236, 1235, 1356$.

We see that the condition in Corollary 4.9 is quite strong. On the other hand, if G contains a Type II vertex then these vertices group themselves into cycles in a natural way.

Lemma 4.10. *Suppose that G contains a Type II vertex u. Then u has a unique Type II out-neighbour, namely $o^-(u)$.*

Proof. Applying the automorphism o^- to the arc $(o(u), u)$, we see that $(u, o^-(u))$ is also an arc. By inspection, $o^-(u)$ is a Type II vertex. Suppose that u' is an arbitrary Type II out-neighbour of u. As (u, u') is an arc, so is $(o(u), o(u'))$. As u' is Type II, $(o(u'), u')$ is an arc. We therefore have paths $o(u) \to u \to u'$ and $o(u) \to o(u') \to u'$, so by k-geodecity we must have $o(u') = u$, i.e. $u' = o^-(u)$. □

It follows immediately that in a vertex-transitive $(d, k; +1)$-digraph all vertices must be Type I.

Lemma 4.11. *If G is vertex-transitive, then every vertex of G is Type I.*

Proof. Suppose that G contains a Type II vertex; by vertex-transitivity, every vertex is Type II. But this contradicts Lemma 4.10. □

In particular, if G is vertex-transitive, then it must satisfy the divisibility condition in Corollary 4.9.

Corollary 4.12. *Let G be a vertex-transitive $(d, k; +1)$-digraph. Then $(k + 1)$ divides $2d + d^2 + d^3 + \cdots + d^{k+1}$.*

In fact, we can significantly extend Corollary 4.9 using the fact that for any vertex u of a vertex-transitive $(d, k; +1)$-digraph the vertex $o^-(u)$ cannot be close to u.

Lemma 4.13. *If G is a vertex-transitive $(d, k; +1)$-digraph, then for any vertex u of G we have $d(u, o^-(u)) \geq k$.*

Proof. Suppose that $d(u, o^-(u)) = t \leq k - 1$. As G is vertex-transitive, the distance from any vertex v of G to $o^-(v)$ is t. Writing $N^+(u) = \{u_1, u_2, \ldots, u_d\}$, let $o^-(u) \in T_{k-2}(u_1)$. As $d(u_2, o^-(u_2)) = t \leq k - 1$, we have $o^-(u_2) \in T(u_2)$. However, as

o^- is an automorphism of G, there is an arc $o^-(u) \to o^-(u_2)$, so that $o^-(u_2)$ also lies in $T(u_1)$. As $o^-(u_2)$ appears twice in the Moore tree, k-geodecity is violated. Hence $t \geq k$. □

Theorem 4.14. *For $1 \leq t \leq k-1$, let Z_{k+t} be the number of distinct directed $(k+t)$-cycles in a vertex-transitive $(d,k;+1)$-digraph G. Then for $2 \leq t \leq k-1$ we have*

$$(M(d,k)+1)(d^t - d^{t-1}) = Z_{k+t}(k+t). \tag{4.1}$$

Proof. Let u be any vertex of G and draw the Moore tree of depth k rooted at u. By Lemma 4.13 all vertices in $T(u)$ have a path of length $\leq k$ to u. For $1 \leq t \leq k-1$, let us say that a vertex v at Level t of the Moore tree is *short* if $d(v,u) \leq k-1$ and *long* if $d(v,u) = k$.

All vertices of $N^+(u)$ must be long by k-geodecity. It is easily seen that for $1 \leq t \leq k-2$ every vertex at Level t has one short out-neighbour and $d-1$ long out-neighbours at Level $t+1$. By induction for $2 \leq t \leq k-1$ there are d^{t-1} short vertices in Level t of the tree. Therefore for $2 \leq t \leq k-1$ the vertex u is contained in $d^t - d^{t-1}$ closed walks of length $k+t$ and these walks must be cycles by k-geodecity. Equation 4.1 follows by double-counting pairs (u, Z), where u is a vertex of G and Z is a directed $(k+t)$-cycle containing u. □

By checking that the divisibility conditions in Theorem 4.14 are satisfied for all t such that $1 \leq t \leq k-1$, computer search shows that the only values of d and k in the range $3 \leq d \leq 12$ and $2 \leq k \leq 10000$ for which there can exist a vertex-transitive $(d,k;+1)$-digraph are
$k = 2$: $d = 3, 6, 9, 12$,
$k = 3$: $d = 6, 10$.
Lemma 4.1 shows that in practice there are no $(d,3;+1)$-digraphs for $d \geq 2$ and no $(d,2;+1)$-digraphs for $d \geq 8$, so the only remaining values of d and k in this range are $(d,k) = (3,2)$ and $(6,2)$. In Section 4.6 we will see that such digraphs also do not exist. This scarcity of vertex-transitive $(d,k;+1)$-digraphs can be taken as evidence in favour of Conjecture 4.2.

There are some simple number-theoretic conditions on d and k that force G to contain a Type II vertex, so that G cannot be vertex-transitive.

Theorem 4.15. *If $d \geq 3$ and $k \geq 2$ satisfy any of the following conditions then any $(d,k;+1)$-digraph contains a Type II vertex:*

- *i) d and k are odd,*
- *ii) $d \equiv 1 \pmod{k+1}$ or $d \equiv -1 \pmod{k+1}$,*
- *iii) $d^2|(k+1)$, or*
- *iv) there is an odd prime p such that $p|(k+1)$ and $d \equiv 2 \pmod{p}$.*

Proof. For part i), suppose that d and k are odd, but G contains only Type I vertices. By Corollary 4.9, $(k+1)$ divides $d(M(d,k)+1)$, so $M(d,k)$ must be odd. However $M(d,k) = 1 + d + d^2 + \cdots + d^k$ contains an even number of odd summands and hence is even.

For part ii), suppose that $d \equiv 1 \pmod{k+1}$. Then

$$d(M(d,k)+1) = d(2 + d + d^2 + \cdots + d^k) \equiv k + 2 \equiv 1 \pmod{k+1},$$

so that $(k+1)$ does not divide $d(M(d,k)+1)$. Similarly if $d \equiv -1 \pmod{k+1}$, then $d(M(d,k)+1) \equiv -2 + 1 - 1 + 1 - \cdots + (-1)^{k+1} \equiv -2 \pmod{k+1}$ if k is even and $d(M(d,k)+1) \equiv -1 \pmod{k+1}$ if k is odd.

For part iii), if d^2 divides $(k+1)$ and $(k+1)$ divides $d(M(d,k)+1)$, then d divides $M(d,k)+1$, which implies that $d = 2$. However, we know that there are no $(2,k;+1)$-digraphs by Lemma 4.1 (or see [132]).

Finally, for part iv) suppose that p is an odd prime such that $p|(k+1)$ and $d \equiv 2 \pmod{p}$; then if every vertex is Type I we must have

$$0 \equiv M(d,k) + 1 \equiv M(2,k) + 1 = 2^{k+1} \pmod{p},$$

implying that p is even, a contradiction. □

Deviating momentarily from our focus in this chapter on digraphs with excess one, this is a suitable place to mention that the same counting arguments apply for a much larger range of values of the excess ϵ if we make the additional assumption of arc-transitivity. Arc-transitivity allows us to further restrict the distance from a vertex u to elements of $O^-(u)$; in fact, the outlier sets $O(u)$ and inverse outlier sets $O^-(u)$ become equivalent in this context.

Lemma 4.16. *Let $\epsilon < d$ and let G be an arc-transitive $(d,k;+\epsilon)$-digraph. Then for all $u \in V(G)$ we have $O(u) = O^-(u)$.*

Proof. Write $N^+(u) = \{u_1, u_2, \ldots, u_d\}$. Suppose that an element v of $O^-(u)$ lies at

distance $t \leq k$ from u. We can assume that $v \in T(u_1)$. By arc-transitivity, there are $d-1$ automorphisms ϕ_i of G, $i = 2, 3, \ldots, d$, that map the arc $u \to u_1$ to the arc $u \to u_i$. Each image $\phi_i(v)$ of v under these automorphisms must also belong to $O^-(u)$, so each branch contains an element of $O^-(u)$. As $\epsilon < d$, one of these elements must be repeated in the Moore tree rooted at u, violating k-geodecity. Therefore we must have $O^-(u) \subseteq O(u)$ and the result follows. □

Corollary 4.17. *If G is an arc-transitive $(d, k; +\epsilon)$-digraph with excess $\epsilon < d$, then $(k+1)$ divides $d(M(d,k)+\epsilon)$ and $(k+t)$ divides $(M(d,k)+\epsilon)(d^t - d^{t-1})$ for $2 \leq t \leq k$.*

Proof. Again we denote the number of distinct directed r-cycles in G by Z_r. Using the same reasoning as in the proof of Theorem 4.14, we see that each vertex of G is contained in d directed $(k+1)$-cycles, so that $d(M(d,k)+\epsilon) = Z_{k+1}(k+1)$, and each vertex is contained in $d^t - d^{t-1}$ directed $(k+t)$-cycles for $2 \leq t \leq k$, so that $(M(d,k)+\epsilon)(d^t - d^{t-1}) = Z_{k+t}(k+t)$. □

Corollary 4.17 represents a step towards proving Conjecture 3.24. Continuing this line of reasoning shows that the divisibility conditions of Corollary 4.17 hold for 2-arc-transitive $(d, k; +\epsilon)$-digraphs with $\epsilon < d^2$; beyond this, we will not venture.

4.2 Diregular digraphs with excess one and degree three

Sillasen has shown that there are no $(2, k; +1)$-digraphs [132]; therefore a reasonable next step is to ask whether there are any $(3, k; +1)$-digraphs. It was proven in [17] that there are no $(3, k; -1)$-digraphs; the strategy of the proof is to show that any two distinct vertices of a $(3, k; -1)$-digraph can have at most one common out-neighbour (and, conversely, at most one common in-neighbour), classify vertices u according to the distance from u to its repeat $r(u)$ and then count the different types of vertices in two different ways to arrive at a contradiction. In this section we show that the first main result of [17], that any two vertices have at most one common out-neighbour, continues to hold in the setting of digraphs with degree three and excess one.

We begin with a lemma that holds generally for $(d, k; +1)$-digraphs; it describes the situation of vertices with identical out-neighbourhoods.

Lemma 4.18. *Let u and v be vertices of a $(d, k; +1)$-digraph such that $N^+(u) = N^+(v)$, where $u \neq v$. Then $v = o(u)$ and $u = o(v)$, i.e. the outlier function o transposes u and v. The same result holds if $N^-(u) = N^-(v)$.*

Proof. Suppose that $N^+(u) = N^+(v)$, but $u \neq v$. Draw the Moore tree of depth k rooted at u; by k-geodecity, u appears only at Level 0, the root position, of this tree. As the Moore tree rooted at v differs from the Moore tree rooted at u only at Level 0, and $u \neq v$, it follows that v cannot reach u by a path of length $\leq k$, so $o(v) = u$ and, by symmetry, $o(u) = v$. The result for in-neighbourhoods follows by the Duality Principle. □

For the remainder of this section let G be a diregular $(3, k; +1)$-digraph with outlier function o. Our first goal is to show that no pair of distinct vertices can have identical out-neighbourhoods; to achieve this we need a lemma for pairs of vertices with exactly two common out-neighbours.

Lemma 4.19. *Let u, v be distinct vertices of G with exactly two common out-neighbours, i.e. $|N^+(u) \cap N^+(v)| = 2$. If we write $N^+(u) = \{u_1, u_2, u_3\}$ and $N^+(v) = \{v_1, v_2, v_3\}$, where $u_1 = v_1$, $u_2 = v_2$ and $u_3 \neq v_3$, then $o(u) = v_3$ and $o(v) = u_3$.*

Proof. Let u and v be as described. This configuration is shown in Figure 4.1. By k-geodecity $u_3 \notin T(u_1) \cup T(u_2)$. Hence there are three possible positions for the vertex u_3 in the Moore tree rooted at v: i) $u_3 = v$, ii) $u_3 \in T(v_3) - \{v_3\}$ or iii) $u_3 = o(v)$. If $u_3 = v$, then we have paths $u \to u_2$ and $u \to u_3 \to u_2$, which is impossible for $k \geq 2$.

Suppose that $u_3 \in T(v_3) - \{v_3\}$. Put $\ell = d(v_3, u_3)$, so that $1 \leq \ell \leq k - 1$. Let w be a vertex in $N^{k-1-\ell}(u_3)$; then $w \in N^{k-1}(v_3)$. The vertex w has three out-neighbours w_1, w_2 and w_3. By k-geodecity none of these out-neighbours can lie in $T(v_3)$. At most two of the out-neighbours can lie in $\{v, o(v)\}$, so it follows that w has an out-neighbour, say w_1, that lies in $T(v_1) \cup T(v_2) = T(u_1) \cup T(u_2)$; without loss of generality $w_1 \in T(u_1)$. Hence there is a path of length $\leq k$ from u to w_1 via u_1. There is also a path from u to w_1 with length $\leq k$ formed from the arc $u \to u_3$, followed by the path from u_3 to w with length $k - 1 - \ell$ and the arc $w \to w_1$. This violates k-geodecity. It follows that option iii) must hold, i.e. $u_3 = o(v)$. Similarly $v_3 = o(u)$. □

Corollary 4.20. *No pair u, v of distinct vertices of G have identical out-neighbourhoods.*

Proof. Suppose that $u \neq v$ but $N^+(u) = N^+(v) = \{u_1, u_2, u_3\}$. The setup is shown in Figure 4.2. By Lemma 4.18 we know that $v = o(u)$ and $u = o(v)$. For $i = 1, 2, 3$ denote the in-neighbour of u_i that does not lie in $\{u, v\}$ by u_i^*. We cannot have $u_1^* = u_2^* = u_3^*$, for otherwise by Lemma 4.18 we would have $o(u) = u_1^* = v$.

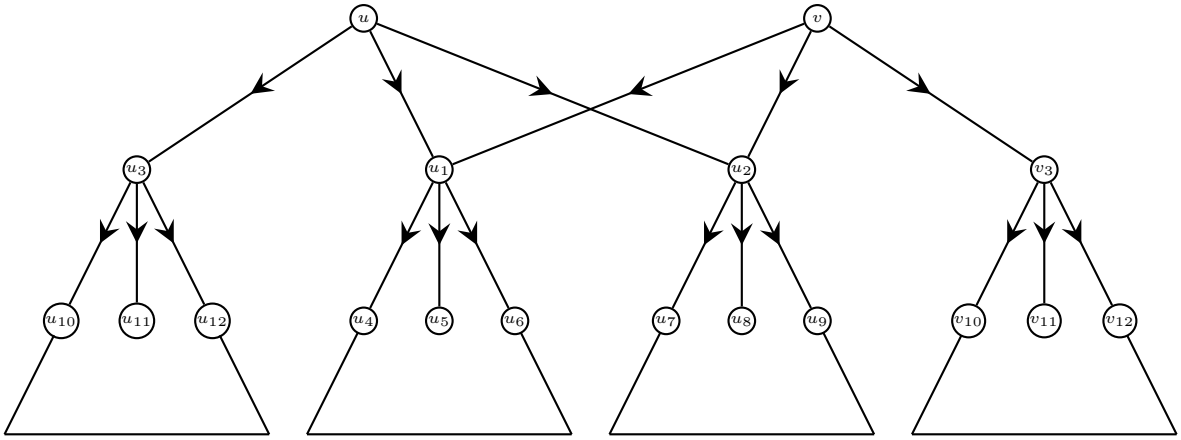

Figure 4.1: Vertices with two common out-neighbours

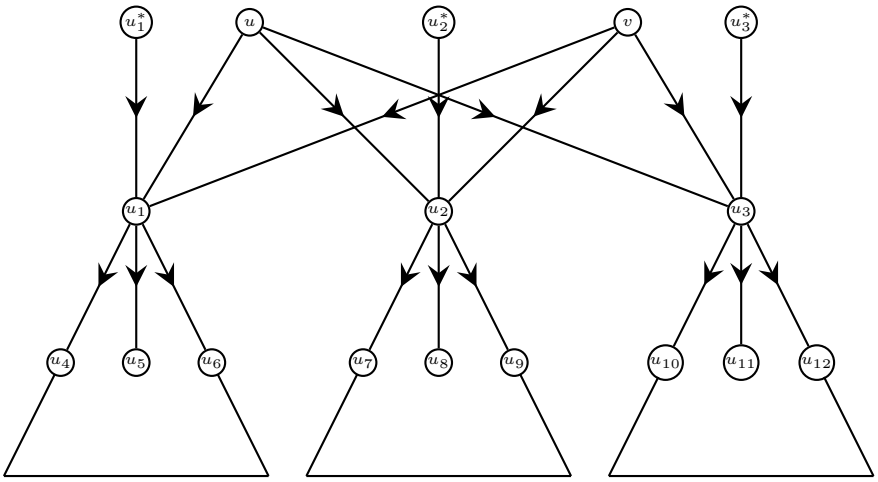

Figure 4.2: Configuration for Corollary 4.20

By the Duality Principle taking the converse G^- of G yields a diregular $(3, k; +1)$-digraph with outlier function $o' = o^-$. In G^- we have $N^+(u_i) = \{u_i^*, u, v\}$ for $i = 1, 2, 3$.

Suppose that $u_i^* \neq u_j^*$. Then in G^- the pair of vertices u_i, u_j has exactly two common out-neighbours, so that by Lemma 4.19 we obtain $o^-(u_i) = u_j^*$ and $o^-(u_j) = u_i^*$. If u_1^*, u_2^*, u_3^* are all distinct, we would then obtain $o^-(u_1) = u_2^* = u_3^*$, a contradiction.

We can thus assume that $u_1^* = u_2^* \neq u_3^*$. Applying Lemma 4.19 to the pairs u_1, u_3 and u_2, u_3 in turn, we deduce that $o^-(u_1) = o^-(u_2) = u_3^*$, again a contradiction, as o is a permutation. □

Having ruled out identical out-neighbourhoods, we can complete the proof of our desired result.

Theorem 4.21. *Any two distinct vertices of a $(3, k; +1)$-digraph G have at most one common out-neighbour and at most one common in-neighbour.*

Proof. Suppose that u, v are distinct vertices with more than one out-neighbour in common. By Corollary 4.20, u and v must have exactly two common out-neighbours. Write $N^+(u) = \{u_1, u_2, u_3\}$ and $N^+(v) = \{v_1, v_2, v_3\}$, where $u_1 = v_1, u_2 = v_2$, but $u_3 \neq v_3$. We label the remaining vertices in accordance with Figure 4.1; in particular if $k \geq 3$, then $N^+(u_1) = \{u_4, u_5, u_6\}$, $N^+(u_2) = \{u_7, u_8, u_9\}$ and $N^+(u_3) = \{u_{10}, u_{11}, u_{12}\}$. By Lemma 4.19 we know that $o(u) = v_3$ and $o(v) = u_3$.

Let $w \in T(u_3) \cap T(v_3)$, with $d(u_3, w) = s$ and $d(v_3, w) = t$. Suppose that $s > t$. Consider the set $N^{k-s}(w)$. By construction, $N^{k-s}(w) \subseteq N^k(u_3)$, so $N^{k-s}(w) \cap T(u_3) = \emptyset$. We have $k + t - s \leq k - 1$, so $N^{k-s}(w) \subseteq T(v_3)$. Hence by k-geodecity $N^{k-s}(w) \cap (T(u_1) \cup T(u_2)) = \emptyset$. As no vertex of $N^{k-s}(w)$ can lie in any of the branches of the Moore tree rooted at u, we must have $N^{k-s}(w) \subseteq \{u, o(u)\}$. Thus the size of the set $N^{k-s}(w)$ satisfies $|N^{k-s}(w)| = 3^{k-s} \leq 2$, which is impossible for $s \leq k - 1$. Therefore $d(u_3, w) = d(v_3, w)$ for every $w \in T(u_3) \cap T(v_3)$.

Consider $N^+(u_3)$ and $N^+(v_3)$. By k-geodecity $N^+(u_3) \cap (T(u_1) \cup T(u_2)) = \emptyset$. Also $v_3 \notin N^+(u_3)$, as $v_3 = o(u)$, and $o(v) = u_3 \notin N^+(u_3)$. Thus $N^+(u_3) \subset \{v\} \cup N^+(v_3)$ and similarly $N^+(v_3) \subset \{u\} \cup N^+(u_3)$. By Corollary 4.20 we cannot have $N^+(u_3) = N^+(v_3)$, so we can assume that $u_{10} = v_{10}$, $u_{11} = v_{11}$, $u_{12} = v$ and $v_{12} = u$. If $k \geq 3$ then u will have distinct $\leq k$-paths to u_1 (and u_2), namely $u \to u_1$ and $u \to u_3 \to v \to u_1$, so $k = 2$. The resulting configuration is displayed in Figure 4.3.

Observe that now u_3 and v_3 have two out-neighbours in common, namely u_{10} and u_{11}, so by Lemma 4.19 we have $o(u_3) = u$ and $o(v_3) = v$. Applying the outlier automorphism to the arcs incident with u, we deduce that $o(u) = v_3$ has arcs to $o(u_3) = u$ and $o(u_1)$ and $o(u_2)$, so $\{o(u_1), o(u_2)\} = \{u_{10}, u_{11}\}$. By 2-geodecity u_{10} can have arcs only to $N^+(u_1)$ and $N^+(u_2)$. As u_{10} has three out-going arcs and cannot have the same out-neighbourhood as u_1 or u_2 by Corollary 4.20, it follows that u_{10} must have two common out-neighbours with either u_1 or u_2; without loss of generality $N^+(u_{10}) = \{u_4, u_5, u_7\}$. Applying Lemma 4.19 to the pair u_1, u_{10} we see that $o(u_1) = u_7$. As we have already determined that $o(u_1) \in \{u_{10}, u_{11}\}$, this is a contradiction. The last part of the theorem follows by the Duality Principle. □

Theorem 4.21 allows us to prove our first non-existence result for degree three, namely that there are no $(3, 2; +1)$-digraphs.

Theorem 4.22. *There are no* $(3, 2; +1)$*-digraphs.*

Proof. Suppose that G is a $(3, 2; +1)$-digraph; by Lemma 4.1 G is diregular. Fix an

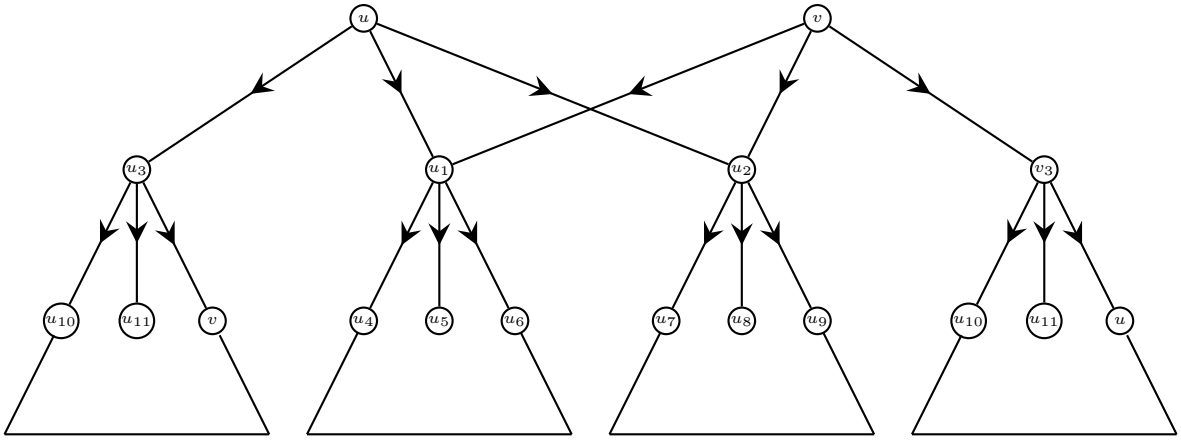

Figure 4.3: Configuration for Theorem 4.21

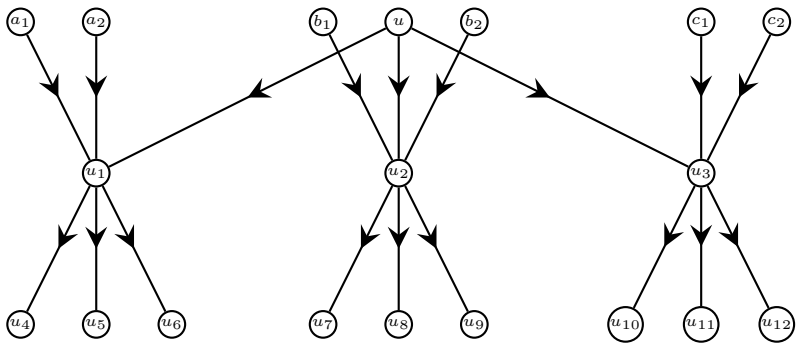

Figure 4.4: The Moore tree for Theorem 4.22

arbitrary vertex u of G with $N^+(u) = \{u_1, u_2, u_3\}$ and draw the Moore tree rooted at u as shown in Figure 4.4. We set $N^-(u_1) = \{u, a_1, a_2\}$, $N^-(u_2) = \{u, b_1, b_2\}$ and $N^-(u_3) = \{u, c_1, c_2\}$.

At least one of the vertices c_1, c_2 is not equal to $o(u)$, say $c_1 \neq o(u)$. By 2-geodecity $c_1 \notin T(u) \cup N^+(u_3)$, so without loss of generality we can assume that $c_1 \in N^+(u_1)$, say $c_1 = u_4$. By Theorem 4.21 c_1 has no arcs to $T(u) - \{u_3\}$, at most one arc to $N^+(u_2)$ and by 2-geodecity has no arcs to $N^+(u_1) \cup N^+(u_3)$. It follows that c_1 must have exactly one arc to $N^+(u_2)$ as well as an arc to $o(u)$. If $c_2 = o(u)$ this would yield two paths of length ≤ 2 from c_1 to u_3, so $c_2 \neq o(u)$. By the same reasoning c_2 has an arc to $o(u)$; however, we now have two distinct vertices with at least two common out-neighbours, contradicting Theorem 4.21. □

4.3 Automorphisms of digraphs with excess one

In [133] Sillasen uses counting arguments to deduce information on the form of the subdigraph of an almost Moore digraph that is induced by the set of vertices fixed by an automorphism. Using the same approach we can deduce a strong result on the

action of automorphisms of a digraph with excess one. This will later help us to analyse the structure of the outlier function of a $(d, k; +1)$-digraph.

Let G be a $(d, k; +1)$-digraph and $\phi \in \mathrm{Aut}(G)$ a non-identity automorphism of G. Denote by $\mathrm{Fix}(\phi)$ the set of vertices of G that are fixed by ϕ and let $\mathrm{FIX}(\phi)$ be the subdigraph induced by $\mathrm{Fix}(\phi)$.

Firstly we show that the fix-set $\mathrm{Fix}(\phi)$ is closed under the action of the outlier automorphism.

Lemma 4.23. *If $u \in \mathrm{Fix}(\phi)$, then $o^j(u) \in \mathrm{Fix}(\phi)$ for all $j \in \mathbb{N}$.*

Proof. Let $u \in \mathrm{Fix}(\phi)$. If $d(u, v) \leq k$, then $d(\phi(u), \phi(v)) = d(u, \phi(v)) \leq k$, so the only vertex of $V(G)$ that lies at distance $\geq k + 1$ from u is $\phi(o(u))$ and so $\phi(o(u)) = o(u)$ and $o(u) \in \mathrm{Fix}(\phi)$. Iteration of o implies the result. □

As the outlier automorphism is fixed-point-free, it follows from Lemma 4.23 that any fix-set $\mathrm{Fix}(\phi)$ cannot consist of a single vertex and, if ϕ fixes just two vertices u, u' of G, then these two vertices are outliers of each other, i.e. $o(u) = u'$ and $o(u') = u$.

Corollary 4.24. *If $|\mathrm{Fix}(\phi)| \leq 2$, then either $\mathrm{Fix}(\phi) = \emptyset$ and $\mathrm{FIX}(\phi)$ is the null digraph, or $|\mathrm{Fix}(\phi)| = 2$ and $\mathrm{FIX}(\phi) \cong 2K_1$.*

We will now assume that $\mathrm{Fix}(\phi)$ contains at least three vertices.

Lemma 4.25. *If $u, v \in \mathrm{Fix}(\phi)$ and P is a path of length $\leq k$ from u to v, then all vertices of P are contained in $\mathrm{Fix}(\phi)$.*

Proof. Let u, v and P be as described. Suppose that there is a vertex $u' \in V(P)$ that is not fixed by ϕ. Then P and $\phi(P)$ are distinct $\leq k$-paths from u to v, contradicting k-geodecity. □

Lemma 4.26. *The digraph $\mathrm{FIX}(\phi)$ is diregular.*

Proof. For any vertex $u \in \mathrm{Fix}(\phi)$ we will denote the out-degree and in-degree of u in the subdigraph $\mathrm{FIX}(\phi)$ by $d^+_\phi(u)$ and $d^-_\phi(u)$ respectively. We will show that for any two (not necessarily distinct) vertices $u, v \in \mathrm{Fix}(\phi)$ we have $d^+_\phi(u) = d^-_\phi(v)$; this implies the desired result. For this pair u, v we will write $N^+(u) = \{u_1, u_2, \ldots, u_d\}$ and $N^-(v) = \{v_1, \ldots, v_d\}$.

Assume that $v \notin o(N^+(u))$. Then for $1 \leq i \leq d$ there is a unique $\leq k$-path P_i from u_i to v. Suppose that $u \not\to v$. By k-geodecity, none of the paths P_i pass through the same in-neighbour of v, so without loss of generality there is a $\leq (k-1)$-path from u_i to v_i for $1 \leq i \leq d$. By Lemma 4.25, it follows that $u_i \in \mathrm{Fix}(\phi)$ if and only if $v_i \in \mathrm{Fix}(\phi)$, so that $d^+_\phi(u) = d^-_\phi(v)$. If $u \to v$, then repeating this reasoning for the out-neighbours of u other than v shows that we still have $d^+_\phi(u) = d^-_\phi(v)$.

Now suppose that $v \in o(N^+(u))$; say $v = o(u_1)$. If $u \not\to v$, then for $2 \leq i \leq d$ we can assume that there is a $\leq (k-1)$-path from u_i to v_i and as before $u_i \in \mathrm{Fix}(\phi)$ if and only if $v_i \in \mathrm{Fix}(\phi)$ for $2 \leq i \leq d$. There is an arc $u \to u_1$, so as o is an automorphism there exists an arc $o(u) \to o(u_1) = v$, giving $o(u) \in N^-(v)$. There are $\leq k$-paths from u to each v_i for $2 \leq i \leq d$, so we must have $o(u) = v_1$. As $o(u) \in \mathrm{Fix}(\phi)$ by Lemma 4.23 we have $v_1 \in \mathrm{Fix}(\phi)$. Also by Lemma 4.23 we have $o^-(v) = u_1 \in \mathrm{Fix}(\phi)$, so again we see that $d^+_\phi(u) = d^-_\phi(v)$. Again the case $u \to v$ is similar.

It follows that $\mathrm{FIX}(\phi)$ is diregular. □

Lemma 4.27. *The digraph* $\mathrm{FIX}(\phi)$ *is an isometric subdigraph of* G *and has diameter* $k+1$.

Proof. As $\mathrm{Fix}(\phi)$ is a subdigraph of G we certainly have $d_{\mathrm{FIX}(\phi)}(u,v) \geq d_G(u,v)$ for all $u, v \in \mathrm{Fix}(\phi)$. Let $u, v \in \mathrm{Fix}(\phi)$ be arbitrary. If $v \in T_k(u) \cap \mathrm{Fix}(\phi)$, then by Lemma 4.25 all vertices of the unique path from u to v with length $\leq k$ in G also belong to $\mathrm{FIX}(\phi)$, so that $d_G(u,v) = d_{\mathrm{FIX}(\phi)}(u,v)$.

By Lemma 4.26, $\mathrm{FIX}(\phi)$ is diregular with degree ≥ 1 (as we are assuming that $|\mathrm{Fix}(\phi)| \geq 3$). Hence if $v = o(u)$ in G, then $o(u)$ has an in-neighbour v' in $\mathrm{Fix}(\phi)$, so that by the preceding argument $d_G(u,v') = d_{\mathrm{FIX}(\phi)}(u,v')$ and thus $d_{\mathrm{FIX}(\phi)}(u, o(u)) = k+1$. Therefore $\mathrm{FIX}(\phi)$ is an isometric subdigraph of G and, since $o(u) \in \mathrm{Fix}(\phi)$ for any $u \in \mathrm{Fix}(\phi)$, the diameter of $\mathrm{FIX}(\phi)$ is exactly $k+1$. □

Corollary 4.28. *The digraph* $\mathrm{FIX}(\phi)$ *is a* $(d', k; +1)$*-digraph for some* d' *in the range* $1 \leq d' \leq d-1$.

Proof. As a subdigraph of G, $\mathrm{FIX}(\phi)$ is k-geodetic. By Lemma 4.26, $\mathrm{FIX}(\phi)$ is diregular with degree d'. We are assuming that $\mathrm{Fix}(\phi)$ contains at least three vertices, so by Lemma 4.25 $\mathrm{FIX}(\phi)$ contains a path and $d' \geq 1$. We are also assuming that ϕ is not the identity automorphism, so ϕ does not fix all vertices of G and $d' \leq d-1$. By diregularity and Lemma 4.27, it follows that $\mathrm{FIX}(\phi)$ has order $M(d',k)+1$, so $\mathrm{FIX}(\phi)$ is a $(d', k; +1)$-digraph. □

As there are no diregular $(2, k; +1)$-digraphs by Lemma 4.1 (see [133]), we have the following result.

Corollary 4.29. *If G is a $(d, k; +1)$-digraph and ϕ is a non-identity automorphism of G, then $\mathrm{FIX}(\phi)$ is either the null digraph, a pair of isolated vertices, a directed $(k+2)$-cycle or a $(d', k; +1)$-digraph, where $3 \leq d' \leq d-1$.*

4.4 Structure of the outlier function

We will now make use of some of the results from the preceding sections to deduce useful information on the permutation structure of the outlier function of a digraph with excess one. Let G be a $(d, k; +1)$-digraph. Recall by Chapter 3 that we are only interested in the case $k \geq 2$. By Theorem 3.15 G is diregular and by Theorem 3.13 the outlier function of G is an automorphism. Therefore every vertex u of G has an associated order $\omega(u)$, which is the smallest integer such that $o^{\omega}(u) = u$. We can immediately apply reasoning similar to that of [42] to make a connection between the vertex orders and the existence of short paths.

Lemma 4.30. *Let $u_0, u_1, \ldots, u_r$ be a path of length r in G, where $r \leq k$, and put $t = \mathrm{lcm}(\omega(u_0), \omega(u_r))$. Then $\omega(u_i)$ divides t for $1 \leq i \leq r-1$.*

Proof. Suppose that for some $1 \leq i \leq r-1$ the order of u_i does not divide t. Then $o^t(u_i) \neq u_i$, so we obtain two $\leq k$-paths $u_0, u_1, \ldots, u_i, \ldots, u_r$ and $o^t(u_0), o^t(u_1), \ldots, o^t(u_i), \ldots, o^t(u_r) = u_0, o^t(u_1), \ldots, o^t(u_i), \ldots, u_r$ from u_0 to u_r, a contradiction. □

Corollary 4.31. *If p is the minimum vertex order of G and W is a walk of length $\leq k$ between two vertices u, v with order p, then every vertex on W has order p.*

Proof. Suppose that there is a vertex w on W such that $\omega(w) > p$. Then W and $o^p(W)$ are two distinct walks of length $\leq k$ between u and v, contradicting k-geodecity. □

We now make two definitions that will help us to analyse the structure of the permutation o.

Definition 4.32. The *index* $\omega(G)$ of a $(d, k; +1)$-digraph G is the value of the smallest vertex order in G, i.e. $\omega(G) = \min\{\omega(u) : u \in V(G)\}$.

Definition 4.33. A $(d, k; +1)$-digraph G is *outlier-regular* if its outlier function o is a regular permutation of $V(G)$, i.e. each cycle in the cycle decomposition of the permutation o has the same length. If each vertex of G has order ω, then G is *ω-outlier-regular*.

As o is an automorphism it follows that any power o^r of o is also an automorphism of G. In Section 4.3 we classified the possible fixed sets of any non-identity automorphism of G. We therefore record the following implication of Corollary 4.29.

Corollary 4.34. *For any integer $r \geq 2$, the set of vertices of G with order dividing r induces one of the following:*

- *the entire digraph G,*
- *the empty digraph,*
- *a pair of vertices that form a transposition in o,*
- *a directed $(k+2)$-cycle, or*
- *a $(d', k; +1)$-digraph, where $3 \leq d' \leq d-1$.*

In Conjecture 4.2 we claimed that there are no $(d, k; +1)$-digraphs for $d, k \geq 2$; one approach to proving this conjecture is to study the properties of a minimal counterexample. Let $k \geq 2$ and suppose that there exists a $(d, k; +1)$-digraph with $d \geq 2$. Then let d' be the smallest possible value of $d \geq 3$ such that there exists a $(d, k; +1)$-digraph; we will refer to a $(d', k; +1)$-digraph as a *minimal $(d, k; +1)$-digraph*. For a fixed k, Corollary 4.34 strongly restricts the structure of the outlier automorphism of a minimal $(d, k; +1)$-digraph.

Corollary 4.35. *A minimal $(d, k; +1)$-digraph G satisfies one of the following:*

- *G is outlier-regular,*
- *the outlier function o of G contains a unique transposition, or*
- *the vertices of G with order $\omega(G)$ form a directed $(k+2)$-cycle.*

In particular this holds for any $(3, k; +1)$-digraph.

Proof. By Corollary 4.34 the automorphism $o^{\omega(G)}$ fixes either i) every vertex of G, in which case every vertex of G has order $\omega(G)$ and G is outlier-regular, ii) two vertices that are outliers of each other, so that $\omega(G) = 2$ and o contains a unique transposition, or iii) a $(k+2)$-cycle. □

If a minimal $(d, k; +1)$-digraph is not outlier-regular, then Corollary 4.35 allows us to deduce the subdigraph induced by the set of vertices with smallest order.

Lemma 4.36. *If a minimal $(d, k; +1)$-digraph G is not outlier-regular, then either its outlier function o contains a unique transposition, or else $\omega(G) = k + 2$ and the vertices with order $k + 2$ induce a directed $(k + 2)$-cycle.*

Proof. Suppose that G is a non-outlier-regular minimal $(d, k; +1)$-digraph with outlier function that does not contain a unique transposition. Then by Corollary 4.35 the vertices with order equal to the index $\omega(G)$ of G induce a directed $(k + 2)$-cycle C. For any vertex u in the cycle its outlier $o(u)$ also has order $\omega(G)$, so the outlier of u must be the vertex preceding u on the cycle C; it follows that $\omega(G) = k + 2$. □

We will find the following classification of this behaviour convenient.

Definition 4.37. A minimal $(d, k; +1)$-digraph G such that the vertices of G with order $\omega(G)$ form a directed $(k + 2)$-cycle is *Type A*, whereas if the outlier function o of G contains a unique transposition, then G is *Type B*.

According to this definition, every minimal $(d, k; +1)$-digraph is either Type A, Type B or outlier-regular. Let us now return to the problem of digraphs with degree three and excess one; if any such digraph exists it is minimal.

Lemma 4.38. *Let G be a $(3, k; +1)$-digraph of Type A. Then $k+2$ divides $\frac{M(3,k)-k-1}{2}$.*

Proof. By Lemma 4.36 we have $\omega(G) = k + 2$ and the vertices with order $k + 2$ induce a $(k + 2)$-cycle C. Pick a vertex u on C and write $N^+(u) = \{u_1, u_2, u_3\}$, where u_1 also lies on C. The automorphism $o^{(k+2)}$ fixes u and u_1, but not u_2 and u_3, so $o^{(k+2)}$ transposes u_2 and u_3. Thus $o^{2(k+2)}$ fixes every vertex in $T_1(u)$ and by Corollary 4.34 every vertex of G has order either $k + 2$ or $2(k + 2)$. If there are r cycles in o with length $2(k + 2)$, then we obtain

$$M(3, k) + 1 = k + 2 + 2r(k + 2)$$

and $k + 2$ divides $\frac{M(3,k)-k-1}{2}$. □

Lemma 4.39. *Let G be a $(3, k; +1)$-digraph of Type B. Then $k \not\equiv 3, 5 \pmod 6$. If $k \equiv 0, 2 \pmod 6$, then G contains two vertices of order two, with all other vertices of G having order six.*

Proof. Assume that G is a non-outlier-regular $(3, k; +1)$-digraph with outlier function o containing a unique transposition. Let u and $o(u)$ be the vertices of G with order two, where $N^+(u) = \{u_1, u_2, u_3\}$. The automorphism o^2 fixes u, but fixes no vertex in $\{u_1, u_2, u_3\}$. We can thus assume that o^2 permutes u_1, u_2, u_3 in a 3-cycle $(u_1u_2u_3)$.

By Theorem 4.21 u and $o(u)$ have at most one common out-neighbour. Suppose that $N^+(u) \cap N^+(o(u)) \neq \emptyset$; we can assume that u_1 is the common out-neighbour of u and $o(u)$. However, applying the automorphism o^2 to G shows that $o^2(u_1)$ is a common out-neighbour of u and $o(u)$ and, since G is Type B we have $o^2(u_1) \neq u_1$, thereby violating Theorem 4.21. It follows that o contains the 6-cycle $(u_1, o(u_1), u_2, o(u_2), u_3, o(u_3))$.

Therefore $\{u\} \cup N^+(u) \subseteq \mathrm{Fix}(o^6)$ and hence o^6 fixes every vertex of G, so that the order of every vertex apart from u and $o(u)$ is either 3 or 6.

Suppose that there is a vertex with order 3. Then o^3 fixes a $(k+2)$-cycle. If there are r cycles in o of length 6, then

$$M(3, k) + 1 = 2 + (k + 2) + 6r.$$

Hence $6|(M(3, k) - k - 3)$. This implies that $k \equiv 1 \pmod 3$.

On the other hand, suppose that all vertices of G have order six, with the exception of the two vertices with order two. Then $6|(M(3, k) - 1)$, which implies that k is even.

Thus if $k \equiv 3 \pmod 6$ or $k \equiv 5 \pmod 6$, then no such digraph can exist. □

Corollary 4.40. *If $k \geq 2$ is such that*

- $k \equiv 3$ *or* $5 \pmod 6$,
- $k + 2$ *does not divide* $\frac{M(3,k)-k-1}{2}$, *and*
- $M(3, k) + 1$ *is prime,*

then there is no $(3, k; +1)$-digraph.

Proof. Assume that G is a $(3, k; +1)$-digraph such that k satisfies each of these conditions. By Lemmas 4.38 and 4.39, G is neither Type A nor Type B and hence must be outlier-regular. As the order of G is prime, it follows that its outlier function o consists of a single cycle of length $M(3, k) + 1$; thus G is vertex-transitive. However, any vertex-transitive digraph with prime order is a circulant digraph (this follows

from the result of [148], the argument of which, as noted in [4], applies equally well to directed graphs), which is not k-geodetic for $k \geq 2$. It follows that there is no $(3, k; +1)$-digraph for]such k. □

The first k for which Corollary 4.40 applies are $k = 3, 15$ and 63. This provides an independent proof of the non-existence of $(3, 3; +1)$-digraphs (this case is covered by the result of [116] for $k = 3$), as well as ruling out the existence of $(3, k; +1)$-digraphs for some larger k.

Corollary 4.41. *There are no* $(3, 3; +1)$, $(3, 15; +1)$- *or* $(3, 63; +1)$-*digraphs.*

4.5 Spectral results

Now that we have more information about the permutation structure of o, we can apply some more powerful spectral results developed in [116]. If A is the adjacency matrix of a $(d, k; +1)$-digraph G with order n, J is the $n \times n$ all-one matrix and P is the permutation matrix associated with the permutation o, then we know by Theorem 1.3 that

$$I + A + A^2 + \cdots + A^k = J - P. \tag{4.2}$$

We will now exploit the connection in Equation 4.2 between the permutation structure of the outlier function o of a $(d, k; +1)$-digraph G and the spectrum of G. We will use the following concise description of the permutation structure of the outlier function o from [116].

Definition 4.42. For any $(d, k; +1)$-digraph G and $1 \leq j \leq M(d, k) + 1$, the number of cycles of length j in the permutation o will be denoted by m_j. The $(M(d, k) + 1)$-tuple $(m_1, m_2, \ldots, m_{M(d,k)+1})$ is the *permutation vector* of G. For $1 \leq j \leq M(d, k) + 1$ we define

- $m'(j)$ is the number of odd cycles in the permutation o with length divisible by j,
- $m''(j)$ is the number of even cycles in the permutation o with length divisible by j, and
- $m(j) = m'(j) + m''(j)$ is the total number of cycles in o with length divisible by j.

Note that as the outlier function is fixed-point-free we always have $m_1 = 0$. We will also need the following family of polynomials derived from the cyclotomic polynomials.

Definition 4.43. For $n, k \geq 1$ the polynomial $F_{n,k}(x)$ is defined by

$$F_{n,k}(x) = \Phi_n(1 + x + x^2 + \cdots + x^k),$$

where $\Phi_n(x)$ is the n-th cyclotomic polynomial.

In [116] Miller et al. derive the following relation between the characteristic polynomial of $J - P$ and the permutation vector of G.

Lemma 4.44 ([116])**.** *The characteristic polynomial of $J - P$ is*

$$(x - M(d,k))(x+1)^{-1} \prod_{j \geq 2, j \text{ even}} (x^j - 1)^{m_j} \prod_{j \geq 3, j \text{ odd}} (x^j + 1)^{m_j}.$$

Theorem 4.45. *There are no 2-outlier-regular $(d, k; +1)$-digraphs.*

Proof. Assume that G is a 2-outlier-regular $(d, k; +1)$-digraph with order $n = M(d,k) + 1$, i.e. the outlier function o of G contains only transpositions. Thus $m_2 = \frac{n}{2}$ and $m_i = 0$ for $i \neq 2$. Therefore by Lemma 4.44 the characteristic polynomial of $J - P$ is

$$(x - M(d,k))(x+1)^{-1}(x^2 - 1)^{n/2} = (x - M(d,k))(x-1)^{\frac{n}{2}}(x+1)^{\frac{n}{2}-1}.$$

It follows from Equation 4.2 that the spectrum of G consists of

- one eigenvalue d,
- $\frac{n}{2}$ eigenvalues λ_i, $1 \leq i \leq \frac{n}{2}$, such that $1 + \lambda_i + \lambda_i^2 + \cdots + \lambda_i^k = 1$ for $1 \leq i \leq \frac{n}{2}$, and
- $\frac{n}{2} - 1$ eigenvalues μ_i such that for $1 \leq i \leq \frac{n}{2} - 1$ we have $1 + \mu_i + \mu_i^2 + \cdots + \mu_i^k = -1$.

For any integer $r \geq 0$ we define

$$\Lambda_r = \sum_{i=1}^{\frac{n}{2}} \lambda_i^r$$

and

$$M_r = \sum_{i=1}^{\frac{n}{2}-1} \mu_i^r.$$

As for all vertices u of G we have $o^-(u) = o(u)$, the reasoning of Theorem 4.14 shows

that each vertex of G is contained in d directed $(k+1)$-cycles. By k-geodecity, any closed $(k+1)$-walk must be a cycle, so it follows from Theorem 1.3 that

$$\mathrm{Tr}(A^r) = d^r + \Lambda_r + M_r = 0, 1 \leq r \leq k, \tag{4.3}$$

and

$$\mathrm{Tr}(A^{k+1}) = d^{k+1} + \Lambda_{k+1} + M_{k+1} = dn. \tag{4.4}$$

Each eigenvalue λ_i satisfies $1 + \lambda_i + \lambda_i^2 + \cdots + \lambda_i^k = 1$; summing this geometric series and rearranging we obtain $\lambda_i(\lambda_i^k - 1) = 0$, so each λ_i is either zero or a k-th root of unity. Hence for $1 \leq r \leq k$ we have $\Lambda_{k+r} = \Lambda_r$. Similarly each eigenvalue μ_i satisfies $\mu_i^{k+1} = 2 - \mu_i$, so that for $1 \leq r \leq k$ we have $\mu_i^{k+r} = 2\mu_i^{r-1} - \mu_i^r$. Thus for $1 \leq r \leq k$ the numbers M_{k+r} satisfy $M_{k+r} = -M_r + 2M_{r-1}$.

In particular $M_{k+1} = -M_1 + 2M_0 = -M_1 + n - 2$ and $\Lambda_{k+1} = \Lambda_1$. Therefore by Equation 4.4 we have

$$\Lambda_1 - M_1 = dn - d^{k+1} - n + 2 = d.$$

Subtracting this from Equation 4.3 with $r = 1$ yields

$$M_1 = -d.$$

For any prime p the polynomial $p + x + x^2 + \cdots + x^k$ is irreducible over $\mathbb{Q}$ [79]. As each μ_i is a solution of $2 + x + x^2 + \cdots + x^k = 0$, it follows that the roots of $2 + x + x^2 + \cdots + x^k$ must appear with equal multiplicity among the μ_i. Therefore k must divide $\frac{n}{2} - 1$. The sum of the roots of $2 + x + x^2 + \cdots + x^k$ is -1; therefore it follows that

$$-d = M_1 = -\frac{1}{k}\left(\frac{n}{2} - 1\right).$$

Rearranging, we obtain

$$n = 2 + d + d^2 + d^3 + \cdots + d^k = 2kd + 2,$$

or, simplifying,

$$2k = 1 + d + d^2 + \cdots + d^{k-1},$$

which is impossible for $d, k \geq 2$. □

In particular, it follows from Lemma 4.16 and Theorem 4.45 that no $(d, k; +1)$-digraph with $d, k \geq 2$ can be arc-transitive.

4.6 2-geodetic digraphs with excess one

In [116] the authors use spectral techniques to show that there are no 2-geodetic digraphs with excess one and degree $d \geq 8$. Sillasen's first paper on the subject [132] proves that there are no $(2, 2; +1)$-digraphs. Theorem 4.22 of the present work further showed that there are no $(3, 2; +1)$-digraphs. This leaves open the existence of $(d, 2; +1)$-digraphs for $d = 4, 5, 6$ and 7. We will see that no $(d, 2; +1)$-digraphs exist for these values of d. We first rule out the existence of outlier-regular $(d, 2; +1)$-digraphs, then use an inductive approach to deal with the remaining cases.

Accordingly we shall now assume that any $(d, 2; +1)$-digraph is outlier-regular. Let G be an outlier-regular $(d, 2; +1)$-digraph with d in the range $4 \leq d \leq 7$. Then the index $\omega(G)$ of G must be a non-unit divisor of the order $2 + d + d^2$ of G. These divisors are displayed in Table 4.1.

d	*Order*	Divisors > 1
4	22	2,11,22
5	32	2,4,8,16,32
6	44	2,4,11,22,44
7	58	2,29,58

Table 4.1: Nontrivial divisors of the orders of the $(d, 2; +1)$-graphs

Theorem 4.45 shows that there are no 2-outlier-regular digraphs, so we have already dealt with the divisors in red. Furthermore, if the index $\omega(G)$ of the digraph is equal to the order $2 + d + d^2$ of the digraph G, then G is vertex-transitive and by Corollary 4.12 the size $2d + d^2 + d^3$ of G must be divisible by 3; this precludes the existence of outlier-regular digraphs with the divisors written in blue in Table 4.45. For the remaining possible structures of the outlier function we will need the exact factorisation of the characteristic polynomial of a $(d, 2; +1)$-digraph from [116].

Lemma 4.46 ([116]). *The characteristic polynomial of a $(d, 2; +1)$-digraph factorises*

in $\mathbb{Q}[x]$ *as*

$$(x-d)x^{a_1}(x+1)^{a_2}(x^2+x+2)^{\frac{m(2)+m'(1)-1}{2}}(x^2+1)^{m(4)} \times \prod_{j\geq 3, j \text{ odd}} F_{j,2}(x)^{\frac{m''(j)}{2}} F_{2j,2}(x)^{\frac{m'(j)}{2}} \prod_{j\geq 6, j \text{ even}} F_{j,2}(x)^{\frac{m(j)}{2}}, \quad (4.5)$$

where a_1 *and* a_2 *are non-negative integers that satisfy the simultaneous equations*

$$a_1 + a_2 = m''(1) \text{ and } d^2 - d + 1 = a_1 - a_2 + 2m(4). \quad (4.6)$$

Lemma 4.47. *An outlier-regular* $(d, 2; +1)$*-digraph cannot have odd index* $\omega(G)$*.*

Proof. Suppose that $\omega(G)$ is odd. Then $m(4) = m''(1) = 0$ and $a_1 = a_2 = 0$. Equation 4.6 then gives $d^2 - d + 1 = 0$, which has no real solutions. □

Lemma 4.47 disposes of all of the green entries in Table 4.1.

Lemma 4.48. *There are no* 22*- or* 44*-outlier-regular* $(6, 2; +1)$*-digraphs.*

Proof. If a $(6, 2; +1)$-digraph G is 22-outlier-regular, then $m(4) = 0$ and $m''(1) = 2$, so the simultaneous equations in Equation 4.6 give $a_1 + a_2 = 2$ and $a_1 - a_2 = 31$, which has no solution in non-negative integers.

Similarly, if G is a 44-outlier-regular $(6, 2; +1)$-digraph, then $m''(1) = 1$ and $m(4) = 1$, so that Equation 4.6 yields $a_1 + a_2 = 1$ and $a_1 - a_2 = 29$, which again does not have non-negative solutions. □

Lemma 4.48 disposes of the pink divisors in Table 4.1.

Lemma 4.49. *There are no outlier-regular* $(d, 2; +1)$*-digraphs.*

Proof. First let $d = 5$ and $\omega \in \{4, 8, 16\}$. Then $m''(1) = m(4) = \frac{32}{\omega}$ and $d^2 - d + 1 = 21$. Equation 4.6 yields $a_1 + a_2 = \frac{32}{\omega}$ and $a_1 - a_2 = 21 - \frac{64}{\omega}$. Solving for a_1 shows that

$$a_1 = \frac{1}{2}\left[21 - \frac{32}{\omega}\right],$$

which is not an integer for $\omega \in \{4, 8, 16\}$. This gets rid of all of the orange entries in Table 4.1.

The only remaining option for an ω-outlier-regular $(d, 2; +1)$-digraph G is that $d = 6$ and $\omega = 4$. Then $m(4) = m''(1) = 44/4 = 11$ and $d^2 - d + 1 = 31$. Equation 4.6 becomes $a_1 + a_2 = 11$ and $a_1 - a_2 = 9$, which has solution $a_1 = 10$ and $a_2 = 1$. It follows from Lemma 4.46 that the spectrum of G is

$$\{6^{(1)}, 0^{(10)}, -1^{(1)}, \left[\frac{-1+\sqrt{7}i}{2}\right]^{(5)}, \left[\frac{-1-\sqrt{7}i}{2}\right]^{(5)}, i^{(11)}, (-i)^{(11)}\}$$

where multiplicities are indicated in round brackets. Summing the third powers of the eigenvalues, it follows that

$$\mathrm{Tr}(A^3) = 240.$$

A vertex is contained in 6 directed triangles if it is Type I and 5 directed triangles if it is Type II. If there are α Type I vertices and β Type II vertices in G, it follows that $6\alpha + 5\beta = 240$ and $\alpha + \beta = 44$. Solving these equations, we have $\alpha = 20$ and $\beta = 24$. Let A be the subdigraph of G induced by the Type I vertices and B the subdigraph induced by the Type II vertices. By Lemma 4.10 it follows that B consists of a collection of 6 directed 4-cycles. Thus $|(A, B)| = |(B, A)| = 120$. Thus each vertex in A has out-neighbourhood entirely contained in B. Each vertex in B has just one out-neighbour in B and so each arc from a vertex u of A allows it to reach just twelve vertices of B by paths of length ≤ 2, which is impossible. □

It follows by Lemma 4.36 that any minimal $(d, 2; +1)$-digraph must be either Type A (with a directed 4-cycle C of vertices with order 4 and all other vertices with order greater than 4) or Type B. We will take an inductive approach. Theorem 4.22 shows that there is no $(3, 2; +1)$-digraph, so we can take any $(4, 2; +1)$-digraph to be minimal, which allows us to show that $(4, 2; +1)$-digraphs do not exist, so that any $(5, 2; +1)$-digraph is minimal and so on. We make the following two observations from Lemma 4.46 and Corollary 4.29 respectively.

Lemma 4.50. *If G is a minimal $(d, 2; +1)$-digraph, then $m''(1)$ is odd.*

Proof. By Lemma 4.46 we have $a_1 + a_2 = m''(1)$ and $a_1 - a_2 = d^2 - d + 1 - 2m(4)$, so $m''(1)$ has the same parity as $d^2 - d + 1$, which is odd. □

Lemma 4.51. *There are exactly two non-zero entries in the permutation vector of a minimal $(d, 2; +1)$-digraph and both cycle lengths of o are even.*

Proof. By Lemma 4.49, a minimal $(d, 2; +1)$-digraph is either Type A, in which case

the smallest non-zero entry of the permutation vector is $m_4 = 1$, or Type B, in which case the smallest entry is $m_2 = 1$.

By Corollary 4.29, for each $r \geq 1$ the automorphism o^r has fix-set of size 0, 2 or 4, or else fixes every vertex of G. Therefore if for some $r \geq 2$ the automorphism o^r fixes 3 or ≥ 5 vertices of G, then o^r is the identity automorphism and every vertex of G has order dividing r. Suppose that the permutation vector contains a non-zero entry $m_j = 0$, where $j \geq 3$ is odd. Then o^j fixes either 3 or ≥ 5 vertices of G, but not the vertices with even order, which is impossible. Likewise, if $i < j$ are both even, i is greater than $\omega(G)$ and m_i and m_j are both non-zero, then o^i fixes at least 6 vertices with order $\omega(G)$ or i, but not the vertices with order j, again a contradiction. □

Theorem 4.52. *There are no* $(4, 2; +1)$*-digraphs.*

Proof. Suppose that G is a $(4, 2; +1)$-digraph. Assume first that G is Type A. Let u be a vertex on the 4-cycle C of vertices with order 4, with $N^+(u) = \{u_1, u_2, u_3, u_4\}$, where u_1 also lies on C. The automorphism o^4 fixes u and u_1, but has no fixed points in $\{u_2, u_3, u_4\}$, so o^2 permutes u_2, u_3 and u_4 in a 3-cycle, say $(u_2u_3u_4)$. Thus o^{12} fixes every vertex of $T(u)$; by Corollary 4.29, o^{12} fixes every vertex of G and so every vertex of G has order $4, 6$ or 12. G has order 22, so we either have $m_4 = 1, m_6 = 3$ or $m_4 = 1, m_6 = 1, m_{12} = 1$. Both are impossible by Lemmas 4.50 and 4.51.

Thus we can assume G to be Type B. Let u be one of the two vertices of G with order 2. The automorphism o^2 fixes u, but permutes its out-neighbours u_1, u_2, u_3 and u_4 without fixed points. Hence without loss of generality o^2 permutes these vertices either as $(u_1u_2)(u_3u_4)$ or $(u_1u_2u_3u_4)$; in either case o^8 fixes every vertex of $T(u)$ and hence all of G, so every vertex has order $2, 4$ or 8. Hence $22 = 2 + 4m_4 + 8m_8$, or $5 = m_4 + 2m_8$. There are three solutions of this equation: i) $m_4 = 1, m_8 = 2$, ii) $m_4 = 3, m_8 = 1$ and iii) $m_4 = 5, m_8 = 0$. By Lemma 4.51 only option iii) can hold. Thus the two non-zero entries of the permutation vector of G are $m_2 = 1, m_4 = 5$ and $m''(1) = 6$, which is even, contradicting Lemma 4.50. □

Having proved that there are no $(4, 2; +1)$-digraphs, we know that any $(5, 2; +1)$-digraph is minimal.

Theorem 4.53. *There is no* $(5, 2; +1)$*-digraph.*

Proof. Assume that G is a $(5, 2; +1)$-digraph. G has order 32. By Theorem 4.52, G is minimal and hence by Lemma 4.49 is either Type A or Type B. Suppose that G is

Type A. As in Theorem 4.52, fix a vertex u on the cycle C of vertices with order 4 and set $N^+(u) = \{u_1, u_2, u_3, u_4, u_5\}$, where $u_1 \in V(C)$. The automorphism o^4 must permute u_2, u_3, u_4 and u_5 amongst themselves without fixed points, so o^4 acts on these vertices either as $(u_2u_3u_4u_5)$ or $(u_2u_3)(u_4u_5)$; in either case o^{16} fixes all vertices of G and every vertex order is $4, 8$ or 16. We have $32 = 4 + 8m_8 + 16m_{16}$, or $7 = 2m_8 + 4m_{16}$. However, the right-hand side is even and the left odd.

Now suppose that G is Type B and let u be a vertex of G belonging to the unique transposition of o. o^2 permutes the vertices of $N^+(u) = \{u_1, u_2, u_3, u_4, u_5\}$ without fixed points; without loss of generality, o^2 acts on these vertices either as i) $(u_1u_2u_3u_4u_5)$ or ii) $(u_1u_2u_3)(u_4u_5)$.

In case i) o^{10} fixes every vertex of G and every vertex order is $2, 5$ or 10, where $30 = 5m_5 + 10m_{10}$. By Lemma 4.51, $m_5 = 0$, so the non-zero entries of the permutation vector are $m_2 = 1, m_{10} = 3$, yielding $m''(1) = 4$, contradicting Lemma 4.50.

In case ii) o^{12} is the identity and every vertex has order $2, 3, 4, 6$ or 12. Lemma 4.51 shows that $m_3 = 0$. We have $30 = 4m_4 + 6m_6 + 12m_{12}$ and Lemma 4.51 shows that just one of m_4, m_6 and m_{12} is non-zero. By Lemma 4.51, as 12 and 4 do not divide 30, we have $m_4 = m_{12} = 0$. If $m_6 > 0$, then $m_2 = 1$ and $m_6 = 5$, giving an even value of $m''(1)$, which is impossible. □

Theorem 4.54. *There is no* $(6, 2; +1)$*-digraph.*

Proof. Suppose that there exists a $(6, 2; +1)$-digraph G with order 44. Suppose that G is Type A; as before, let $u \to u_1$ be an arc of the 4-cycle of vertices with order 4. We can assume that the automorphism o^4 permutes the other out-neighbours $\{u_2, u_3, u_4, u_5, u_6\}$ either as i) $(u_2u_3u_4u_5u_6)$ or ii) $(u_2u_3u_4)(u_5u_6)$. In case i) every vertex of G has order $4, 5, 10$ or 20; by Lemma 4.51 $m_5 = 0$. If $m_{20} > 0$, then by Lemma 4.51 we have $m_4 = 1, m_{10} = 0, m_{20} = 2$. By Lemma 4.46, this yields $a_1 + a_2 = 3$ and $a_1 - a_2 = 25$, which would imply that a_2 is negative. Therefore $m_4 = 1, m_{10} = 4, m_{20} = 0$, giving $a_1 + a_2 = 5, a_1 - a_2 = 29$, which again is impossible.

In case ii) every vertex order is $4, 6, 8, 12$ or 24. We have $40 = 6m_6 + 8m_8 + 12m_{12} + 24m_{24}$. As none of $6, 12$ or 24 are divisors of 40, Lemma 4.51 shows that $m_8 = 5, m_6 = m_{12} = m_{24} = 0$, so that $m''(1) = 6$ is even, violating Lemma 4.50.

Now suppose that G is Type B. Let u be a vertex in the unique transposition of o.

We can assume that o^2 permutes the vertices of $N^+(u)$ in one of four ways: i) $(u_1u_2u_3u_4)(u_5u_6)$, ii) $(u_1u_2u_3u_4u_5u_6)$, iii) $(u_1u_2u_3)(u_4u_5u_6)$ or iv) $(u_1u_2)(u_3u_4)(u_5u_6)$. For Case i), every vertex has order 2, 4 or 8, but neither 4 nor 8 divide 42, contradicting Lemma 4.51.

In Cases ii), iii) and iv) each vertex order is $2, 3, 4, 6$ or 12, with $42 = 3m_3 + 4m_4 + 6m_6 + 12m_{12}$. By Lemma 4.51 we know that $m_3 = 0$ and just one of m_4, m_6 and m_{12} is non-zero. As 4 and 12 do not divide 42, we must have $m_4 = m_{12} = 0$ and $m_6 = 7$, so that $m''(1) = 8$ is even, a contradiction. □

Theorem 4.55. *There are no* $(7, 2; 1)$*-digraphs.*

Proof. Assume that G is a $(7, 2; +1)$-digraph. G has order 58. Suppose that G is Type A and $u \to u_1$ is an arc of the 4-cycle of vertices with order 4. Then we can assume that o^4 permutes $\{u_2, u_3, u_4, u_5, u_6, u_7\} = N^+(u) - \{u_1\}$ in one of the following ways: i) $(u_2u_3u_4u_5)(u_6u_7)$, ii) $(u_2u_3)(u_4u_5)(u_6u_7)$, iii) $(u_2u_3u_4u_5u_6u_7)$ or iv) $(u_2u_3u_4)(u_5u_6u_7)$.

In Cases i) and ii) every vertex order is $4, 8$ or 16 and $54 = 8m_8 + 16m_{16}$. However neither 8 nor 16 divides 54, violating Lemma 4.51. We can thus assume that either case iii) or iv) holds and every vertex order is $4, 6, 8, 12$ or 24, with $54 = 6m_6 + 8m_8 + 12m_{12} + 24m_{24}$. Lemma 4.51 shows that $m_8 = m_{12} = m_{24} = 0$ and $m_6 = 9$. Then $m''(1) = 10$ is even, contradicting Lemma 4.50.

Therefore assume that G is Type B and let u be a vertex with order 2. o^2 permutes the elements of $N^+(u) = \{u_1, u_2, u_3, u_4, u_5, u_6, u_7\}$ in one of the following ways: i) $(u_1u_2u_3u_4u_5u_6u_7)$, ii) $(u_1u_2u_3u_4u_5)(u_6u_7)$, iii) $(u_1u_2u_3u_4)(u_5u_6u_7)$ or iv) $(u_1u_2u_3)(u_4u_5)(u_6u_7)$.

In Case i) all vertex orders are $2, 7$ or 14, so by Lemma 4.51, $m_2 = 1, m_7 = 0, m_{14} = 4$. Then $m''(1) = 5$ and $m(4) = 0$, so that $a_1 + a_2 = 5$ and $a_1 - a_2 = 43$, which has no suitable solutions.

In Case ii) all vertex orders are $2, 4, 5, 10$ or 20, $m_5 = 0$ and $56 = 4m_4 + 10m_{10} + 20m_{20}$. 10 and 20 do not divide 56, so $m_2 = 1, m_4 = 14$. In Cases iii) and iv) all vertex orders are $2, 3, 4, 6, 8, 12$ or 24 and $56 = 3m_3 + 4m_4 + 6m_6 + 8m_8 + 12m_{12} + 24m_{24}$. Lemma 4.51 shows that the only valid solutions are $m_2 = 1$ and $m_8 = 7$ and again $m_2 = 1, m_4 = 14$. In the former case $m''(1)$ is even, so we have shown that we can assume that $m_2 = 1$ and $m_4 = 14$. Thus $m''(1) = 15$ and $m(4) = 14$, giving $a_1 + a_2 = 15$, $a_1 - a_2 = 43 - 28 = 15$, giving

$a_1 = 15$ and $a_2 = 0$. It follows from Lemma 4.46 that the spectrum of G is, counted by multiplicity,

$$\{7, 0^{(15)}, \left[\frac{-1+\sqrt{7}i}{2}\right]^{(7)}, \left[\frac{-1-\sqrt{7}i}{2}\right]^{(7)}, i^{(14)}, -i^{(14)}\}.$$

Adding up the third powers of these eigenvalues, we see that the trace of A^3 is $\mathrm{Tr}(A^3) = 378$. A vertex lies in 7 directed triangles if it is Type I and 6 if it is Type II; therefore if there are α Type I vertices in G and β Type II vertices, then Theorem 1.3 shows that

$$7\alpha + 6\beta = 378, \alpha + \beta = 58.$$

Solving these equations gives $\alpha = 30, \beta = 28$. As a vertex has the same type as its outlier, it follows that the subdigraph B induced by the Type II vertices consists of 7 directed 4-cycles and there is a set A of 28 vertices v such that $d(v, o^-(v)) = 2$, the other two Type I vertices being u and $o(u)$.

B has size 28 and $(B, V(G) - B) = (V(G) - B, B) = 168$. This means that the subdigraph induced by $A' = A \cup \{u, o(u)\}$ has size 42. Fix a vertex $v \in A'$. The outlier $o(v)$ of v also lies in A', so v can reach every vertex of B by ≤ 2-paths. The vertex v has 7 out-going arcs. Suppose that the out-degree of v in the subdigraph induced by A' is ≤ 2. Each arc from v to B allows v to reach 2 vertices of B; therefore the largest possible number of vertices of B that v could reach by ≤ 2-paths would be achieved if v has two out-neighbours in A', each of which has out-neighbourhood contained in B ; however, this would still only allow v to reach 24 of the 28 vertices of B. It follows that the minimum out-degree in A' is ≥ 3, which implies that the size of the subdigraph induced by A' is ≥ 90, a contradiction. □

This completes the remaining cases in the classification of $(d, 2; +1)$-digraphs from Lemma 4.1 (see [116]). Combined with the results in Lemma 4.1, we see that to find a digraph with excess one, we must look at digraphs that have degree at least three and are at least 5-geodetic.

Theorem 4.56. *If $d, k \geq 2$ and $\epsilon(d, k) = 1$, then $d \geq 3$ and $k \geq 5$.*

Chapter 5

Diregularity of digraphs with small excess

5.1 Background

There are various methods for constructing digraphs with small excess, including voltage graph constructions and searches in the class of Cayley graphs; we will make use of the latter method in Section 9.5. Such constructions naturally yield diregular digraphs. As their structure is much weaker than diregular digraphs, it is much more difficult to construct digraphs with small excess that are not diregular and for the same reason nice counting arguments that work for diregular digraphs break down in the general setting.

Experience with searching for geodetic cages suggests that it is harder for a non-diregular k-geodetic digraph to have order close to the Moore bound. This motivates the following conjecture.

Conjecture 5.1. *All (d, k)-geodetic-cages are diregular (i.e. the geodetic cages coincide with the balanced cages).*

In Section 9.5 we determine the geodetic cages for three pairs of (d, k); we will see that in these small cases Conjecture 5.1 holds. This conjecture appears to be quite deep.

In fact, our intuition is somewhat misleading, for if Conjecture 5.1 holds then it is only barely true. In [137] and [138] it is shown that from a diregular digraph of order n, maximum out-degree d and diameter k that contains a pair of vertices with identical out-neighbourhoods there can be derived a non-diregular digraph of order $n-1$, maximum out-degree d and diameter $\leq k$ by means of a 'vertex deletion scheme'. By these means large non-diregular digraphs are constructed from Kautz digraphs in [137]. We now describe a 'vertex-splitting' construction that enables us to derive a non-diregular $(d, k; +(\epsilon+1))$-digraph from a $(d, k; +\epsilon)$-digraph.

Theorem 5.2 (Vertex-splitting construction)**.** *If there exists a $(d, k; +\epsilon)$-digraph, then for any $0 \leq r \leq d$ there also exists a non-diregular $(d, k; +(\epsilon+1))$-digraph with*

minimum in-degree $\leq d - r$.

Proof. Let G be a $(d, k; +\epsilon)$-digraph and choose a vertex u with in-degree $\geq d$. Form a new digraph G' by adding a new vertex w to G, setting $N^+(w) = N^+(u)$ and redirecting $d - r$ arcs that are incident to u to be incident to w. Colloquially, the vertex u is split into two vertices. G' is easily seen to also be k-geodetic with minimum out-degree $\geq d$. □

It follows from Theorem 5.2 that the order of a smallest possible non-diregular k-geodetic digraph with minimum out-degree d exceeds $N(d, k)$ by at most one. This suggests the following strengthened form of Conjecture 5.1.

Conjecture 5.3. *All smallest possible non-diregular k-geodetic digraphs with minimum out-degree d can be derived from a diregular (d, k)-geodetic cage by the vertex-splitting construction.*

We already know from Lemma 4.1 that all digraphs with excess one are diregular. In this chapter we will use counting arguments to rule out the existence of k-geodetic digraphs with out-degree two and excess two that are not diregular. This will pave the way for our complete classification of such digraphs in Chapter 6. This result is the analogue for the directed degree/geodecity problem of the result of [137] that there are no non-diregular digraphs with out-degree two and defect two. Finally in Section 5.4 we give some indications of the structure of non-diregular $(2, k; +3)$-digraphs.

To aid us in our discussion we define the sets S and S' of a non-diregular $(d, k; +\epsilon)$-digraph as follows.

Definition 5.4.

$$S = \{u \in V(G) : d^-(u) < d\}, S' = \{v \in V(G) : d^+(v) > d\}.$$

Therefore S is the set of vertices with 'too small' in-degree and S' is the set of vertices with 'too large' in-degree. In the following for convenience we will also refer to outlier sets as Ω-sets.

5.2 Basic structural results

We begin our investigation of non-diregular digraphs with small excess with two fundamental lemmas that connect the sets S and S' to outlier sets and

out-neighbourhoods. We will assume in these lemmas that the digraphs are out-regular. By Lemma 3.10 this assumption will be true if the excess satisfies $\epsilon < M(d, k-1)$; this inequality will hold in all cases of interest in this chapter.

Lemma 5.5. *For every vertex u of an out-regular, but non-diregular $(d, k; +\epsilon)$-digraph G we have*

$$S \subseteq \bigcap_{u \in V(G)} O(N^+(u)).$$

Proof. Let $v \in S$ and $u \in V(G)$. Write $N^+(u) = \{u_1, u_2, \ldots, u_d\}$ and suppose that $v \notin O(u_i)$ for $1 \leq i \leq d$. Let $v \notin N^+(u)$. Then for $1 \leq i \leq d$ there is a $\leq k$-path from u_i to v and so for $1 \leq i \leq d$ there is a $\leq (k-1)$-path from u_i to $N^-(v)$. As $d^-(v) \leq d-1$ it follows by the Pigeonhole Principle that there exists an in-neighbour v^* of v with two $\leq k$-paths from u to v^*, contradicting k-geodecity. Only trivial changes are necessary to deal with the case $v \in N^+(u)$. □

The second lemma is a generalisation of Lemma 2.2 of [132].

Lemma 5.6. *For every vertex u of an out-regular, but non-diregular $(d, k; +\epsilon)$-digraph G the set S' satisfies*

$$S' \subseteq \bigcap_{u \in V(G)} N^+(O(u)).$$

Proof. Let $v' \in S'$ and $u \in V(G)$. Suppose for a contradiction that $v' \notin N^+(O(u))$. Then every in-neighbour of v' is reachable by a $\leq k$-path from u. If $u \notin N^-(v')$, then by the Pigeonhole Principle there must exist an out-neighbour u^* of u with two $\leq (k-1)$-paths to $N^-(v')$, so that there are two $\leq k$-paths from u^* to v', a contradiction. The result follows similarly if $u \in N^-(v')$. □

As every vertex of an out-regular $(d, k; +\epsilon)$-digraph has exactly ϵ outliers, this provides us with a bound on the size of the sets S and S'. This generalises Lemma 2.3 of [132].

Corollary 5.7. *The size of the sets S and S' are bounded above by*

$$|S|, |S'| \leq \epsilon d.$$

There are also natural restrictions on the in-degrees of vertices in S and S'.

Lemma 5.8. *For every vertex $v' \in S'$ we have $d+1 \leq d^-(v') \leq d+\epsilon$.*

Proof. Let $v' \in S'$ and consider the Moore tree of depth k rooted at v'. Write $N^+(v') = \{v'_1, v'_2, \ldots, v'_d\}$. Every in-neighbour of v' lies in $(\bigcup_{i=1}^d T(v'_i)) \bigcup O(v')$. By k-geodecity, at most one in-neighbour of v' lies in any set $T(v'_i)$. As there are d such sets and ϵ vertices in $O(v')$, the result follows. □

Lemma 5.9. $\sum_{v \in S}(d - d^-(v)) = \sum_{v' \in S'}(d^-(v') - d)$.

Proof. By Lemma 3.10, the average in-degree must be d. □

Lemma 5.10. *If there is a $v' \in S'$ with $d^-(v') = d+\epsilon$, then every Ω-set is contained in $N^-(v')$.*

Proof. Let $u \in V(G)$ with $N^+(u) = \{u_1, u_2, \ldots, u_d\}$. Suppose that $u \notin N^-(v')$. In each of the d sets $T(u_i)$ there lies at most one in-neighbour of v'. It follows that every outlier of u must be an in-neighbour of v'. The case $u \in N^-(v')$ is similar. □

5.3 Digraphs with out-degree two and excess two

In this section we will assume that G is a k-geodetic digraph with minimum out-degree $d = 2$ and excess $\epsilon = 2$, where $k \geq 2$. We will occasionally have to consider the case $k = 2$ separately. We now state the main result of this chapter.

Theorem 5.11 (Main Theorem)**.** *There are no non-diregular $(2, k; +2)$-digraphs for $k \geq 2$.*

We will proceed to derive a list of possible in-degree sequences for G. Analysing each in turn, we will obtain a contradiction in each case, thereby proving the main theorem. Before embarking upon this program, we mention a final important lemma that connects the case of excess two with previous work on digraphs with excess one. This result generalises the proof strategy of Theorem 2 of [116] and can be viewed as the 'reverse operation' to the vertex-splitting construction in Theorem 5.2.

Lemma 5.12 (Amalgamation Lemma)**.** *Suppose that G contains vertices u_1, u_2 such that for all vertices $u \in V(G)$ we have $O(u) \cap \{u_1, u_2\} \neq \emptyset$. Then $N^+(u_1) \neq N^+(u_2)$.*

Proof. Suppose that $N^+(u_1) = N^+(u_2)$. Denote the graph resulting from the amalgamation of vertices u_1, u_2 by G^*. Inspection shows that if G^* is not k-geodetic,

then neither is G. G^* is therefore a $(2, k; +1)$-digraph, contradicting Lemma 4.1. □

5.3.1 There are no vertices in G with in-degree four

By Lemma 5.8, all vertices in S' have in-degree three or four. In this section we shall prove that all vertices in S' must have in-degree three. If G contained a vertex with in-degree zero, deleting this vertex would yield a digraph with out-degree two and excess one, which is impossible by Lemma 4.1; hence every vertex in S has in-degree one, so that by Lemma 5.9 we have $|S| = \sum_{v' \in S'}(d^-(v') - 2)$. By Corollary 5.7 we have $|S| \leq 4$, so it follows that if G contains a vertex of in-degree four, then the possible in-degree sequences of G are $(1, 1, 2, \ldots, 2, 4)$, $(1, 1, 1, 1, 2, \ldots, 2, 4, 4)$, $(1, 1, 1, 2, \ldots, 2, 3, 4)$ and $(1, 1, 1, 1, 2, \ldots, 2, 3, 3, 4)$. We can narrow down the possibilities further as follows.

Lemma 5.13. *If G contains a vertex v' with in-degree four, then $|S| = 4$.*

Proof. Suppose that $|S| \leq 3$ and let $d^-(v') = 4$. By k-geodecity, every vertex has at most one $\leq k$-path to v'. The smallest possible number of initial vertices of $\leq k$-paths to v' is achieved if $S \subset N^-(v')$ and $d(v'', v') \geq k$ for $v'' \in S' - \{v'\}$, so that

$$M(2, k) + 2 \geq |T_{-k}(v')| \geq 4 + 3M(2, k-2) + M(2, k-1) = 2 + M(2, k) + M(2, k-2),$$

which is impossible for $k \geq 2$. □

The only possible in-degree sequences for G are thus $(1, 1, 1, 1, 2, \ldots, 2, 4, 4)$ and $(1, 1, 1, 1, 2, \ldots, 2, 3, 3, 4)$. We need one final piece of structural information and then we can proceed to analyse the possible in-degree sequences.

Corollary 5.14. *If $|S| = 4$ and there is a vertex $v' \in S'$ with in-degree four, then $S = N^-(v')$ and all Ω-sets are contained in S. If $\Omega \subset S$ is an outlier set, then so is $S - \Omega$.*

Proof. Putting $\epsilon = 2$ in Lemma 5.10, we see that $O(u) \subseteq N^-(v')$ for all $u \in V(G)$. Hence for any vertex u we have by Lemma 5.5

$$S \subseteq O(N^+(u)) \subseteq N^-(v').$$

As $|S| = |N^-(v')| = 4$, we must have equality in the above inclusion, i.e. $S = N^-(v')$.

Let $O(u) = \Omega$. Write $u^- \in N^-(u)$ and $N^+(u^-) = \{u, u^+\}$. By Lemma 5.5 we have

$$\Omega \cup O(u^+) = O(u) \cup O(u^+) = O(N^+(u^-)) = S,$$

so we must have $O(u^+) = S - \Omega$. □

We are now in a position to show that neither of the remaining in-degree sequences can arise.

Theorem 5.15. *There are no* $(2, k; +2)$*-digraphs with in-degree sequence* $(1, 1, 1, 1, 2, \ldots, 2, 4, 4)$ *for* $k \geq 2$.

Proof. Let v_1', v_2' be the vertices with in-degree four. By Corollary 5.14, $S = N^-(v_1') = N^-(v_2')$ and v_1' is not an outlier, so it follows that $v_2' \in T^-(v)$ for some $v \in S$. But as $N^-(v_2') = S$, it follows that there is a $\leq k$-cycle through v, contradicting k-geodecity. □

Theorem 5.16. *There are no* $(2, k; +2)$*-digraphs with in-degree sequence* $(1, 1, 1, 1, 2, \ldots, 2, 3, 3, 4)$ *for* $k \geq 2$.

Proof. Let v' be the vertex with in-degree four and let w_1, w_2 be the vertices with in-degree three. Write $S = \{v_1, v_2, v_3, v_4\}$. By Corollary 5.14, $N^-(v') = S$ and no vertex outside S is an outlier. Without loss of generality, suppose that $O(v') = \{v_1, v_2\}$. By Corollary 5.14, $\{v_3, v_4\}$ is also an Ω-set. By Lemma 5.6 we can thus assume that

$$v_1, v_3 \in N^-(w_1), v_2, v_4 \in N^-(w_2).$$

Again by Lemma 5.6, $\{v_1, v_3\}$ and $\{v_2, v_4\}$ cannot be Ω-sets. The only other possible Ω-sets are $\{v_1, v_4\}$ and $\{v_2, v_3\}$. We see then that $\Omega \cap \{v_1, v_3\} \neq \emptyset$ for all Ω-sets and $N^+(v_1) = N^+(v_3)$, contradicting the Amalgamation Lemma. □

It follows that no vertex of G has in-degree ≥ 4. By Lemma 5.9 and Corollary 5.7, we must therefore have $|S| = |S'|$ and $|S| \leq 4$, which leaves us with only four in-degree sequences to analyse, namely $(1, 2, \ldots, 2, 3), (1, 1, 2, \ldots, 2, 3, 3), (1, 1, 1, 2, \ldots, 2, 3, 3, 3)$ and $(1, 1, 1, 1, 2, \ldots, 2, 3, 3, 3, 3)$. For $|S| = r$, we will write $S = \{v_1, \ldots, v_r\}, S' = \{v_1', \ldots, v_r'\}$.

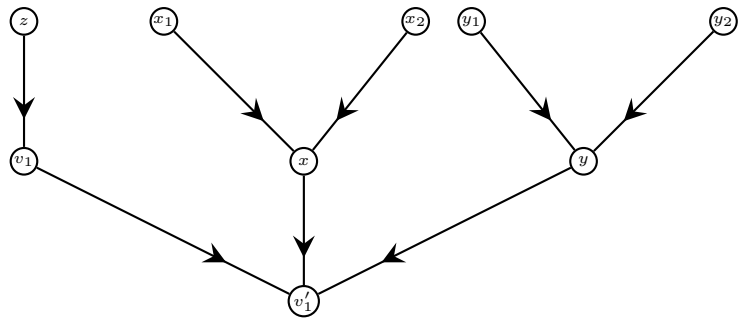

Figure 5.1: Subdigraph of any $(2,2;+2)$-digraph with in-degree sequence $(1,2,\ldots,2,3)$

5.3.2 Degree sequence $(1,2,\ldots,2,3)$

Theorem 5.17. *There are no $(2,k;+2)$-digraphs with in-degree sequence $(1,2,\ldots,2,3)$ for $k \geq 3$.*

Proof. We obtain a lower bound for $|T_{-k}(v_1')|$ by assuming that $v_1 \in N^-(v_1')$. By k-geodecity, all vertices in $T_{-k}(v_1')$ are distinct, so

$$M(2,k)+2 \geq |T_{-k}(v_1')| \geq 2+M(2,k-2)+2M(2,k-1) = 1+M(2,k)+M(2,k-2).$$

This inequality is not satisfied for $k \geq 3$. □

This leaves open the question of whether there exists a non-diregular $(2,2;+2)$-digraph with the given in-degree sequence. By the argument of the preceding theorem, such a digraph must contain the subdigraph shown in Figure 5.1, which also displays the vertex-labelling that we shall employ. We proceed to show that no such digraph exists.

Evidently v_1' is not an outlier. Note that all arcs added to the subdigraph in Figure 5.1 must terminate in the set $\{z, x_1, x_2, y_1, y_2\}$. G is out-regular with degree $d = 2$, so we can assume without loss of generality that $z \to x_1$. By 2-geodecity, $x_1 \not\to z$ and $x_1 \not\to x_2$, so we can assume that $x_1 \to y_1$. Similarly, we must either have $y_1 \to z$ or $y_1 \to x_2$.

Lemma 5.18. *The out-neighbourhood of y_1 is $N^+(y_1) = \{y, x_2\}$.*

Proof. Assume for a contradiction that $y_1 \to z$. $x \not\to x_1$ or x_2 by 2-geodecity. Also, $x \not\to z$, or we would have two paths $x_1 \to y_1 \to z$ and $x_1 \to x \to z$. Similarly, $x \not\to y_1$, or there would be paths $x_1 \to y_1$ and $x_1 \to x \to y_1$. Therefore $x \to y_2$. We now

analyse the possible out-neighbours of y. $y \not\to y_1, y_2$ and if $y \to x_1$, then there would be paths $y_1 \to z \to x_1$ and $y_1 \to y \to x_1$. Likewise $y \not\to z$, so $y \to x_2$. We now see that $v_1' \not\to x_2$ or y_2; for example, if $v_1' \to y_2$, then there would be paths $x \to y_2$ and $x \to v_1' \to y_2$. Since v_1' cannot be adjacent to two vertices linked by an arc, we see that v_1' cannot have two out-neighbours in $N^{-2}(v_1')$ without violating 2-geodecity. Hence we are forced to conclude that $y_1 \to x_2$. □

Theorem 5.19. *There are no* $(2, 2; +2)$*-digraphs with in-degree sequence* $(1, 2, \ldots, 2, 3)$.

Proof. By Lemma 5.18, we have $y_1 \to x_2$. There are five possibilities for $N^+(v_1')$, namely $\{z, x_2\}, \{z, y_1\}$, $\{z, y_2\}, \{x_1, y_2\}$ and $\{x_2, y_2\}$; we discuss each case in turn.

Case i): $N^+(v_1') = \{z, x_2\}$

If $v_1 \to y_1$, then we have paths $z \to x_1 \to y_1$ and $z \to v_1 \to y_1$, so $v_1 \not\to y_1$. Likewise, v_1 is not adjacent to z, x_1 or x_2. Thus $v_1 \to y_2$. Similarly, $x_2 \to y_2$. We must now have $x \to y_1$. However, this gives us paths $x_1 \to y_1$ and $x_1 \to x \to y_1$, which is impossible.

Case ii) $N^+(v_1') = \{z, y_1\}$

By 2-geodecity, $y \to x_1$; however, this yields paths $y \to v_1' \to y_1$ and $y \to x_1 \to y_1$.

Case iii): $N^+(v_1') = \{z, y_2\}$

As there are paths $x \to v_1' \to z$, $x \to v_1' \to y_2$ we cannot have $x \to z$ or $x \to y_2$. Obviously $x \not\to x_1, x_2$, so $x \to y_1$. Now there are paths $x_1 \to y_1$ and $x_1 \to x \to y_1$, a contradiction.

Case iv): $N^+(v_1') = \{x_1, y_2\}$

By 2-geodecity, we have successively $v_1 \to x_2$, $x \to z$ and $y \to z$. But now as each of z, x_1 and x_2 already has in-degree two, we are led to conclude that $y_2 \to y_1$, violating 2-geodecity.

Case v): $N^+(v_1') = \{x_2, y_2\}$

By 2-geodecity, v_1 cannot be adjacent to any of z, x_1, x_2, y_1 or y_2.

Having exhausted all possibilities, our proof is complete. □

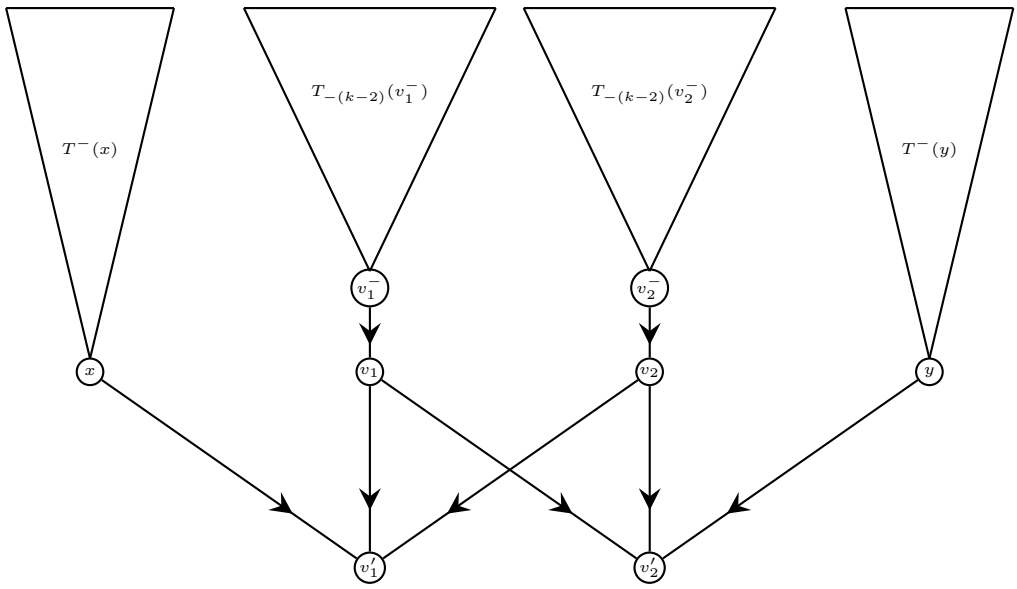

Figure 5.2: Configuration for in-degree sequence $(1, 1, 2, \ldots, 2, 3, 3)$

5.3.3 Degree sequence $(1, 1, 2, \ldots, 2, 3, 3)$

We shall assume firstly that $k \geq 3$ and deal with the special case of $k = 2$ separately.

Lemma 5.20. *If $k \geq 3$, then for each $v' \in S'$ we have $S \subset N^-(v')$.*

Proof. Let $v' \in S'$ and consider $T_{-k}(v')$. Suppose that neither v_1 nor v_2 lies in $N^-(v')$. Then for $k \geq 2$, by k-geodecity

$$M(2, k) + 2 \geq 4 + 2M(2, k-3) + 2M(2, k-1) = 2 + M(2, k) + M(2, k-2),$$

a contradiction. Now suppose that $|S \cap N^-(v')| = 1$. We would then have

$$M(2, k) + 2 \geq 3 + 2M(2, k-1) + M(2, k-3) = 2 + M(2, k) + M(2, k-3),$$

which again is impossible for $k \geq 3$. □

Hence we can set $N^-(v_1') = \{v_1, v_2, x\}, N^-(v_2') = \{v_1, v_2, y\}$. This situation is displayed in Figure 5.2, where $N^-(v_i) = \{v_i^-\}$ for $i = 1, 2$. As the in-neighbourhoods of v_1' and v_2' have at least v_1 and v_2 in common, we immediately obtain the following corollary on the positions of v_1' and v_2'.

Corollary 5.21. *$d(v_1', v_2') \geq k$ and $d(v_2', v_1') \geq k$. If $d(v_1', v_2') = k$, then $v_1' \in N^{-(k-1)}(y)$, and similarly if $d(v_2', v_1') = k$, then $v_2' \in N^{-(k-1)}(x)$.*

Corollary 5.22. $|O^-(v_1)| = |O^-(v_2)| = 2^k + 1$.

Proof. By k-geodecity, $v_2, v_1', v_2' \notin T^-(v_1)$, so $|T_{-k}(v_1)| = 1 + M(2, k-1)$, yielding $|O^-(v_1)| = M(2,k) + 2 - (1 + M(2, k-1)) = 2^k + 1$. Similarly for v_2. □

Corollary 5.23. *If $d(v_1', v_2') = k$, then $|O^-(y)| = 1$ and if $v_2' \in O(v_1')$, then $|O^-(y)| = 2$. Similarly, $|O^-(x)| = 1$ if $d(v_2', v_1') = k$ and $|O^-(x)| = 2$ if $v_1' \in O(v_2')$.*

Proof. Similar to the proof of Corollary 5.22. □

Lemma 5.24. $|O^-(v_1')| = |O^-(v_2')| = 1$.

Proof. Consider $|T_{-k}(v')|$, where $v' \in S'$. Counting distinct vertices of G,

$$M(2,k) + 2 = 3 + 2M(2, k-2) + M(2, k-1) + |O^-(v')| = 1 + M(2,k) + |O^-(v')|.$$

Rearranging, we obtain $|O^-(v')| = 1$. □

Lemma 5.25. *The vertices x and y are distinct.*

Proof. Suppose that $x = y$. Then $N^-(v_1') = N^-(v_2')$, so that we must have $v_1' \in O(v_2'), v_2' \in O(v_1')$ and hence by Corollary 5.23 $|O^-(x)| = 2$. As $N^+(v_1) = N^+(v_2) = N^+(x)$, by k-geodecity we have $O(v_1) = \{v_2, x\}, O(v_2) = \{v_1, x\}, O(x) = \{v_1, v_2\}$, so $O^-(x) = \{v_1, v_2\}$. By Lemma 5.6, every Ω-set must intersect $\{v_1, v_2, x\}$, so it follows that every Ω-set contains an element of $\{v_1, v_2\}$, contradicting the Amalgamation Lemma. □

Lemma 5.26. *Let Ω be an outlier set. Then either $\Omega \cap S \neq \emptyset$ or $\Omega = \{x, y\}$. $\{x, y\}$ is an Ω-set.*

Proof. By Lemma 5.6 and the Amalgamation Lemma. □

Let α denote the number of vertices of G with outlier set $\{v_1, v_2\}$ and β the number of vertices with outlier set $\{x, y\}$.

Lemma 5.27. $\alpha = \beta + 1$.

Proof. By Corollary 5.22, v_1 and v_2 appear in $2(2^k + 1) - \alpha = 2^{k+1} + (2 - \alpha)$ Ω-sets. By Lemma 5.26, any Ω-set that does not contain either v_1 or v_2 must equal $\{x, y\}$. It follows that

$$M(2,k) + 2 = 2^{k+1} + 1 = 2^{k+1} + 2 - \alpha + \beta,$$

implying the result. □

Corollary 5.28. *$v_2 \in O(v_1)$, $v_1 \in O(v_2)$ and $d(v_1', v_2') = d(v_2', v_1') = k$.*

Proof. Suppose that $d(v_1, v_2) \leq k$. Then we must have

$$S' \cap T^-(v_2) = N^+(v_1) \cap T^-(v_2) \neq \emptyset,$$

contradicting k-geodecity. Thus $v_2 \in O(v_1)$ and similarly $v_1 \in O(v_2)$.

Suppose that $v_2' \in O(v_1')$. Then v_1 and v_2 have no out-neighbours in $T^-(y)$, so

$$O(v_1) = \{v_2, y\}, O(v_2) = \{v_1, y\}.$$

By Corollary 5.23, $|O^-(y)| = 2$, so $\{x, y\}$ is not an Ω-set, contradicting Lemma 5.26. $v_1' \in O(v_2')$ is impossible for the same reason. □

Theorem 5.29. *There are no $(2, k; +2)$-digraphs with in-degree sequence $(1, 1, 2, \ldots, 2, 3, 3)$ for $k \geq 3$.*

Proof. It follows from Corollaries 5.23 and 5.28 and Lemma 5.26 that there is a unique vertex z such that $O(z) = \{x, y\}$. Furthermore, no other Ω-set contains x or y. Hence, by Lemma 5.27, $\alpha = 2, \beta = 1$. Denote the two vertices with Ω-set $\{v_1, v_2\}$ by w, w'. Write $N^+(w) = \{w_1, w_2\}, N^+(w') = \{w_1', w_2'\}$.

It is easily seen that $\{w, w'\} \cap \{x, y\} = \emptyset$. Suppose that $w = x$ and set $w_2 = v_1'$. By Corollary 5.28, we must have $y \in N^{k-1}(v_1')$, so by k-geodecity $x, y, v_1, v_2 \notin T(w_1)$, so $O(w_1) = \{v_1', v_2'\}$, contradicting Lemma 5.26. The other cases are identical.

As $O(w) = \{v_1, v_2\}$, $x, y \in T(w_1) \cup T(w_2)$. Suppose that x and y lie in the same branch, e.g. $x, y \in T(w_1)$. By k-geodecity and the definition of w, $\{x, y, v_1, v_2\} \cap (\{w\} \cup T(w_2)) = \emptyset$, so that $O(w_2) = \{v_1', v_2'\}$, which is impossible by Lemma 5.26. Hence we can assume $x \in T(w_1), y \in T(w_2)$. Then $N^-(v_2') \cap T(w_1) = N^-(v_1') \cap T(w_2) = \emptyset$, so $v_2' \in O(w_1), v_1' \in O(w_2)$. Applying the same analysis to w', we see that we can assume $v_2' \in O(w_1'), v_1' \in O(w_2')$. By Lemma 5.24, it follows that $w_1 = w_1'$ and $w_2 = w_2'$, so that $N^+(w) = N^+(w')$. As $O(w) = \{v_1, v_2\}$, we must have $w' \in T_k(w)$. Hence there is a $\leq k$-cycle through either w_1 or w_2. □

Now we turn to the case $k = 2$. The argument of Lemma 5.20 shows that each member of S' has an in-neighbour in S. This allows us to deduce the following lemma.

Lemma 5.30. *Neither element of S' is adjacent to the other.*

Proof. Suppose that $v_2' \to v_1'$. If $|N^-(v_1') \cap S| = 1$, then the order of G would be at least 10, whereas $|V(G)| = M(2,2) + 2 = 9$. Hence $|N^-(v_1') \cap S| = 2$ and since v_2' also has an in-neighbour in S, there would be an element of S with two ≤ 2-paths to v_1'. □

Theorem 5.31. *There are no $(2,2;+2)$-digraphs with in-degree sequence $(1,1,2,\ldots,2,3,3)$.*

Proof. If $S \subset N^-(v_1') \cap N^-(v_2')$, then the argument for $k \geq 3$ remains valid, so we can assume that $N^-(v_1') = \{v_1, x, y\}$, where $\{x, y\} \cap (S \cup S') = \emptyset$. Simple counting shows that $O^-(v_1') = \emptyset$. We will write $N^-(x) = \{x_1, x_2\}, N^-(y) = \{y_1, y_2\}, N^-(v_1) = \{z\}$. Without loss of generality, there are four possibilities: i) $v_2 = z, v_2' = x_1$, ii) $v_2 = x_1, v_2' = z$, iii) $v_2 = y_1, v_2' = x_1$ and iv) $v_2 = x_1, v_2' = x_2$.

Case i) $v_2 = z, v_2' = x_1$:

v_2' has three in-neighbours. By Lemma 5.30, $v_1' \notin N^-(v_2')$. By 2-geodecity, $N^-(v_2') \cap T^-(x) = \emptyset$. v_1 and $z = v_2$ cannot both be in-neighbours of v_2', so v_2' must have exactly two in-neighbours in $T^-(y)$; necessarily $y_1, y_2 \in N^-(v_2')$ but $y \notin N^-(v_2')$. If $v_2 \to v_2'$, then there is no vertex other than x that v_2' can be adjacent to without violating 2-geodecity, so we must have $v_1 \to v_2'$ and $v_2' \to v_2$. As we already have a 2-path $v_2 \to v_1 \to v_2'$, v_2 cannot be adjacent to v_2', y_1 or y_2, so $v_2 \to x_2$. As all in-neighbours of v_2 and v_2' are accounted for, we must have $y \to x_2$. But now the only possible out-neighbourhood of v_1' is $\{y_1, y_2\}$, which gives two 2-paths from v_1' to v_2'.

Case ii) $v_2 = x_1, v_2' = z$:

As $v_1 \not\to v_2'$, Lemma 5.20 shows that $v_2 \to v_2'$. Without loss of generality, $N^-(v_2')$ must be one of $\{v_2, x_2, y_1\}, \{v_2, x_2, y\}$ or $\{v_2, y_1, y_2\}$. Suppose that $N^-(v_2') = \{v_2, x_2, y_1\}$. Then $v_2' \to y_2$ and $N^+(v_1')$ is either $\{v_2, y_2\}$ or $\{x_2, y_2\}$. If $N^+(v_1') = \{v_2, y_2\}$, then we can deduce that $x \to y_1$, $y \to x_2$ and $y_2 \to x_2$, so that there are paths $y_2 \to x_2$ and $y_2 \to y \to x_2$, so assume that $N^+(v_1') = \{x_2, y_2\}$. As y can already reach x_2 by a 2-path, there is an arc $y \to v_2$. v_2 has a unique in-neighbour, so $y_2 \to x_2$ and hence there are paths $v_1' \to x_2$ and $v_1' \to y_2 \to x_2$.

If $N^-(v_2') = \{v_2, x_2, y\}$, then y_1 cannot be adjacent to any of v_2', v_2, x_2 or y_2 without violating 2-geodecity. Hence we can assume that $N^-(v_2') = \{v_2, y_1, y_2\}$. Now we must

have $v_2' \to x_2$. Without loss of generality, $x_2 \to y_1$ and $x \to y_2$. We cannot have $y \to x_2$, or there would be paths $y_1 \to y \to x_2$ and $y_1 \to v_2' \to x_2$, so $y \to v_2$. v_1' cannot be adjacent to both y_1 and y_2, so $v_1' \to x_2$ and hence also $v_1' \to y_2$. Now the only possible remaining arc is $v_1 \to y_1$, so that we have paths $v_2' \to v_1 \to y_1$ and $v_2' \to x_2 \to y_1$, which is impossible.

Case iii) $v_2 = y_1, v_2' = x_1$:

$N^-(v_2')$ must be either $\{z, v_2, y_2\}$ or $\{v_1, v_2, y_2\}$. In the first case, there are no vertices other than x that v_2' can be adjacent to without violating 2-geodecity, so $N^-(v_2') = \{v_1, v_2, y_2\}$. By 2-geodecity, $v_2' \to z$. If $y \to z$, then there would be distinct ≤ 2-paths from v_2 to z, so $y \to x_2$. v_1' is not adjacent to both v_2 and y_2 and is not adjacent to x_2, or there would be two ≤ 2-paths from y to x_2, so we see that $v_1' \to z$, implying that there are paths $v_1 \to v_2' \to z$ and $v_1 \to v_1' \to z$.

Case iv) $v_2 = x_1, v_2' = x_2$:

As $v_2 \not\to v_2'$, we have $v_1 \to v_2'$ and $N^-(v_2') = \{v_1, y_1, y_2\}$. Hence $v_2' \to z$. As y_1 can already reach z by a 2-path, $y \not\to z$, so $y \to v_2$. z must be adjacent to y_1 or y_2, but can already reach v_2' via v_1, yielding a contradiction.

Having dealt with every possibility, the result is proven. □

5.3.4 Degree sequence $(1, 1, 1, 2, \ldots, 2, 3, 3, 3)$

This represents the most difficult case to deal with. Again, we will discuss the cases $k = 2$ and $k \geq 3$ separately.

Lemma 5.32. *If $k \geq 2$, then for every $u \in V(G)$ we have $|O(u) \cap S| = 1$ or 2. There exists an Ω-set contained in S.*

Proof. Let $u \in V(G)$ be arbitrary. Let u^- be an in-neighbour of u and let u^+ be the other out-neighbour of u^-. By Lemma 5.5, if $S \cap O(u) = \emptyset$, then we would have $S \subseteq O(u^+)$. Since $|S| = 3$ and $|O(u^+)| = 2$, this is impossible. In fact, as $S \subseteq O(u) \cup O(u^+)$, at least one of $O(u)$ and $O(u^+)$ must be entirely contained in S. □

Lemma 5.33. *If $k \geq 2$, then for each $v' \in S'$, $S \cap N^-(v') \neq \emptyset$.*

Proof. Assume that v' is an element of S' such that $S \cap N^-(v') = \emptyset$. Then we obtain

a lower bound for $|T_{-k}(v')|$ by assuming that all members of S lie in $N^{-2}(v')$, whilst v' is at distance $\geq k$ from the remaining members of S'. Recalling that $M(2,k) = 0$ for $k < 0$, this yields

$$|T_{-k}(v')| \geq 6+3M(2,k-3)+M(2,k-2)+M(2,k-1) = 3+M(2,k)+M(2,k-3),$$

a contradiction. □

For $i = 1,2,3$, we will say that a vertex $v' \in S'$ is Type i if $|S \cap N^-(v')| = i$. As each member of S has out-degree two, it follows that if for $i = 1,2,3$ there are N_i vertices of Type i then $N_1 + 2N_2 + 3N_3 \leq 6$. We now determine the number of vertices of each type.

Lemma 5.34. *Let $k \geq 2$. Suppose that $v' \in S'$ is Type 1, with $N^-(v') \cap S = \{v\}$. Then for $v^* \in S - \{v\}$ we have $d(v^*, v') = 2$ and for $v'' \in S' - \{v'\}$ we have $d(v'', v') = k$. Also $O^-(v') = \emptyset$.*

Proof. The results for $k = 2$ follow by simple counting, so assume that $k \geq 3$. Let v', v be as described. Consider $T_{-k}(v')$. We obtain a lower bound for $|T_{-k}(v')|$ by assuming that $S - \{v\} \subset N^{-2}(v')$ and that $(S' - \{v'\}) \cap T^-(v') = \emptyset$. Hence

$$|V(G)| \geq |T_{-k}(v')| \geq 5+2M(2,k-3)+M(2,k-2)+M(2,k-1) = 2+M(2,k) = |V(G)|.$$

Clearly, if v' were any closer to the remaining members of S' or if v' were any further from the vertices in $S - \{v\}$, $|T_{-k}(v')|$ would have order greater than $2 + M(2,k)$, which is impossible by k-geodecity. Evidently all vertices of G lie in $T_{-k}(v')$, so $O^-(v') = \emptyset$. □

Our reasoning for the cases $k \geq 3$ and $k = 2$ must now part company, so we will now assume that $k \geq 3$ and return to the case $k = 2$ presently.

Lemma 5.35. *For $k \geq 3$, no two elements of S' are adjacent to one another.*

Proof. Suppose that there is an arc (v', v'') in G, where $v', v'' \in S'$. Consider $T_{-k}(v'')$. We obtain a lower bound for $|T_{-k}(v'')|$ by assuming that v'' is Type 2 and that v' is Type 1, whilst v'' lies at distance $\geq k$ from the remaining vertex in S'. Then by inspection

$$|T_{-k}(v'')| \geq 4+M(2,k-1)+2M(2,k-2)+M(2,k-3) = 2+M(2,k)+M(2,k-3),$$

which is impossible for $k \geq 3$. □

Lemma 5.36. *There are no Type 3 vertices.*

Proof. Suppose for a contradiction that $v_1' \in S'$ is a Type 3 vertex, i.e. $N^-(v_1') = S$. As $N_1 + 2N_2 + 3N_3 \leq 6$, S' must contain a Type 1 vertex. We can assume that v_2' is Type 1 and $N^+(v_1) = \{v_1', v_2'\}, N^+(v_2) = \{v_1', v_3'\}$. It follows by Lemma 5.34 that $v_2 \in N^{-2}(v_2')$. Therefore we must have $N^+(v_2) \cap N^-(v_2') = \{v_1', v_3'\} \cap N^-(v_2') \neq \emptyset$, which contradicts Lemma 5.35. □

Lemma 5.37. *There is a Type 2 vertex.*

Proof. Assume for a contradiction that each vertex in S' is Type 1. Suppose that the sets $S \cap N^-(v_i')$, $i = 1, 2, 3$ are not all distinct; say (v_1, v_1') and (v_1, v_2') are arcs in G. Since v_1 has out-degree two, we can assume that (v_2, v_3') is also an arc. By Lemma 5.34, we have $v_1 \in N^{-2}(v_3')$. As the out-neighbours of v_1 are v_1' and v_2', it follows that either (v_1', v_3') or (v_2', v_3') is an arc, contradicting Lemma 5.35.

Hence we can assume that $N^+(v_i) = \{v_i', v_i^+\}$ for $i = 1, 2, 3$ where $v_i^+ \notin S'$ for $i = 1, 2, 3$. By Lemma 5.32, there is an outlier set Ω contained in S. By Lemma 5.6, S' must be contained in $N^+(\Omega)$; by inspection this is impossible. □

Lemma 5.38. *There is a Type 1 vertex.*

Proof. Suppose that $N_2 = 3$. We can set $N^-(v_i') \cap S = S - \{v_i\}$ for $i = 1, 2, 3$. Then for $i \neq j$ we must have $d(v_i', v_j') \geq k$, as $N^-(v_i') \cap N^-(v_j') \neq \emptyset$. As $N^+(v_3) = \{v_1', v_2'\}$, it follows that $v_3' \in O(v_3)$. By Lemma 5.6, $S' \subseteq N^+(O(v_3))$. By Lemma 5.35, $N^+(v_3') \cap S' = \emptyset$, so, as G has out-degree $d = 2$, this is not possible. □

Lemma 5.39. *Let v' be a Type 2 vertex. Then $S \cap N^-(v')$ is not an Ω-set. Also, every vertex in G can reach exactly one member of $S \cap N^-(v')$ by a $\leq k$-path. If $v', v'' \in S'$ are both Type 2 vertices, then $S \cap N^-(v') \neq S \cap N^-(v'')$.*

Proof. For definiteness, suppose that v_1' is a Type 2 vertex, with $S \cap N^-(v_1') = \{v_1, v_2\}$. Suppose that $\{v_1, v_2\}$ is an Ω-set. By Lemma 5.6, $S' \subseteq N^+\{v_1, v_2\}$. We can thus suppose that there are arcs (v_1, v_2') and (v_2, v_3') in G. By Lemma 5.38 we can assume that v_2' is Type 1. By Lemma 5.34, $v_2 \in N^{-2}(v_2')$ so that $N^+(v_2) \cap N^-(v_2') = \{v_1', v_3'\} \cap N^-(v_2') \neq \emptyset$, contradicting Lemma 5.35. Therefore $\{v_1, v_2\}$ is not an Ω-set.

Let u be a vertex that can reach both v_1 and v_2 by a $\leq k$-path. Let $u^- \in N^-(u)$ and $N^+(u^-) = \{u, u^+\}$. By Lemma 5.5 we must then have $O(u^+) = \{v_1, v_2\}$, a contradiction. Suppose now that v_1' and v_2' are Type 2 vertices and $S \cap N^-(v_1') = S \cap N^-(v_2') = \{v_1, v_2\}$. Then $N^+(v_1) = N^+(v_2)$, which by the preceding argument contradicts the Amalgamation Lemma. □

Corollary 5.40. *There are two Type 1 vertices and a unique Type 2 vertex.*

Proof. Suppose that v_1' and v_2' are Type 2 vertices, so that v_3' is Type 1. By Lemma 5.39 we can assume that $S \cap N^-(v_1') = \{v_1, v_2\}, S \cap N^-(v_2') = \{v_1, v_3\}$ and $v_2 \in N^-(v_3')$. By Lemma 5.34, we then have $v_1, v_3 \in N^{-2}(v_3')$. It follows that v_1 has an out-neighbour in $N^-(v_3')$, contradicting Lemma 5.35. □

We can therefore assume for the remainder of this subsection that v_1' and v_2' are Type 1 and v_3' is Type 2. Write x for the in-neighbour of v_3' that does not lie in S.

Lemma 5.41. $S \cap N^-(v_1') = S \cap N^-(v_2')$.

Proof. Suppose that $S \cap N^-(v_1') \neq S \cap N^-(v_2')$. By Lemma 5.34, without loss of generality we can put

$$v_1 \in N^-(v_1'), v_2, v_3 \in N^{-2}(v_1'), v_2 \in N^-(v_2') \text{ and } v_1, v_3 \in N^{-2}(v_2').$$

We cannot have $N^+(v_1) \subset S'$, or $v_1 \in N^{-2}(v_2')$ would imply that two vertices of S' are adjacent. Thus $v_1 \notin N^-(v_3')$. Similar reasoning applies to v_2. However, there are two members of S in $N^-(v_3')$, a contradiction. □

We can now set without loss of generality $v_1 \in N^-(v_1') \cap N^-(v_2')$, $v_2, v_3 \in N^{-2}(v_1') \cap N^{-2}(v_2')$ and $S \cap N^-(v_3') = \{v_2, v_3\}$. It follows from Lemma 5.39 that for every vertex u we have $|O(u) \cap \{v_2, v_3\}| = 1$. We can assume that $v_3 \in O(v_1), v_2 \notin O(v_1)$. Write $N^+(v_2) = \{v_3', v_2^+\}$ and $N^+(v_3) = \{v_3', v_3^+\}$. By the Amalgamation Lemma $v_2^+ \neq v_3^+$.

Lemma 5.42. *v_3' is not an outlier.*

Proof. Suppose that for some outlier set we have $v_3' \in \Omega$. By Lemma 5.35, $N^+(v_3') \cap S' = \emptyset$, so that we cannot have $S' \subseteq N^+(\Omega)$, contradicting Lemma 5.6. □

As there is a $\leq k$-path from v_1 to v_2, either v_1' or v_2' lies in $T^-(v_2)$; assume that $v_1' \in T^-(v_2)$. Suppose that $d(v_1', v_2) \leq k-2$. There is a path of length 2 from v_2 to v_1', so there would be a $\leq k$-cycle through v_1', which is impossible. It follows that $d(v_1', v_2) = k-1$, so that $d(v_1', v_3') = k$.

As v_1 must lie in $T_{-k}(v_3')$, we must have $v_2' \in T^-(v_3')$. If $d(v_2', v_3') \leq k-2$, then there would be two $\leq k$-paths from v_2 and v_3 to v_3'. Thus $d(v_2', v_3') = k-1$. If v_2' lies in $N^{-(k-2)}(v_2)$ or $N^{-(k-2)}(v_3)$, there would be a $\leq k$-cycle in G through v_2 or v_3 respectively. Hence $v_2' \in N^{-(k-2)}(x)$ and $v_1' \notin T^-(x)$.

Corollary 5.43. *x is not an outlier.*

Proof. As $v_2' \in N^{-(k-2)}(x)$ and $v_1', v_3', v_2, v_3 \notin T^-(x)$, $|T_{-k}(x)| = M(2,k)+2$. □

Lemma 5.44. *$v_1 \notin \{v_2^+, v_3^+\}$, i.e. v_1 is not an out-neighbour of v_2 or v_3.*

Proof. Suppose that $v_1 = v_2^+$. Denote the in-neighbour of v_1' that does not belong to $\{v_1, v_3^+\}$ by v_1^* and the in-neighbour of v_2' that does not belong to $\{v_1, v_3^+\}$ by v_2^*. By Lemma 5.34, v_1' and v_2' are not outliers and $d(v_2', v_1') = d(v_3', v_1') = k$. We cannot have $v_2' \in T^-(v_1)$, or there would be a k-cycle through v_1. Also $v_2' \notin T^-(v_3^+)$, or there would be a k-cycle through v_3^+. Likewise, $v_3' \notin T^-(v_1)$, or there would be a $(k-1)$-cycle through v_2, and $v_3' \notin T^-(v_3^+)$, or there would be two $\leq k$-paths from v_3 to v_3^+. It follows that $v_2', v_3' \in N^{-(k-1)}(v_1^*)$ and likewise we have $v_1', v_3' \in N^{-(k-1)}(v_2^*)$. As $S \cap T^-(v_1^*) = S \cap T^-(v_2^*) = \emptyset$, it follows that $|T_{-k}(v_1^*)| = |T_{-k}(v_2^*)| = M(2,k)+2$, so that $O^-(v_1^*) = O^-(v_2^*) = \emptyset$. By Lemma 5.6, possible Ω-sets are

$$\{v_2, v_1\}, \{v_2, v_3^+\}, \{v_3, v_1\}, \{v_3, v_3^+\}.$$

But then every Ω-set contains either v_1 or v_3^+ and $N^+(v_1) = N^+(v_3^+)$, contradicting the Amalgamation Lemma. □

Theorem 5.45. *There are no $(2,k;+2)$-digraphs with in-degree sequence $(1,1,1,2,\ldots,2,3,3,3)$ for $k \geq 3$.*

Proof. By Lemma 5.44, $N^-(v_1') = N^-(v_2') = \{v_1, v_2^+, v_3^+\}$. By Lemma 5.34, we have $v_2' \in N^{-k}(v_1')$. But it is easy to see that whether v_2' lies in $T^-(v_1), T^-(v_2^+)$ or $T^-(v_3^+)$, there will be a k-cycle through v_1, v_2^+ or v_3^+ respectively. □

It remains only to deal with the case $k = 2$. First we need to prove the equivalent of Lemma 5.35, i.e. that S' is an independent set.

Lemma 5.46. *For $k = 2$, no two members of S' are adjacent.*

Proof. Suppose that $v_2' \to v_1'$. By 2-geodecity, v_1' must be Type 2, v_2' is Type 1 and $O^-(v_1') = \emptyset$. By the same reasoning, if $v_3' \to v_2'$, then v_2' would be Type 2, a contradiction. Hence we can assume that
$N^-(v_1') = \{v_1, v_2, v_2'\}, N^-(v_2') = \{v_3, x, y\}, N^-(v_1) = \{z\}$ and $N^-(v_2) = \{v_3'\}$, where $d^-(x) = d^-(y) = d^-(z) = 2$.

Obviously $v_2 \not\to v_3'$, so v_3' is either Type 1 or Type 2. Suppose that $v_3 \to v_3'$. Then v_2' cannot be adjacent to v_3', or there would be two ≤ 2-paths from v_3 to v_3'. Hence $v_2' \to z$. This implies that x and y are not adjacent to z, as they can already reach z via v_2'. Therefore x and y are adjacent to v_3'. Now v_3' cannot be adjacent to any of v_3, x or y, so $v_3' \to z$, thereby creating paths $v_3 \to v_3' \to z$ and $v_3 \to v_2' \to z$. Alternatively, one can see that $N^-(v_2') = N^-(v_3')$, which is impossible, since $|T_{-2}(v_2')| = 9$. Therefore $v_3 \not\to v_3'$. Applying the same approach to x and y, we see that these vertices also have no arcs to v_3'. Hence all of v_3, x and y are adjacent to z. However, as $d^-(z) = 2$, this is not possible. □

Lemma 5.47. *Every vertex in S' is Type 2.*

Proof. Suppose that S' contains a Type 1 vertex; say v_1' is Type 1, with
$N^-(v_1') = \{v_1, x, y\}$, where $d^-(x) = d^-(y) = 2$. Write
$N^-(v_1) = \{z\}, N^-(x) = \{x_1, x_2\}, N^-(y) = \{y_1, y_2\}$.

Note that we cannot have $|N^-(x) \cap S'| = 2$ or $|N^-(y) \cap S'| = 2$. For suppose that $y_1 = v_2', y_2 = v_3'$. v_1' is not an in-neighbour of either of these vertices by Lemma 5.46. By 2-geodecity no in-neighbourhood can contain both end-points of an arc, so the in-neighbourhoods of v_2' and v_3' must consist of one vertex from $\{z, v_1\}$ and both of x_1, x_2. However, x_1 and x_2 have out-degree two, so this is not possible. The same argument shows that we cannot have $|N^-(x) \cap S'| = |N^-(y) \cap S'| = 1$, for then v_2' and v_3' would have to be adjacent, in violation of Lemma 5.46. There are thus two possibilities up to isomorphism: i) $v_2' = z, v_3' = x_1, v_2 = x_2, v_3 = y_1$ or ii) $v_2' = z, v_3' = x_1, v_2 = y_1, v_3 = y_2$.

In case i), as S' is independent we must have $N^-(v_3') = \{v_1, v_3, y_2\}$. However, no arc from v_3' can be inserted to $N^{-2}(v_1')$ without violating either 2-geodecity or Lemma 5.46.

In case ii), we must have $N^-(v_3') = S$, so that v_2' cannot have any in-neighbours in S,

contradicting Lemma 5.33. Therefore S' contains no Type 1 vertices. From $N_1 + 2N_2 + 3N_3 \leq 6$, it now follows that every vertex of S' is Type 2 and $N^+(v_i) \subset S'$ for $i = 1, 2, 3$. □

Distinct vertices from S cannot have identical out-neighbourhoods; for example, if $N^+(v_1) = N^+(v_2) = \{v_1', v_2'\}$, then v_3' could not be Type 2. For $i = 1, 2, 3$, we can therefore set $N^-(v_i') = (S - \{v_i\}) \cup \{x_i\}$, where $d^-(x_i) = 2$. As $S' \cap N^-(S') = \emptyset$, we see that $N^+(v_i) \cap T^-(v_i') = \emptyset$ for $i = 1, 2, 3$, so that $O^-(v_i') = \{v_i\}$ for $i = 1, 2, 3$. We now have enough information to complete the proof.

Theorem 5.48. *There are no* $(2, 2; +2)$*-digraphs with in-degree sequence* $(1, 1, 1, 2, 2, 2, 3, 3, 3)$.

Proof. Write $N^-(v_i) = \{z_i\}$ for $i = 1, 2, 3$ and put $N^-(x_1) = \{y_1, y_2\}$. There are three distinct cases to consider, depending on the position of v_2' and v_3' in $T_{-2}(v_1')$: i) $v_2' = z_2, v_3' = z_3$, ii) $v_2' = z_2, v_3' = y_1$ and iii) $v_2' = y_1, v_3' = y_2$.

Consider case i). v_1' is adjacent to neither v_2' nor v_3' by Lemma 5.46 and cannot be adjacent to both elements of $N^-(x_1)$ by 2-geodecity. Hence we can assume that $N^+(v_1') = \{v_1, y_2\}$. Hence v_1' has paths of length two to v_2' and v_3' via v_1. It follows that y_2 cannot be adjacent to any of v_1, v_2', v_3' or y_1 without violating 2-geodecity.

In case ii), the only vertex other than v_1 and v_2 that can be an in-neighbour of v_3' is z_3, but in this case v_3' cannot be adjacent to any of y_2, z_3, v_1 or v_2', so we have a contradiction. Finally, in case iii) there are two 2-paths from v_1 to x_1. □

5.3.5 Degree sequence $(1, 1, 1, 1, 2, \ldots, 2, 3, 3, 3, 3)$

We turn to our final in-degree sequence. In this case the abundance of elements in S and S' enables us to easily classify all Ω-sets of G. A parity argument based on the number of occurrences of the outlier sets then allows us to obtain a contradiction.

Lemma 5.49. *For every vertex* u*,* $O(N^+(u)) = S$*,* $N^+(O(u)) = S'$ *and* $O(u) \subset S$*. If* Ω *is an outlier set, so is* $S - \Omega$*.*

Proof. By Lemmas 5.5 and 5.6 we have $S \subseteq O(N^+(u))$ and $S' \subseteq N^+(O(u))$. As $|S| = |S'| = 4$, we must have equality in the inclusions. If $O(u) = \Omega$, let u^-, u^+ be such that $N^+(u^-) = \{u, u^+\}$; then we must have $O(u) \cup O(u^+) = S$, so that $O(u) \subset S$ and $O(u^+) = S - \Omega$. □

Corollary 5.50. *For all $v' \in S'$, $|N^-(v') \cap S| = 2$.*

Proof. Let $N^+(v') = \{w_1, w_2\}$. Let $O(w_1) = \Omega_1, O(w_2) = \Omega_2$, where $\Omega_1 \cup \Omega_2 = S$. Write $N^+(w_1) = \{w_3, w_4\}$ and $N^+(w_2) = \{w_5, w_6\}$. By k-geodecity, at most one in-neighbour of v' lies in $T(w_3)$ and at most one lies in $T(w_4)$ and furthermore $w_1 \notin N^-(v')$. It follows that an in-neighbour of v' lies in Ω_1. Applying the argument to w_2, another in-neighbour of v' lies in Ω_2. Hence $|N^-(v') \cap S| \geq 2$ for all $v' \in S'$.

Suppose that $|N^-(v'_1) \cap S| = 3$. As $|N^-(v'_i) \cap S| \geq 2$ for $i = 2, 3, 4$, we must have $\sum_{i=1}^{4} d^+(v_i) \geq 9$, which is impossible. □

Lemma 5.51. *No two elements of S have the same out-neighbourhood.*

Proof. Suppose that $V \subset S$, $|V| = 2$ and $|N^+(V)| = 2$. By Lemma 5.49, V is not an Ω-set, as $N^+(V) \neq S'$. Suppose that there exists a vertex u that can reach both vertices of V by $\leq k$-paths. Then by Lemma 5.49 $O(u) = S - V$, so that $S - (S - V) = V$ must be an Ω-set, a contradiction. Now we have a pair of vertices with identical out-neighbourhoods and with non-empty intersection with every Ω-set, violating the Amalgamation Lemma. □

Lemma 5.52. *There are only two distinct Ω-sets.*

Proof. Let $u \in V(G)$ and $N^+(u) = \{u_1, u_2\}$ and write $O(u_1) = \Omega_1, O(u_2) = \Omega_2$, where $\Omega_1 \cup \Omega_2 = S$. By Lemma 5.51, for $1 \leq i, j \leq 4$ and $i \neq j$

$$N^-(v'_i) \cap S \neq N^-(v'_j) \cap S.$$

None of the sets $N^-(v'_i) \cap S$ can be Ω-sets, since any such set has at most three out-neighbours. There are $\binom{4}{2}$ two-element subsets of S, all of which are accounted for by the two outlier sets Ω_1 and Ω_2 and the four sets $N^-(v'_i) \cap S$. □

Theorem 5.53. *There are no $(2, k; +2)$-digraphs with in-degree sequence $(1, 1, 1, 1, 2, \ldots, 2, 3, 3, 3, 3)$ for $k \geq 2$.*

Proof. Let the distinct outlier sets of G be Ω_1 and Ω_2. As G has odd order $2^{k+1} + 1$, one of these sets must occur more frequently as an Ω-set than the other. Take an arbitrary vertex u with $O(u) = \Omega_1$ and consider $T_k(u) \cup \Omega_1$, which contains all vertices of G without repetitions. By Lemmas 5.49 and 5.52, for every vertex w of G with out-neighbours w_1, w_2, we have $O(w_1) = \Omega_1, O(w_2) = \Omega_2$ or vice versa, so half of

the vertices in $T_k(u) - \{u\}$ have outlier set Ω_1 and half have outlier set Ω_2. As $O(u) = \Omega_1$ and each element of Ω_1 has outlier-set Ω_2, it follows that the set Ω_2 occurs $2^k + 1$ times as an Ω-set and Ω_1 occurs 2^k times. However, repeating the argument with a vertex u with $O(u) = \Omega_2$ leads to the opposite conclusion, a contradiction. □

This concludes the proof of the main theorem of this chapter.

5.4 Digraphs with degree two and excess three

In the preceding section we saw that all $(2, k; +2)$-digraphs are diregular. This raises the question of whether a $(2, k; +3)$-digraph must be diregular for $k \geq 3$. In this section we briefly indicate our best results on the structure of a non-diregular $(2, k; +3)$-digraph.

Suppose that G is a non-diregular $(2, k; +3)$-digraph. By Corollary 5.7, the size of the sets S and S' is bounded above by 6 and by Lemma 5.8 the largest possible in-degree of a vertex in S' is 5. Firstly we show that this upper limit on the in-degree cannot be met.

Theorem 5.54. *The largest possible in-degree of a vertex in S' is 4.*

Proof. Suppose that $v' \in S'$ has in-degree $d^-(v') = 5$. We can obtain a lower bound for the number of vertices in $T_{-k}(v')$ by assuming that every vertex in $N^-(v')$ lies in S, as well as one vertex in $N^{-2}(v')$; this yields

$$|T_{-k}(v')| \geq 7 + 4M(2, k-2) + M(2, k-3) = 2^{k+1} + 2^{k-2} + 2,$$

which is too large. □

Now we examine the case of a vertex v' in S' with in-degree 4.

Theorem 5.55. *If $v' \in S'$ has in-degree $d^-(v') = 4$, then $|S| \geq 4$.*

Proof. If $|S| \leq 3$, then we get a lower bound for the size of $T_{-k}(v')$ by assuming that $S \subset N^-(v')$; this gives the bound

$$|T_{-k}(v')| \geq 4 + M(2, k-1) + 3M(2, k-2) = 2^{k+1} + 2^{k-1},$$

which is too large for $k \geq 3$. □

Theorem 5.56. *If there is a vertex $v' \in S'$ with in-degree $d^-(v') = 4$ and $|S| = 4$, then $S = N^-(v')$.*

Proof. Suppose that $N^-(v') \neq S$. Then we get a lower bound for $|T_{-k}(v')|$ by assuming that $|S \cap N^-(v')| = 3$ and the other member of S lies in $N^{-2}(v')$; this yields

$$|T_{-k}(v')| \geq 5 + M(2, k-3) + 2M(2, k-2) + M(2, k-1) = 2^{k+1} + 2^{k-2} + 1,$$

which is too large for $k \geq 3$. Therefore $S = N^-(v')$. □

The size of S also cannot be too small.

Theorem 5.57. *The set S has size at least two.*

Proof. Suppose that $|S| = 1$. Then S' consists of a single vertex v' with in-degree 3. We obtain a lower bound on the size of $T_{-k}(v')$ by assuming that the single vertex v of S satisfies $v \to v'$, which yields the bound

$$M(2, k) + 3 \geq |T_{-k}(v')| \geq M(2, k) + M(2, k-2) + 1,$$

which is impossible for $k \geq 3$. □

These results significantly restrict the possible in-degree sequences of a non-diregular $(2, k; +3)$-digraph; however, the large number of remaining in-degree sequences means that we as yet have no proof that $(2, k; +3)$-digraphs must be diregular.

Chapter 6

Diregular digraphs with small excess

In Section 5 we showed that any digraphs with out-degree two and excess two must be diregular. In this chapter we use this result as a stepping stone to a complete classification of digraphs with out-degree two and excess two. In Section 6.2 we prove that there are no $(2, k; +2)$-digraphs for $k \geq 3$. We consider the case $k = 2$ separately in Section 6.3; we will see that there do exist $(2, 2; 2)$-digraphs, which will give our first non-trivial examples of geodetic cages. In Section 6.4 we push our method further to classify diregular $(2, k; +3)$-digraphs for $k \geq 4$. The case $k = 3$ is considered separately in Section 6.5.

We also record here the labelling convention that we will employ for vertices at distance $\leq k$ from a vertex u of G. The out-neighbours of u will be labelled according to $N^+(u) = \{u_1, u_2\}$ and vertices at a greater distance from u are labelled inductively as follows: $N^+(u_1) = \{u_3, u_4\}, N^+(u_2) = \{u_5, u_6\}, N^+(u_3) = \{u_7, u_8\}$ and so on. See Figure 6.1 for an example. In this chapter we will also say that a vertex u can *reach* a vertex v in a digraph G if there is a $\leq k$-path from u to v.

6.1 The Neighbourhood Lemma

By Lemma 4.1, the outlier function of a digraph G with excess one is an automorphism of G [132]. This parallels the result of [15] that the repeat function of a digraph with defect one is also an automorphism. As was demonstrated in Chapter 4, this is a very useful result. However for larger values of the defect δ or excess ϵ this result no longer holds. For small defect it was shown in [131] that a more general multiset relation $N^+(R(u)) = R(N^+(u))$ holds. We now prove the Neighbourhood Lemma for digraphs with small excess, which will be our fundamental tool in this chapter. For a set-valued function Ψ of the vertices of a digraph G and a subset $U \subseteq V(G)$ we define the multiset $\Psi(U)$ to be the union of the sets $\Psi(u), u \in U$, counted by multiplicity.

Lemma 6.1 (Neighbourhood Lemma)**.** *Let G be a diregular $(d, k; +\epsilon)$-digraph for any $d, k \geq 2$ and $\epsilon \geq 1$. Then for any vertex u of G we have $O(N^+(u)) = N^+(O(u))$ as multisets.*

Proof. As G is diregular, any vertex can occur at most d times in either multiset. Suppose that a vertex v occurs t times in $N^+(O(u))$. Let $N^-(v) = \{v_1, v_2, \ldots, v_t, v_{t+1}, \ldots, v_d\}$ and $N^+(u) = \{u_1, u_2, \ldots, u_d\}$, where $O(u) \cap N^-(v) = \{v_1, v_2, \ldots, v_t\}$. Suppose that $u \notin N^-(v)$. Since no set $T(u_i)$ contains more than one in-neighbour of v by k-geodecity, there are exactly $d - t$ out-neighbours of u that can reach v by a $\leq k$-path, so that v occurs t times in $O(N^+(u))$. A similar argument deals with the case $u \in N^-(v)$. As both multisets have size $d\epsilon$, this implies the result. □

6.2 Diregular digraphs with degree two and excess two

We will now make use of the Neighbourhood Lemma in order to show that there are no diregular $(2, k; +2)$-digraphs for $k \geq 3$. We know from Chapter 5 that all digraphs with out-degree two and excess two are diregular, so this implies that $\epsilon(2, k) \geq 3$ for $k \geq 3$. The case $k = 2$ will need to be handled separately in the next section.

The strategy used in [118] to deal with digraphs with degree two and defect two is to use counting arguments on two directed Moore trees rooted at vertices that share a unique common out-neighbour. We commence our analysis of $(2, k; +2)$-digraphs by showing that there must exist such a pair of vertices. For even ϵ this follows from a simple parity argument; in Section 6.4 we will have to use a slightly more sophisticated approach to establish the existence of such a pair.

Lemma 6.2. *If G is a diregular $(2, k; +\epsilon)$-digraph, where ϵ is even, then G contains a pair of vertices u, v with a single common out-neighbour, i.e. $|N^+(u) \cap N^+(v)| = 1$.*

Proof. Suppose for a contradiction that G contains no such pair of vertices. Define a map $\phi : V(G) \to V(G)$ as follows. Let u^+ be an out-neighbour of a vertex u and let $\phi(u)$ be the in-neighbour of u^+ distinct from u. By our assumption, it is easily verified that ϕ is a well-defined bijection with no fixed points and with square equal to the identity. It follows that G must have even order, whereas $M(2, k) + \epsilon$ is odd. □

On the other hand, it is conceivable that a digraph with small excess could contain a pair of vertices with identical out- or in-neighbourhoods (we will see that this does actually occur for geodetic cages - see Figure 6.7); however in such a case the outlier sets of these vertices are strongly constrained. The following lemma is a generalisation of Lemma 4.18.

Lemma 6.3. *For $k \geq 2$, let u and v be distinct vertices of a $(2, k; +2)$-digraph such*

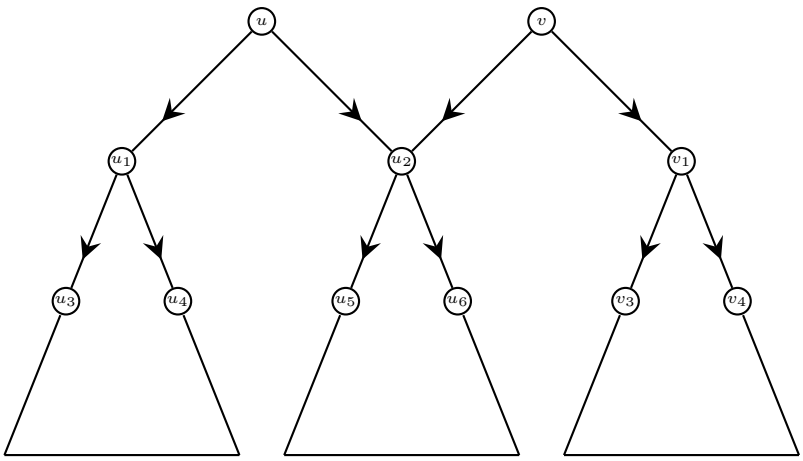

Figure 6.1: Configuration for $k \geq 3$

that $N^+(u) = N^+(v) = \{u_1, u_2\}$. *Then* $u_1 \in O(u_2), u_2 \in O(u_1)$ *and there exists a vertex* x *such that* $O(u) = \{v, x\}, O(v) = \{u, x\}$.

Proof. Suppose that u can reach v by a $\leq k$-path. Then $v \in T(u_1) \cup T(u_2)$. As $N^+(v) = N^+(u)$, it follows that there would be a $\leq k$-cycle through v, contradicting k-geodecity. If $O(u) = \{v, x\}$, then $x \neq v$ and $x \notin T(u_1) \cup T(u_2)$, so that v cannot reach x by a $\leq k$-path. Similarly, if u_1 can reach u_2 by a $\leq k$-path, then we must have $\{u, v\} \cap T(u_1) \neq \emptyset$, which is impossible. □

We will now prove the following classification of $(2, k; +2)$-digraphs.

Theorem 6.4. *There are no diregular* $(2, k; +2)$*-digraphs for* $k \geq 3$.

For the remainder of this section G will stand for a diregular $(2, k; +2)$-digraph, where $k \geq 2$; we will investigate the properties of G and arrive at a contradiction, thereby proving Theorem 6.4. By Lemma 6.2 we can fix a pair of vertices u, v of G with a unique common out-neighbour. In accordance with our vertex-labelling convention, we have the situation in Figure 6.1. A triangle based at a vertex x represents the set $T(x)$.

We now proceed to determine the possible outlier sets of u and v.

Lemma 6.5. *We have* $v \in N^{k-1}(u_1) \cup O(u)$ *and* $u \in N^{k-1}(v_1) \cup O(v)$. *Furthermore, if* $v \in O(u)$, *then* $u_2 \in O(u_1)$, *whilst if* $u \in O(v)$, *then* $u_2 \in O(v_1)$.

Proof. The vertex v cannot lie in $T(u)$, or else the vertex u_2 would be repeated in $T_k(u)$. Also, $v \notin T(u_2)$, or there would be a $\leq k$-cycle through v. Therefore, if

$v \notin O(u)$, then $v \in N^{k-1}(u_1)$. Likewise for the other result. If $v \in O(u)$, then neither in-neighbour of u_2 lies in $T(u_1)$, so that $u_2 \in O(u_1)$. □

Lemma 6.6. *Let $w \in T(v_1)$, with $d(v_1, w) = l$. Suppose that $w \in T(u_1)$, with $d(u_1, w) = m$. Then either $m \leq l$ or $w \in N^{k-1}(u_1)$. The analogous result obtained by interchanging the roles of u_1 and v_1 also holds.*

Proof. Let w be as described and suppose that $m > l$. Consider the set $N^{k-m}(w)$. By construction, $N^{k-m}(w) \subseteq N^k(u_1)$, so by k-geodecity $N^{k-m}(w) \cap T(u_1) = \emptyset$. At the same time, we have $l + k - m \leq k - 1$, so $N^{k-m}(w) \subseteq T(v_1)$. This implies that $N^{k-m}(w) \cap T(v_2) = N^{k-m}(w) \cap T(u_2) = \emptyset$. As $V(G) = \{u\} \cup T(u_1) \cup T(u_2) \cup O(u)$, it follows that $N^{k-m}(w) \subseteq \{u\} \cup O(u)$. Therefore $|N^{k-m}(w)| = 2^{k-m} \leq 3$. By assumption $0 \leq m \leq k - 1$, so it follows that $m = k - 1$. □

Corollary 6.7. *If $w \in T(v_1)$, then either $w \in \{u\} \cup O(u)$ or $w \in T(u_1)$ with $d(u_1, w) = k - 1$ or $d(u_1, w) \leq d(v_1, w)$.*

Proof. By k-geodecity and Lemma 6.6. □

Corollary 6.8. *$v_1 \in N^{k-1}(u_1) \cup O(u)$ and $u_1 \in N^{k-1}(v_1) \cup O(v)$.*

Proof. We prove the first inclusion. By Corollary 6.7, $v_1 \in \{u\} \cup O(u) \cup \{u_1\} \cup N^{k-1}(u_1)$. By k-geodecity, $v_1 \neq u$ and by construction, $v_1 \neq u_1$. □

We now have enough information to identify one member of $O(u)$ and $O(v)$.

Lemma 6.9. *$v_1 \in O(u)$ and $u_1 \in O(v)$.*

Proof. We prove that $v_1 \in O(u)$. Suppose that neither v_1 nor v lies in $O(u)$. Then by Lemma 6.5 and Corollary 6.8 we have $v, v_1 \in N^{k-1}(u_1)$. As v_1 is an out-neighbour of v, it follows that v_1 appears twice in $T_k(u_1)$, violating k-geodecity. Therefore $O(u) \cap \{v, v_1\} \neq \emptyset$.

Now assume that $v_1, v_3 \in T_k(u)$. Again by Corollary 6.8, $v_1 \in N^{k-1}(u_1)$. By k-geodecity we also have $v_3 \in T(u_1)$. However, $v_3 \in N^+(v_1)$, so v_3 appears twice in $T_k(u_1)$, which is impossible. Hence $O(u) \cap \{v_1, v_3\} \neq \emptyset$. Similarly, $O(u) \cap \{v_1, v_4\} \neq \emptyset$. Therefore, if $v_1 \notin O(u)$, then $\{v, v_3, v_4\} \subseteq O(u)$. Since these vertices are distinct, this is a contradiction and the result follows. □

Lemma 6.9 allows us to conclude that for vertices sufficiently close to v_1 one of the potential situations mentioned in Corollary 6.7 cannot occur.

Lemma 6.10. $T_{k-3}(v_1) \cap N^{k-1}(u_1) = T_{k-3}(u_1) \cap N^{k-1}(v_1) = \emptyset$.

Proof. Let $w \in T_{k-3}(v_1) \cap N^{k-1}(u_1)$. Consider the position of the vertices of $N^+(w)$ in $T_k(u) \cup O(u)$. As $v_1 \notin N^+(w)$, it follows from Lemma 6.9 that at most one of the vertices of $N^+(w)$ can be an outlier of u, so let us write $w_1 \in N^+(w) - O(u)$. By k-geodecity, $w_1 \notin T(u_1) \cup \{u\}$. Hence $w_1 \in T(u_2) = T(v_2)$. However, w_1 also lies in $T(v_1)$, so this violates k-geodecity. □

Corollary 6.11. *There is at most one vertex in $T_{k-3}(v_1) - \{v_1\}$ that does not lie in $T(u_1)$; for all other vertices $w \in T_{k-3}(v_1) - \{v_1\}$, $d(u_1, w) = d(v_1, w)$. A similar result for $T_{k-3}(u_1) - \{u_1\}$ also holds.*

Proof. By Corollary 6.7 and Lemma 6.10 any vertex of $T_{k-3}(v_1) - \{v_1\}$ that does not lie in $T(u_1)$ must lie in $\{u\} \cup O(u)$. By k-geodecity, $u \notin T_{k-3}(v_1)$. Furthermore by Lemma 6.9 we have $v_1 \in O(u)$, so at most one vertex of $T_{k-3}(v_1) - \{v_1\}$ can belong to $O(u)$. Thus, with at most one exception, every vertex $w \in T_{k-3}(v_1) - \{v_1\}$ must lie in $T_{k-2}(u_1)$ and $d(u_1, w) \leq d(v_1, w)$. Since any such w does not belong to $\{v\} \cup N^{k-1}(v_1) \cup O(v)$, we can interchange the roles of u and v in this argument to conclude that $d(v_1, w) \leq d(u_1, w)$, so that $d(u_1, w) = d(v_1, w)$. □

Corollary 6.11 does not tell us anything in the case $k = 3$; thus in the next lemma we extend Corollary 6.11 to yield information on $k = 3$.

Lemma 6.12. *For $k = 3$, $N^+(u_1) \cap N^2(v_1) = N^+(v_1) \cap N^2(u_1) = \emptyset$.*

Proof. Suppose that $v_3 = u_7$. By the reasoning of Lemma 6.10 we can set $u = v_7$ and $O(u) = \{v_1, v_8\}$. $v \notin O(u)$ and by 3-geodecity $v \notin N^+(u_3)$, so we can assume that $v = u_9$. $u_3 \to v_3$ implies that $u_3 \notin T(v_1)$, so $O(v) = \{u_1, u_3\}$. We must have $\{u_4, u_8, u_{10}\} = \{v_4, v_9, v_{10}\}$. As $u_4 \to v$, it follows that $v_4 = u_8$ and hence $\{u_4, u_{10}\} = \{v_9, v_{10}\}$, which is impossible. □

By Lemma 6.9 u_1 is an outlier of v for $k \geq 3$, so that neither v_3 nor v_4 can be equal to u_1. It follows from Corollary 6.11 and Lemma 6.12 that either $N^+(u_1) = N^+(v_1)$ or u_1 and v_1 have a single common out-neighbour, with one vertex of $N^+(v_1)$ being an outlier of u.

Lemma 6.13. $N^2(u) \neq N^2(v)$

Proof. Let $N^2(u) = N^2(v)$, with $N^+(u_1) = N^+(v_1) = \{u_3, u_4\}$. Suppose that $v \notin O(u)$. By Lemma 6.5, $v \in N^{k-2}(u_3) \cup N^{k-2}(u_4)$. But then there is a k-cycle through v. It follows that $O(u) = \{v, v_1\}, O(v) = \{u, u_1\}$. By Lemma 6.5 it follows that $u_2 \in O(u_1) \cap O(v_1)$. Therefore by Lemma 6.3 $O(u_1) = \{u_2, v_1\}, O(v_1) = \{u_2, u_1\}$.

Consider the in-neighbour u' of u_1 that is distinct from u. We have either $|N^+(u') \cap N^+(u)| = 1$ or $|N^+(u') \cap N^+(u)| = 2$. In the first case, it follows from Lemma 6.9 that $u_2 \in O(u')$. Every vertex of G is an outlier of exactly two vertices, so $u' = u_1$ or v_1. In either case, we have a contradiction. Therefore $N^+(u') = N^+(u)$. It now follows from Lemma 6.3 that $u' \in O(u) = \{v, v_1\}$, which is impossible. □

By Lemma 6.13 we have $N^+(u_1) \neq N^+(v_1)$, implying that u_1 and v_1 have a unique common out-neighbour, so that we can assume that $u_3 = v_3$, $O(u) = \{v_1, v_4\}$ and $O(v) = \{u_1, u_4\}$. As u_1, v_1 have a unique common out-neighbour u_3, we can apply the above analysis to the pair u_1, v_1 to conclude that we can set $u_9 = v_9$, $O(u_1) = \{v_4, v_{10}\}$ and $O(v_1) = \{u_4, u_{10}\}$ without loss of generality. This yields the following corollary.

Corollary 6.14. *Without loss of generality,*
$u_3 = v_3, u_9 = v_9, O(u) = \{v_1, v_4\}, O(v) = \{u_1, u_4\}, O(u_1) = \{v_4, v_{10}\}$ *and* $O(v_1) = \{u_4, u_{10}\}$.

We are now in a position to complete the proof of Theorem 6.4 by deriving a contradiction.

Theorem 6.4. *There are no diregular* $(2, k; +2)$*-digraphs for* $k \geq 3$.

Proof. Let u, v be a pair of vertices with a unique common out-neighbour in a diregular $(2, k; +2)$-digraph G. By Corollary 6.14 we can label the vertices of G as in Figure 6.2, where $O(u) = \{v_1, v_4\}$, $O(v) = \{u_1, u_4\}$, $O(u_1) = \{v_4, v_{10}\}$ and $O(v_1) = \{u_4, u_{10}\}$. It follows that $u, v \notin \{u_1, u_4, v_1, v_4\}$, so by Lemma 6.5 we have $d(u, v) = d(v, u) = k$. In fact, $u_3 = v_3$ implies that $v \in N^{k-2}(u_4)$ and $u \in N^{k-2}(v_4)$. Let $k \geq 4$. Then $u, v \notin \{u_{10}, v_{10}\}$, so $u, v \in T_k(u_1) \cap T_k(v_1)$. If $u \in T(u_3) = T(v_3)$, then u would appear twice in $T_k(v_1)$, so $u \in N^{k-1}(u_4)$. However, as u and v have a common out-neighbour, this violates k-geodecity.

Finally, suppose that $k = 3$. The above analysis will hold unless $u = v_{10}$ and $v = u_{10}$. Let $N^-(u_1) = \{u, u'\}, N^-(v_1) = \{v, v'\}$. It is evident that $v' \notin \{v_1, v_4\}$, so that

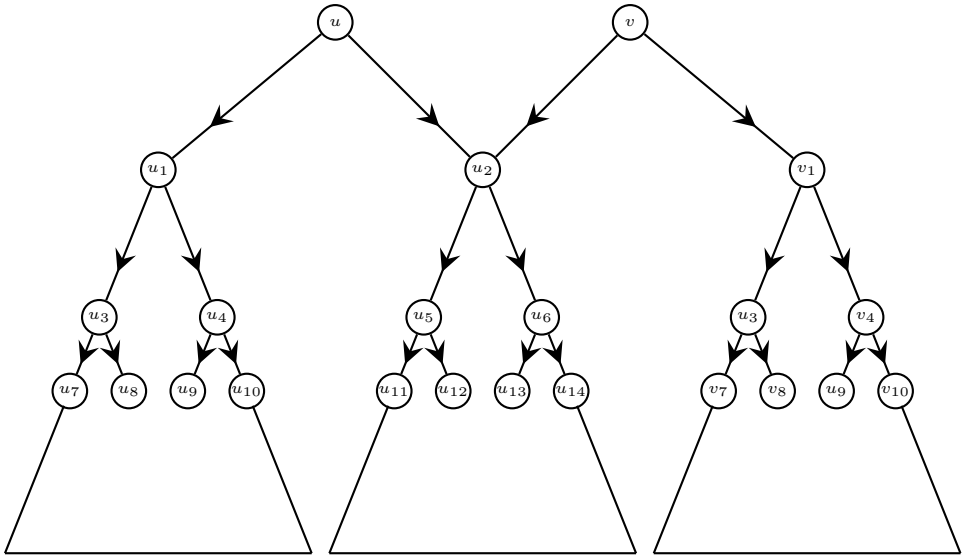

Figure 6.2: Labelling for proof of Theorem 6.4

$v' \in T_3(u)$. As $v \in N^+(u_4)$, we must have $v' \in N^2(u_2)$. Similarly $u' \in N^2(u_2)$. Since u_1 and v_1 have a common out-neighbour, we can assume that $u' \in N^+(u_5)$ and $v' \in N^+(u_6)$. v_4 can be the outlier of only two vertices, namely u and u_1, so $v_4 \in N^3(u_2)$ and likewise $u_4 \in N^3(u_2)$. By 3-geodecity $v_4 \in N^2(u_5)$ and $u_4 \in N^2(u_6)$. It follows that $u, v \notin N^3(u_2)$, so $u \notin T_3(u_1) \cup T_3(u_2)$. Hence $O(u) = N^-(u) = \{v_1, v_4\}$, which again is impossible. □

6.3 Classification of $(2, 2; +2)$-digraphs

We now classify the $(2, 2; +2)$-digraphs up to isomorphism. We will prove the following theorem.

Theorem 6.15. *There are exactly two $(2, 2; +2)$-digraphs, which are displayed in Figures 6.4 and 6.7.*

Let G be an arbitrary diregular $(2, 2; +2)$-digraph. G has order $M(2, 2) + 2 = 9$. By Lemma 6.2, G contains a pair of vertices u, v such that $|N^+(u) \cap N^+(v)| = 1$; we will assume that $u_2 = v_2$, so that we have the situation shown in Figure 6.3.

We can immediately deduce some information on the possible positions of v and v_1 in $T_2(u)$.

Lemma 6.16. *If $v \notin O(u)$, then $v \in N^+(u_1)$. If $v_1 \notin O(u)$, then $v_1 \in N^+(u_1)$.*

Proof. $v \notin T(u_2)$ by 2-geodecity. $v \neq u$ by construction. If we had $v = u_1$, then there

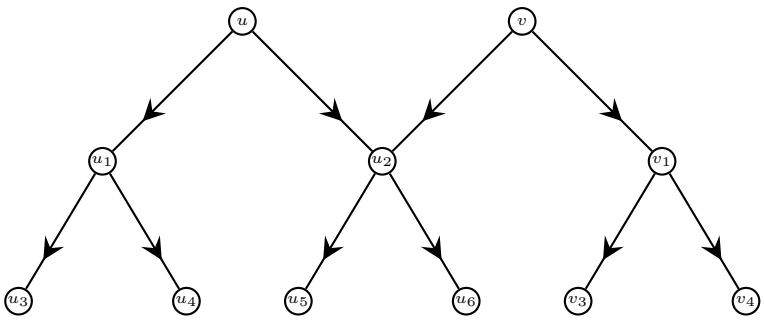

Figure 6.3: The vertices u and v

would be two distinct ≤ 2-paths from u to u_2. Also $v_1 \notin \{u\} \cup T(u_2)$ by 2-geodecity and by assumption $u_1 \neq v_1$. □

Since v and v_1 cannot both lie in $N^+(u_1)$ by 2-geodecity, we have the following corollary.

Corollary 6.17. $O(u) \cap \{v, v_1\} \neq \emptyset$.

We will call a pair of vertices u, v with a single common out-neighbour *bad* if at least one of

$$O(u) \cap \{v_1, v_3\} = \emptyset, O(u) \cap \{v_1, v_4\} = \emptyset, O(v) \cap \{u_1, u_3\} = \emptyset, O(v) \cap \{u_1, u_4\} = \emptyset.$$

holds. Otherwise such a pair will be called *good*.

Lemma 6.18. *There is a unique* $(2, 2; +2)$*-digraph containing a bad pair.*

Proof. Assume that there exists a bad pair u, v. Without loss of generality, $O(u) \cap \{v_1, v_3\} = \emptyset$. By Lemma 6.16 we can set $v_1 = u_3$. By 2-geodecity $v_3 = u$. We cannot have $v_4 = v_3 = u$, so v_4 must be an outlier of u. By Corollary 6.17 it follows that $O(u) = \{v, v_4\}$.

Consider the vertex u_1. By Lemma 6.16, if $u_1 \notin O(v)$, then $u_1 \in N^+(v_1)$. However, as $v_1 = u_3$, there would be a 2-cycle through u_1. Hence $u_1 \in O(v)$. As $O(u) = \{v, v_4\}$, we have $V(G) = \{u, u_1, u_2, u_3 = v_1, u_4, u_5, u_6, v, v_4\}$ and $O(v) = \{u_1, u_4\}$. As neither u nor v lies in $T(u_1)$, we must also have $u_2 \in O(u_1)$. As u_1 can reach u_1, v_1, u_4, u and v_4, it follows that without loss of generality we either have $O(u_1) = \{u_2, v\}$ and $N^+(u_4) = \{u_5, u_6\} = N^+(u_2)$ or $O(u_1) = \{u_2, u_6\}$ and $N^+(u_4) = \{v, u_5\}$. In either case, v, u_1 is a good pair.

Suppose firstly that $N^+(u_2) = N^+(u_4)$. Then v is an outlier of u and u_1. As each vertex is the outlier of exactly two vertices, v_1 must be able to reach v by a ≤ 2-path.

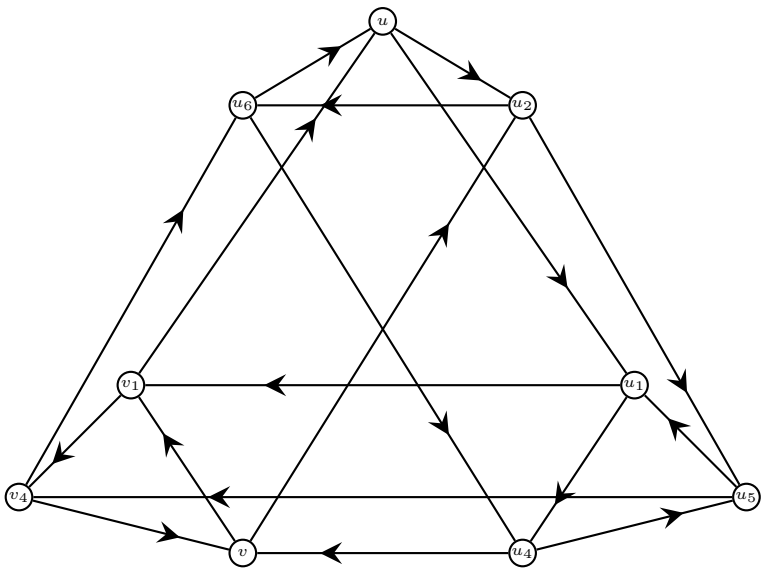

Figure 6.4: The unique $(2, 2; +2)$-digraph containing a bad pair

Hence $v_4 \to v$. Likewise u_2 can reach v, so without loss of generality $u_5 \to v$. Suppose that $O(u_2) \cap \{u, u_1\} = \emptyset$. As u and v have a common out-neighbour, we must have $u_6 \to u$. Since $u \to u_1$, by 2-geodecity we must have $u_5 \to u_1$. However, this is a contradiction, as v and u_1 also have a common out-neighbour. Therefore, at least one of u, u_1 is an outlier of u_2. By Lemma 6.3 u_4 is an outlier of u_2. Therefore either $O(u_2) = \{u, u_4\}$ or $O(u_2) = \{u_1, u_4\}$. If $O(u_2) = \{u, u_4\}$, then u_2 must be able to reach u_1, v_1 and v_4. $u_5 \to v$ and $v \to v_1$, so $v_1 \in N^+(u_6)$. As $u_1 \to v_1$, we must have $N^+(u_5) = \{v, u_1\}$. As v and u_1 have a common out-neighbour, this violates 2-geodecity. Hence $O(u_2) = \{u_1, u_4\}$ and u_2 can reach u, v_1 and v_4. As $v \to v_1$, $v_1 \in N^+(u_6)$. As $v_1 \to v_4$, it follows that $N^+(u_5) = \{v, v_4\}$. However, $v_4 \to v$, so this again violates 2-geodecity.

We are left with the case $O(u_1) = \{u_2, u_6\}$ and $N^+(u_4) = \{v, u_5\}$. Then $v_1 \in O(u_2)$, as neither v nor u_1 lies in $T(u_2)$. Observe that u_2 and u_4 have a single common out-neighbour, so by Corollary 6.17 $O(u_2) \cap \{u_4, v\} \neq \emptyset$. Therefore either $O(u_2) = \{v_1, u_4\}$ or $O(u_2) = \{v_1, v\}$. Suppose firstly that $O(u_2) = \{v_1, u_4\}$. Then $N^2(u_2) = \{u, v, u_1, v_4\}$. As $N^+(u_4) = \{v, u_5\}$, $u_5 \not\to v$, so $u_6 \to v$. As $N^+(u) \cap N^+(v) \neq \emptyset$, $u_5 \to u$. $u \to u_1$, so necessarily $N^+(u_6) = \{v, u_1\}$. However, $v_1 \in N^+(u_1) \cap N^+(v)$, contradicting 2-geodecity.

Hence $O(u_2) = \{v_1, v\}$ and $N^2(u_2) = \{u, u_1, u_4, v_4\}$. As $u_4 \to u_5$, $u_5 \not\to u_4$. Thus $u_6 \to u_4$. Now $u_1 \to u_4$ and $u \to u_1$ implies that $N^+(u_5) = \{u_1, v_4\}$ and $N^+(u_6) = \{u, u_4\}$. Finally we must have $N^+(v_4) = \{v, u_6\}$. This gives us the $(2, 2, +2)$-digraph shown in Figure 6.4. $\square$

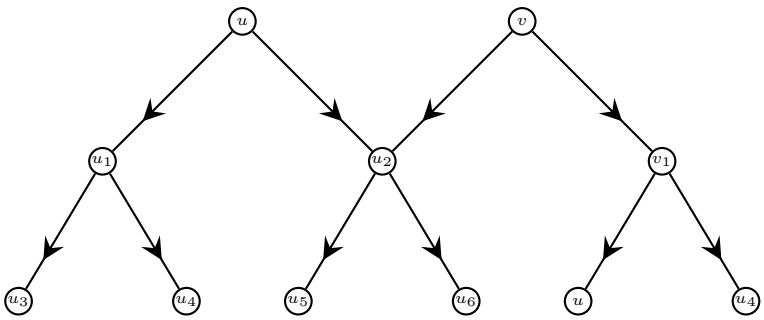

Figure 6.5: Case 1 configuration

We can now assume that all pairs given by Lemma 6.2 are good. Let us fix a pair u, v with a single common out-neighbour. It follows from Corollary 6.17 and the definition of a good pair that $v_1 \in O(u)$; otherwise $O(u)$ would contain v, v_3 and v_4, which is impossible. Likewise $u_1 \in O(v)$.

Considering the positions of v_3 and v_4, we see that there are without loss of generality four possibilities: 1) $u = v_3, u_4 = v_4$, 2) $u = v_3, O(u) = \{v_1, v_4\}$, 3) $N^+(u_1) = N^+(v_1)$ and 4) $u_3 = v_3, O(u) = \{v_1, v_4\}$. A suitable relabelling of vertices shows that case 4 is equivalent to case 1.a) below, so we will examine cases 1 to 3 in turn.

Case 1: $\mathbf{u = v_3, u_4 = v_4}$

Depending upon the position of v, we must either have $O(u) = \{v_1, v\}$ and $O(v) = \{u_1, u_3\}$ or $v = u_3$.

Case 1.a): $\mathbf{O(u) = \{v_1, v\}, O(v) = \{u_1, u_3\}}$

In this case $V(G) = \{u, u_1, u_2, u_3, u_4, u_5, u_6, v, v_1\}$. u_1 and v_1 have a single common out-neighbour, namely u_4, so, as we are assuming all such pairs to be good, we have $u_3 \in O(v_1), u \in O(u_1)$. By 2-geodecity, $N^+(u_4) \subset \{u_5, u_6, v\}$, so without loss of generality either $N^+(u_4) = \{u_5, u_6\}$ or $N^+(u_4) = \{u_5, v\}$.

Suppose that $N^+(u_4) = \{u_5, u_6\}$. By elimination, $O(v_1) = \{v, u_3\}$. As G is diregular, every vertex is an outlier of exactly two vertices; v is an outlier of u and v_1, so both u_1 and u_2 can reach v by a ≤ 2-path. Hence $v \in N^+(u_3)$. As $v \to v_1$, we see that v_1 is an outlier of u_1; as u is also an outlier of u_1, we have $O(u_1) = \{u, v_1\}$ and $N^+(u_3) = \{v, u_2\}$. As $v \to u_2$, this is impossible.

Now consider $N^+(u_4) = \{u_5, v\}$. We now have $O(v_1) = \{u_3, u_6\}$. Thus $u_3 \in O(v) \cap O(v_1)$, so $u_3 \in T_2(u_4)$. v is not adjacent to u_3, so $u_3 \in N^+(u_5)$. u_2 and u_4 have u_5 as a unique common out-neighbour, so $u_6 \in O(u_4), v \in O(u_2)$. As

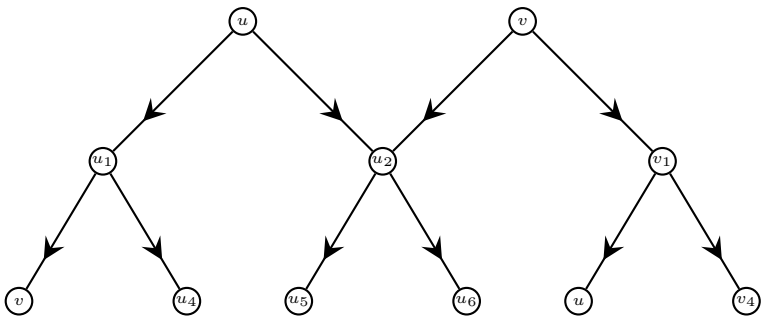

Figure 6.6: Case 2 configuration

$u_6 \in O(v_1) \cap O(u_4)$, u_1 can reach u_6. Hence $u_6 \in N^+(u_3)$. Neither u nor v lie in $T(u_1)$, so $u_2 \in O(u_1)$. Therefore either $O(u_1) = \{u, u_2\}$ or $O(u_1) = \{u_2, v_1\}$. If $O(u_1) = \{u, u_2\}$, then $N^+(u_3) = \{u_6, v_1\}$. u_2 can't reach v_1, since $v, u_3 \notin T(u_2)$, so $O(u_2) = \{v, v_1\}$ and $N^2(u_2) = \{u, u_1, u_3, u_4\}$. As $u_4 \to u_5$, $u_4 \in N^+(u_6)$. $u_1 \to u_4$, so $N^+(u_5) = \{u_1, u_3\}$. As $u_1 \to u_3$, this is a contradiction. Thus $O(u_1) = \{u_2, v_1\}$, so that $N^+(u_3) = \{u, u_6\}$. u_1 must have an in-neighbour apart from u, which must be either u_5 or u_6. As $u_1 \to u_3$, we have $u_1 \in N^+(u_6)$. By elimination, v and v_1 must also have in-neighbours in $\{u_5, u_6\}$. As u_1 and v_1 have a common out-neighbour, we have $N^+(u_5) = \{u_3, v_1\}, N^+(u_6) = \{u_1, v\}$. However, both u_3 and v_1 are adjacent to u, violating 2-geodecity.

Case 1.b): $\mathbf{v = u_3}$

There exists a vertex x such that $V(G) = \{u, u_1, u_2, v, u_4, u_5, u_6, v_1, x\}$, $O(u) = \{v_1, x\}$ and $O(v) = \{u_1, x\}$. As $x \in O(u) \cap O(v)$, u_1 and u_2 can reach x, so without loss of generality $x \in N^+(u_4) \cap N^+(u_5)$. As u_5 and u_4 have a common out-neighbour, $u_5 \in O(u_1)$. Also, u_1 and v_1 have u_4 as a unique common out-neighbour, so $u \in O(u_1)$ and $O(u_1) = \{u, u_5\}$. Thus $N^+(u_4) = \{x, u_6\}$. Observe that u_2 and u_4 have the out-neighbour u_6 in common. Thus $x \in O(u_2)$, whereas we already have $x \in O(u) \cap O(v)$, a contradiction.

Case 2: $\mathbf{u = v_3, O(u) = \{v_1, v_4\}}$

As v is not equal to v_1 or v_4, v must lie in $T_2(u)$. Without loss of generality, $v = u_3$. Hence $V(G) = \{u, u_1, u_2, v, u_4, u_5, u_6, v_1, v_4\}$ and $O(v) = \{u_1, u_4\}$. We have the configuration shown in Figure 6.6. Hence u_1 can reach u_1, v, u_4, u_2 and v_1, so we have without loss of generality one of the following: a) $O(u_1) = \{u, v_4\}, N^+(u_4) = \{u_5, u_6\}$, b) $O(u_1) = \{u, u_5\}, N^+(u_4) = \{u_6, v_4\}$, c) $O(u_1) = \{u_5, u_6\}, N^+(u_4) = \{u, v_4\}$ or d) $O(u_1) = \{u_5, v_4\}, N^+(u_4) = \{u, u_6\}$.

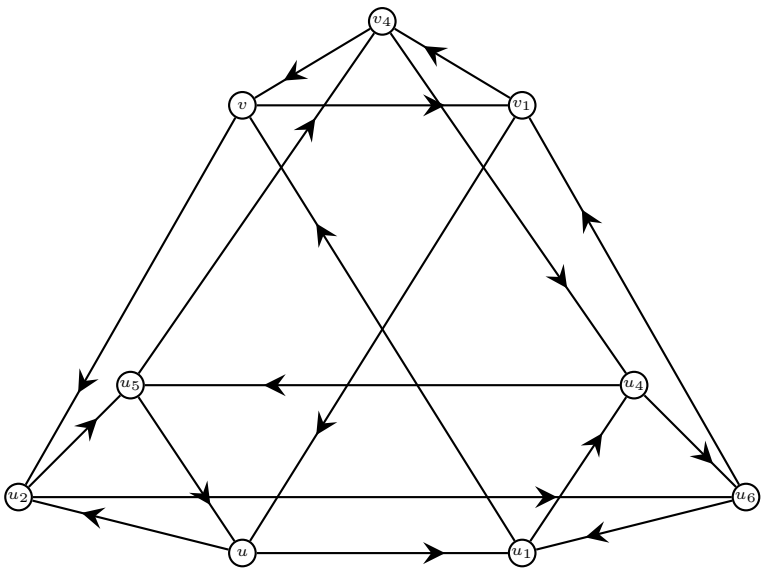

Figure 6.7: A second $(2, 2; +2)$-digraph

Case 2.a): $\mathbf{O(u_1) = \{u, v_4\}, N^+(u_4) = \{u_5, u_6\}}$

As $v_4 \in O(u) \cap O(u_1)$, u_2 can reach v_4 and without loss of generality $v_4 \in N^+(u_5)$. $N^+(u_2) = N^+(u_4)$, so by Lemma 6.3 $u_2 \in O(u_4), u_4 \in O(u_2), u_5 \in O(u_6)$ and $u_6 \in O(u_5)$. Hence $u_4 \in O(v) \cap O(u_2)$, so v_1 can reach u_4, so $u_4 \in N^+(v_4)$. Neither u_5 nor u_6 lies in $N^+(v_4)$, so $O(v_1) = \{u_5, u_6\}$ and $N^+(v_4) = \{u_4, v\}$. Hence $O(v_4) = \{u, u_1\}$. Observe that $N^+(u_1) = N^+(v_4)$, so that $v \in O(u_4)$. Therefore $v \notin N^+(u_5) \cup N^+(u_6)$, yielding $O(u_2) = \{u_4, v\}, N^2(u_2) = \{v_4, v_1, u, u_1\}$. As $v_1 \to v_4$ and $N^+(u_1) = N^+(v_4)$, we must have $N^+(u_5) = \{v_4, u\}, N^+(u_6) = \{v_1, u_1\}$. This yields the digraph in Figure 6.7. Unlike the digraph in Figure 6.4, this digraph contains pairs of vertices with identical out-neighbourhoods, so the two are not isomorphic.

Case 2.b): $\mathbf{O(u_1) = \{u, u_5\}, N^+(u_4) = \{u_6, v_4\}}$

As $u_4 \to v_4$, $u_4 \notin N^+(v_4)$, so $u_4 \in O(v_1)$. Hence $u_4 \in O(v) \cap O(v_1)$, so u_2 can reach u_4. As $u_4 \to u_6$, we must have $u_5 \to u_4$. u_2 and u_4 have u_6 as a common out-neighbour, so $v_4 \in O(u_2), u_5 \in O(u_4)$. Therefore $v_4 \in O(u) \cap O(u_2)$, so that u_6 can reach v_4, but $v_4 \notin T(u_6)$, so $N^+(u_6)$ contains an in-neighbour of v_4. $u_4 \notin N^+(u_6)$, so we must have $u_6 \to v_1$. We have $u_5 \in O(u_4) \cap O(u_1)$, so v_1 can reach u_5 and hence $v_4 \to u_5$. v_1 cannot reach u_6, as $u_2, u_4 \notin T(v_1)$, so $O(v_1) = \{u_4, u_6\}, N^+(v_4) = \{u_5, v\}$. Now u_2 and v_4 have u_5 as a unique common out-neighbour, so $u_6 \in O(v_4), v \in O(u_2)$. Thus $O(u_2) = \{v, v_4\}$ and $N^2(u_2) = \{u_4, v_1, u, u_1\}$. Taking into account adjacencies between members of $N^2(u_2)$, it follows that $N^+(u_5) = \{u_4, u\}, N^+(u_6) = \{u_1, v_1\}$. However, u_2, u_4 now constitutes a bad pair, contradicting our assumption.

Case 2.c): $\mathbf{O(u_1) = \{u_5, u_6\}, N^+(u_4) = \{u, v_4\}}$

As $u_4 \to v_4$, $u_4 \notin N^+(v_4)$. Hence $u_4 \in O(v) \cap O(v_1)$, implying that u_2 can reach u_4. Without loss of generality, $u_5 \to u_4$. There are three possibilities: i) $O(v_1) = \{u_4, u_6\}, N^+(v_4) = \{v, u_5\}$, ii) $O(v_1) = \{u_4, u_5\}, N^+(v_4) = \{v, u_6\}$ and iii) $O(v_1) = \{u_4, v\}, N^+(v_4) = \{u_5, u_6\}$.

i) $O(v_1) = \{u_4, u_6\}, N^+(v_4) = \{v, u_5\}$

u_1 and v_4 have v as a unique common out-neighbour, so $u_4 \in O(v_4)$. However, this contradicts $v_4 \to u_5 \to u_4$.

ii) $O(v_1) = \{u_4, u_5\}, N^+(v_4) = \{v, u_6\}$

Neither u_4 nor v_1 lie in $T(u_2)$, so $v_4 \in O(u_2)$. Now observe that u_2 and v_4 have u_6 as unique common out-neighbour, so $v \in O(u_2)$, yielding $O(u_2) = \{v, v_4\}$ and $N^2(u_2) = \{u_4, u_1, u, v_1\}$. As $u_4 \to u$ and $u \to u_1$, we must have $N^+(u_5) = \{u_4, u_1\}, N^+(u_6) = \{u, v_1\}$, a contradiction, since $u_1 \to u_4$.

iii) $O(v_1) = \{u_4, v\}, N^+(v_4) = \{u_5, u_6\}$

We now have $N^+(u_2) = N^+(v_4)$, so $u_2 \in O(v_4), v_4 \in O(u_2), u_5 \in O(u_6), u_6 \in O(u_5)$. Also $N^+(u_4) = N^+(v_1)$, so $u_4 \in O(v_1), v_1 \in O(u_4)$ and $u \in O(v_4)$. $u \in O(v_4)$ implies that $u \notin N^+(u_5) \cup N^+(u_6)$, so we see that $u \in O(u_2)$ and hence $O(u_2) = \{u, v_4\}$ and $N^2(u_2) = \{u_4, u_1, v, v_1\}$. As $u_1 \to u_4$ and $u_1 \to v$, we have $N^+(u_5) = \{u_4, v\}, N^+(u_6) = \{u_1, v_1\}$. It is not difficult to show that this yields a $(2,2,+2)$-digraph isomorphic to that in Figure 6.7.

Case 2.d): $\mathbf{O(u_1) = \{u_5, v_4\}, N^+(u_4) = \{u, u_6\}}$

In this case $v_4 \in O(u) \cap O(u_1)$, so u_2 can reach v_4. u_4 and v_1 have unique common out-neighbour u, so $v_4 \in O(u_4), u_6 \in O(v_1)$. If $u_6 \to v_4$, then we would have $u_4 \to u_6 \to v_4$, contradicting $v_4 \in O(u_4)$, so $u_5 \to v_4$. This also implies that $u_5 \notin N^+(v_4)$, so $u_5 \in O(v_1)$, yielding $O(v_1) = \{u_5, u_6\}$ and $N^+(v_4) = \{v, u_4\} = N^+(u_1)$. Now $v_4, u_1 \notin T(u_2)$, so $O(u_2) = \{v, u_4\}$ and $N^2(u_2) = \{v_1, v_4, u, u_1\}$. As $v_1 \to v_4$ and $v_1 \to u$, it follows that $N^+(u_5) = \{v_4, u\}, N^+(u_6) = \{u_1, v_1\}$. However, we now have paths $u_4 \to u \to u_1$ and $u_4 \to u_6 \to u_1$, which is impossible.

Case 3: $\mathbf{N^+(u_1) = N^+(v_1)}$

It is easy to see by 2-geodecity that $V(G) = \{u, u_1, u_2, u_3, u_4, u_5, u_6, v, v_1\}$, $O(u) = \{v, v_1\}$ and $O(v) = \{u, u_1\}$. As $u_1, v_1 \notin T(u_2)$, we have $O(u_2) = \{u_3, u_4\}$ and $N^2(u_2) = \{u, u_1, v, v_1\}$. Without loss of generality, $N^+(u_5) = \{u, v_1\}, N^+(u_6) = \{v, u_1\}$. u and v have in-neighbours apart from u_5 and u_6 respectively, so without loss of generality $u_3 \to u, u_4 \to v$. Likewise, u_5 and u_6 have in-neighbours other than u_2, so, as $u_5 \to u$ and $u_6 \to v$, we must have $N^+(u_3) = \{u, u_6\}, N^+(u_4) = \{v, u_5\}$. But now we have paths $u_3 \to u \to u_1$ and $u_3 \to u_6 \to u_1$, violating 2-geodecity.

Corollary 6.19. *There is a unique $(2, 2; +2)$-digraph containing no bad pairs.*

This completes our analysis of diregular $(2, 2; +2)$-digraphs and, by the results of the preceding chapter, we have now classified all $(2, 2, ; +2)$-digraphs. By Theorem 5.2 smallest non-diregular $(2, 2; +\epsilon)$-digraphs have excess $\epsilon = 3$.

6.4 Diregular digraphs with degree two and excess three

In the preceding sections we succeeded in classifying all digraphs with out-degree two and excess two. We will now bring the approach of Section 6.2 to bear on diregular digraphs with out-degree two and excess three to prove the following result.

Theorem 6.20. *There are no diregular $(2, k; +3)$-digraphs for $k \geq 4$.*

Therefore in this section G will stand for a diregular $(2, k; +3)$-digraph for some $k \geq 3$. We will show now that there are no diregular $(2, k; +3)$ digraphs for $k \geq 4$; the case $k = 3$ is dealt with separately in the next section.

An important step in our argument for $(2, k; +2)$-digraphs was to find a pair of vertices with exactly one common out-neighbour. We accomplished this for even ϵ in Lemma 6.2. This is slightly more difficult for odd ϵ; for $\epsilon = 3$ we can accomplish this using Heuchenne's characterisation of line digraphs [88], which tells us that a digraph is a line digraph if and only if any two out-neighbourhoods are either disjoint or identical, i.e. if and only if the out-neighbourhoods constitute a partition of $V(G)$.

Theorem 6.21. *For $k \geq 3$, any diregular $(2, k; +3)$-digraph G contains a pair of vertices u, v with exactly one common out-neighbour.*

Proof. Let G be a diregular $(2, k; +3)$-digraph without the required pair of vertices.

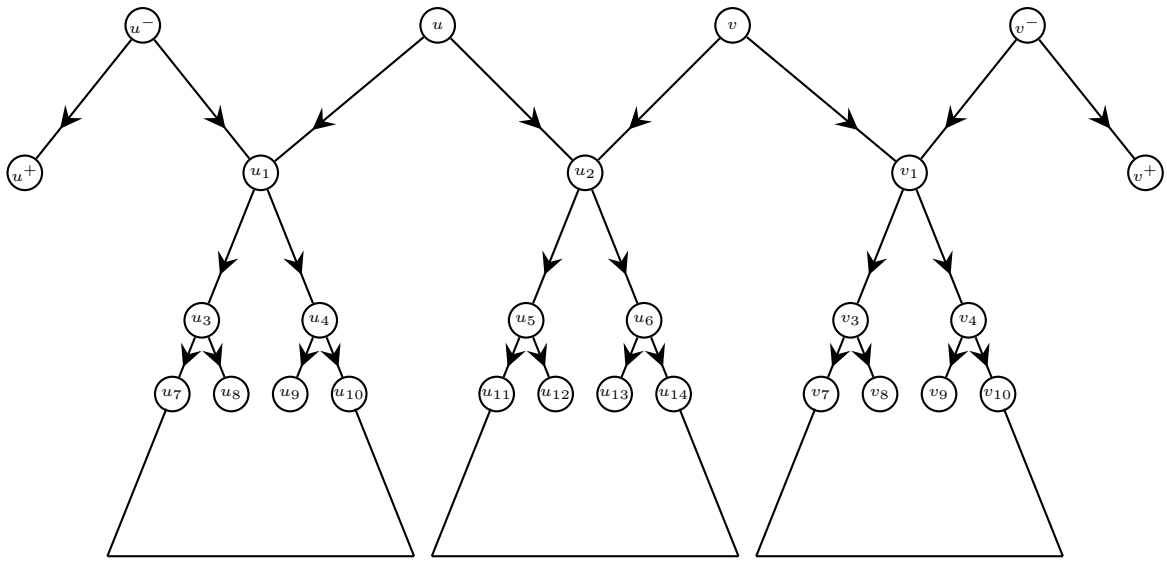

Figure 6.8: Configuration for $k \geq 3$

Then all out-neighbourhoods are either disjoint or identical. Then by Heuchenne's condition G is the line digraph of a digraph H with degree two [88]. H must be at least $(k-1)$-geodetic. As $2|V(H)| = |V(G)|$, H must be a $(2, k-1; +2)$-digraph. Since the line digraphs of the $(2,2)$-geodetic-cages derived in Section 6.3 are not 3-geodetic and there are no $(2, k; +2)$-digraphs for $k \geq 3$ by Theorem 6.4, we have a contradiction. □

We have seen that there exists a $(2,2)$-cage in which distinct vertices share identical out-neighbourhoods. We will therefore need the following trivial extension of Lemma 6.3 (the proof is similar, so we omit it).

Lemma 6.22. *Let z, z' be vertices of a $(d, k; +\epsilon)$-digraph H for some $\epsilon \geq 1$. If $N^+(z) = N^+(z')$, then there exists a set X of $\epsilon - 1$ vertices of H such that $O(z) = \{z'\} \cup X, O(z') = \{z\} \cup X$.*

We now fix an arbitrary pair of vertices u, v of G with a unique out-neighbour in common. We will assume that $u_2 = v_2$, so that, following the vertex labelling convention established earlier, we have the situation shown in Figure 6.8. We will also write $N^-(u_1) = \{u, u^-\}, N^-(v_1) = \{v, v^-\}, N^+(u^-) = \{u_1, u^+\}$ and $N^+(v^-) = \{v_1, v^+\}$. It is easily seen that $u^- \neq v, v^- \neq u$.

We can make some immediate deductions concerning the position of the vertices u, v and u_2 in the diagram in Figure 6.8.

Lemma 6.23. *$v \in N^{k-1}(u_1) \cup O(u)$ and $u \in N^{k-1}(v_1) \cup O(v)$. If $v \in O(u)$, then $u_2 \in O(u_1)$ and if $u \in O(v)$, then $u_2 \in O(v_1)$.*

Proof. v cannot lie in $T(u)$, or the vertex u_2 would be repeated in $T_k(u)$. Also, $v \notin T(u_2)$, or there would be a $\leq k$-cycle through v. Therefore, if $v \notin O(u)$, then $v \in N^{k-1}(u_1)$. Likewise for the other result. If $v \in O(u)$, then neither in-neighbour of u_2 lies in $T(u_1)$, so that $u_2 \in O(u_1)$. □

The following lemma is the main tool in our analysis.

Lemma 6.24 (Contraction Lemma)**.** *Let $w \in T(v_1)$, with $d(v_1, w) = l$. Suppose that $w \in T(u_1)$, with $d(u_1, w) = m$. Then either $m \leq l$ or $w \in N^{k-1}(u_1)$. A similar result holds for $w \in T(u_1)$.*

Proof. Let w be as described and suppose that $m > l$. Consider the set $N^{k-m}(w)$. By construction, $N^{k-m}(w) \subseteq N^k(u_1)$, so by k-geodecity $N^{k-m}(w) \cap T(u_1) = \emptyset$. At the same time, we have $l + k - m \leq k - 1$, so $N^{k-m}(w) \subseteq T(v_1)$. This implies that $N^{k-m}(w) \cap T(v_2) = N^{k-m}(w) \cap T(u_2) = \emptyset$. As $V(G) = \{u\} \cup T(u_1) \cup T(u_2) \cup O(u)$, it follows that $N^{k-m}(w) \subseteq \{u\} \cup O(u)$. Therefore $|N^{k-m}(w)| = 2^{k-m} \leq 4$, so either $m = k - 1$ or $m = k - 2$. Suppose that $m = k - 2$; then $N^2(w) = \{u\} \cup O(u)$. Neither v nor v_1 lies in $N^2(w)$, so that neither v nor v_1 lies in $O(u)$. By k-geodecity and Lemma 6.23, $v \in N^{k-1}(u_1)$ and $v_1 \in T(u_1)$, so that v_1 appears twice in $T_k(u_1)$. Thus $m = k - 1$. □

The Contraction Lemma has the following immediate consequence.

Corollary 6.25. *If $w \in T(v_1)$, then either $w \in \{u\} \cup O(u)$ or $w \in T(u_1)$ with $d(u_1, w) = k - 1$ or $d(u_1, w) \leq d(v_1, w)$.*

This allows us to restrict the possible positions of u_1 and v_1 in Figure 6.8.

Corollary 6.26. *$v_1 \in N^{k-1}(u_1) \cup O(u)$ and $u_1 \in N^{k-1}(v_1) \cup O(v)$.*

Proof. We prove the first inclusion. By Corollary 6.25, $v_1 \in \{u\} \cup O(u) \cup \{u_1\} \cup N^{k-1}(u_1)$. By k-geodecity $v_1 \neq u$ and by construction $v_1 \neq u_1$. □

Corollary 6.27. *If $v_1 \notin O(u)$, then $O(u) = \{v, v_3, v_4\}$, with a similar result for v.*

Proof. Suppose that $v_1 \notin O(u)$, so that $v_1 \in N^{k-1}(u_1)$ by Corollary 6.26. If $v \notin O(u)$, then by Lemma 6.23 we would have $v \in N^{k-1}(u_1)$, so that u_1 has a path of length k

to v_1; however, as u_1 has a path of length $k-1$ to v_1, this would violate k-geodecity. As a result, we must conclude that if $v_1 \notin O(u)$, then $v \in O(u)$.

Consider now the vertex v_3. By k-geodecity, $v_3 \notin \{u\} \cup T(u_2)$, so if $v_3 \notin O(u)$, then $v_3 \in T(u_1)$; however, as u_1 has a path of length k to v_3 via v_1, this again violates k-geodecity. Therefore $v_3 \in O(u)$ and similarly $v_4 \in O(u)$. There are three vertices in $O(u)$, so we must have $O(u) = \{v_1, v_3, v_4\}$ if $v_1 \notin O(u)$. □

Lemma 6.28. *For $k \geq 3$, either $v_1 \in O(u)$ or $u_1 \in O(v)$.*

Proof. Suppose that $O(u) = \{v, v_3, v_4\}, O(v) = \{u, u_3, u_4\}$. By the Neighbourhood Lemma,

$$O(\{u_1, u_2\}) = O(N^+(u)) = N^+(O(u)) = \{u_2, v_1, v_7, v_8, v_9, v_{10}\}$$

and

$$O(\{v_1, u_2\}) = O(N^+(v)) = N^+(O(v)) = \{u_2, u_1, u_7, u_8, u_9, u_{10}\}.$$

By Corollary 6.26, $v_1 \in N^{k-1}(u_1)$ and $u_1 \in N^{k-1}(v_1)$, so we must have $u_1, v_1 \in O(u_2)$. As $O(u_2) \subset N^+(O(u))$, it follows that $u_1 \in N^2(v_1)$, so $k \leq 3$. Now set $k = 3$. We can put $u_9 = v_1, v_9 = u_1$. As $N^2(v_1) \cap O(u) = \emptyset$ and $u \notin N^2(v_1)$, $\{v_7, v_8, v_{10}\} = \{u_7, u_8, u_{10}\}$. $u_{10} \in N^2(v_1)$ implies that there are two distinct ≤ 3-paths from u_4 to u_{10}, contradicting 3-geodecity. □

We will now identify an outlier of u and v using the Neighbourhood Lemma.

Theorem 6.29. *For $k \geq 3$, $v_1 \in O(u)$ and $u_1 \in O(v)$.*

Proof. Assume for a contradiction that $O(v) = \{u, u_3, u_4\}$ and $v_1 \in O(u)$. Let $k \geq 4$. v can reach u_1 by a $\leq k$-path, so by Corollary 6.26 $u_1 \in N^{k-1}(v_1)$. Suppose that $x \in (T_{k-2}(u_1) - \{u_1\}) \cap N^{k-1}(v_1)$ and write $N^+(x) = \{x_1, x_2\}$. Clearly $x_1, x_2 \notin \{u, u_3, u_4\}$, so $x_1, x_2 \in T_k(v)$. However, by k-geodecity $x_1, x_2 \notin T(u_2) \cup T(v_1)$, so we are forced to conclude that $x_1 = x_2 = v$, which is absurd. It follows from the Contraction Lemma that for any vertex $w \in T_{k-2}(u_1) - \{u_1, u_3, u_4\}$ we have $d(u_1, w) = d(v_1, w)$. In particular, $N^2(u_1) = N^2(v_1)$. However, as $u_1 \in N^{k-1}(v_1)$, this implies the existence of a $(k-1)$-cycle through u_1.

Now set $k = 3$. We can put $v_9 = u_1$. $N^2(u_1) \cap O(v) = \emptyset$, so $N^2(u_1) \subset \{v, v_3, v_4, v_7, v_8, v_{10}\}$. v_4 has paths of length 3 to every vertex in $N^2(u_1)$, so

$v_4, v_{10} \notin N^2(u_1)$, yielding $N^2(u_1) = \{v, v_3, v_7, v_8\}$. Without loss of generality, $u_7 = v_3$. $u_7 \not\to u_8$, so $u_8 = v$ and $N^+(v_3) = N^+(u_7) = N^+(u_4)$, which is impossible. □

The next stage of our approach is to show that exactly one member of $N^+(v_1)$ is also an outlier of u and similarly for v. This will be accomplished by analysing the possible positions of u_3, u_4, v_3, v_4 in Figure 6.8. The possibilities are described in the following lemma.

Lemma 6.30. *For $k \geq 4$, $\{u_3, u_4\} \subset \{v_3, v_4\} \cup O(v)$ and $\{v_3, v_4\} \subset \{u_3, u_4\} \cup O(u)$.*

Proof. Let $u_3 \notin N^+(v_1) \cup O(v)$. By Corollary 6.25 and Theorem 6.29, $u_3 \in N^{k-1}(v_1)$. By k-geodecity, $u_7, u_8 \notin T(u_2) \cup T(v_1)$. Also for $k \geq 4$ we cannot have $v \in N^+(u_3)$. Therefore $O(v) = \{u_1, u_7, u_8\}$. Hence v can reach u_4 by a $\leq k$-path. We cannot have $u_4 \in N^{k-1}(v_1)$, or the same argument would imply that $N^+(u_4) \subset O(v) = \{u_1, u_7, u_8\}$. By Corollary 6.25 we can assume that $u_4 = v_4$. As $u \notin O(v)$, $u \in N^{k-1}(v_1)$. Since $u_4 = v_4$, to avoid k-cycles we must conclude that $u \in N^{k-2}(v_3)$. Likewise $u_3 \in N^{k-2}(v_3)$. However, as there is a path $u \to u_1 \to u_3$, v_3 has a $(k-2)$-path and a k-path to u_3, which violates k-geodecity. □

Firstly, we show using the Neighbourhood Lemma that $O(u)$ does not contain both out-neighbours of v_1 and vice versa.

Lemma 6.31. *For $k \geq 4$, $N^+(u_1) \cap N^+(v_1) \neq \emptyset$.*

Proof. Suppose that $\{u_3, u_4\}$ and $\{v_3, v_4\}$ are disjoint. Then by Theorem 6.29 and Lemma 6.30 we have $O(u) = \{v_1, v_3, v_4\}, O(v) = \{u_1, u_3, u_4\}$. The Neighbourhood Lemma yields

$$N^+(O(v)) = \{u_3, u_4, u_7, u_8, u_9, u_{10}\} = O(v_1) \cup O(u_2).$$

Recall that $N^-(u_1) = \{u^-, u\}$, $N^-(v_1) = \{v^-, v\}$, $N^+(u^-) = \{u_1, u^+\}$ and $N^+(v^-) = \{v_1, v^+\}$. Then as $u_2 \notin \{u^+, v^+\}$, it follows by Theorem 6.29 that $u^+ \in O(u)$ and $v^+ \in O(v)$. If $u^+ = v_1$, then, as $T(u_2) \cap (T(u_1) \cup T(v_1)) = \emptyset$, examining $T_k(u^-)$ we see that we would have $T(u_2) \subseteq \{u^-\} \cup O(u^-)$, so that $M(2, k-1) \leq 4$, which is impossible. Without loss of generality, $u^+ = v_3, v^+ = u_3$. Then v_1 and u^- have v_3 as a unique common out-neighbour, so by Theorem 6.29

$$u_1 \in O(v_1) \subset \{u_3, u_4, u_7, u_8, u_9, u_{10}\},$$

which contradicts k-geodecity. □

It will now be demonstrated that u cannot reach both out-neighbours of v_1 by $\leq k$-paths, so that $O(u)$ contains exactly one out-neighbour of v_1, again with a similar result for v.

Lemma 6.32. *For $k \geq 4$, $N^+(u_1) \neq N^+(v_1)$.*

Proof. Let $N^+(u_1) = N^+(v_1) = \{u_3, u_4\}$. If u can reach v by a $\leq k$-path, so that $v \in N^{k-1}(u_1)$, then there would be a k-cycle through v, so $v \in O(u)$ and $u \in O(v)$. Hence by Lemmas 6.22 and 6.23, there exists a vertex x such that $O(u_1) = \{v_1, u_2, x\}$ and $O(v_1) = \{u_1, u_2, x\}$. Since $u_1, v_1 \notin T(u_2)$, $u_3, u_4 \in O(u_2)$. Applying Theorem 6.29 to the pairs u, u^- and u, v, we see that $u^+, v_1 \in O(u)$. As $N^+(u_1) = N^+(v_1)$, we cannot have $u^+ \in \{v, v_1\}$. Therefore $O(u) = \{v, v_1, u^+\}$ and similarly $O(v) = \{u, u_1, v^+\}$.

Suppose that $u^+ = v^+$. Then u^- and v^- have a single common out-neighbour, so that $v_1 \in O(u^-), u_1 \in O(v^-)$. Hence $u_1 \in O(v) \cap O(v_1) \cap O(v^-)$. As G is diregular, a simple counting argument shows that every vertex is an outlier of exactly three distinct vertices. As $u_2 \notin \{v, v_1, v^-\}$, it follows that u_2 can reach u_1 by a k-path; likewise u_2 can reach v_1. Therefore $u^-, v^- \in N^{k-1}(u_2)$; however, as $u^+ = v^+$, this is impossible. Hence $u^+ \neq v^+$.

The Neighbourhood Lemma gives

$$N^+(O(u)) = \{v_1, u_2, u_3, u_4\} \cup N^+(u^+) = O(u_1) \cup O(u_2)$$

and

$$N^+(O(v)) = \{u_1, u_2, u_3, u_4\} \cup N^+(v^+) = O(v_1) \cup O(u_2).$$

It follows that $O(u_2)$ contains a vertex $z \in N^+(u^+) \cap N^+(v^+)$. Therefore $u^+, v^+ \notin T(u_2)$. Examining $T_k(u^-)$, we see that u^+ does not lie in $T(u_1) - \{u_1\} = T(v_1) - \{v_1\}$. As already mentioned, $u^+ \neq v, v_1$. Therefore v cannot reach u^+ by a $\leq k$-path, so $u^+ \in O(v) = \{u, u_1, v^+\}$, a contradiction. □

Since u, v was an arbitrary pair of vertices with a unique common out-neighbour, Lemmas 6.30, 6.31 and 6.32 imply the following result.

Corollary 6.33. *For $k \geq 4$, if u, v are vertices with a single out-neighbour u_2 in common, then $v_1 \in O(u), u_1 \in O(v)$ and $|O(u) \cap N^+(v_1)| = |O(v) \cap N^+(u_1)| = 1$.*

Thanks to Corollary 6.33 we can assume that $u_3 = v_3$, $u_4 \neq v_4$, $v_1, v_4 \in O(u)$ and $u_1, u_4 \in O(v)$. Repeated applications of Corollary 6.33 allow us to prove that there are no diregular $(2, k; +3)$-digraphs for $k \geq 4$ by inductively identifying outliers of u_2.

Theorem 6.20. *There are no diregular $(2, k; +3)$-digraphs for $k \geq 4$.*

Proof. Let $k \geq 5$. As $u_3 \in N^+(u_1) \cap N^+(v_1)$, $u_3 \in O(u_2)$. The pair u_1, v_1 have u_3 as a unique common out-neighbour, so by Corollary 6.33 we can assume that $u_9 = v_9$, $u_{10} \neq v_{10}$. $u_4, v_4, u_9 \notin T(u_2)$, so $u_9 \in O(u_2)$. The pair u_4, v_4 have u_9 as a unique common out-neighbour, so we can assume that $u_{21} = v_{21}, u_{22} \neq v_{22}$. As $u_{10}, v_{10}, u_{21} \notin T(u_2)$, $u_{21} \in O(u_2)$. Continuing further we see that $u_{45} \in O(u_2)$. In fact, it follows inductively that $O(u_2)$ contains at least $k - 1$ distinct vertices, which is impossible, as G has excess $\epsilon = 3$.

Now set $k = 4$. By the foregoing reasoning, we can write $O(u_2) = \{u_3, u_9, u_{21}\}, O(u) = \{v_1, v_4, z\}, O(v) = \{u_1, u_4, z'\}$ for some vertices z, z' and assume that $u_3 = v_3, u_9 = v_9, u_{21} = v_{21}$ and that u_{22} and v_{22} have a single common out-neighbour. By 4-geodecity, $u, v, u_1, v_1, u_4, v_4 \notin O(u_2)$. Taking into account adjacencies among u, v, u_1 and v_1, we can assume that $u_{23} \to u, u_{25} \to v_1, u_{27} \to v$ and $u_{29} \to u_1$. As $u_1 \to u_4$, $u_4 \notin N^3(u_6)$. If $u_4 \in N^2(u_{11})$, then u_{11} has two distinct ≤ 4-paths to u_4. Thus $u_4 \in N^2(u_{12})$. However, now there are distinct ≤ 4-paths from u_{12} to u_9, violating 4-geodecity. □

6.5 Classification of $(2, 3; +3)$-digraphs

The methods of Section 6.4 do not settle the issue of the existence of a $(2, 3; +3)$-digraph. We now demonstrate how these ideas can be extended to show that there are no such digraphs.

Let G be a diregular $(2, 3; +3)$-digraph and fix an arbitrary pair of vertices u and v with a single out-neighbour u_2 in common. Theorem 6.29 identifies v_1 as an outlier of u and u_1 as an outlier of v. As in the preceding section, we will analyse the possible positions of u_3, u_4, v_3 and v_4 in $T_3(u)$ and $T_3(v)$. Our first goal is to show that at least one out-neighbour of v_1 is an outlier of u and vice versa. Call a pair of vertices u, v with $|N^+(u) \cap N^+(v)| = 1$ *bad* if either $O(u) \cap N^+(v_1) = \emptyset$ or $O(v) \cap N^+(u_1) = \emptyset$. Suppose that G contains a bad pair u, v; without loss of generality $u_3, u_4 \in T(v_1) - \{v_1\}$.

Lemma 6.34. *If G contains a bad pair, then $|\{u_3, u_4\} \cap N^2(v_1)| \leq 1$.*

Proof. Suppose that $u_3, u_4 \in N^2(v_1)$. By 3-geodecity applied to $T_3(v_1)$ and $T_3(u)$, we have $N^2(u_1) \cap T(v_1) = N^2(u_1) \cap T(u_2) = \emptyset$, so that $N^2(u_1) = \{v\} \cup O(v)$. As $u_1 \in O(v)$, there would thus be a 2-cycle through u_1. □

As at most one vertex in $\{u_3, u_4\}$ can lie in $N^2(v_1)$ by Lemma 6.34 and there is no arc between u_3 and u_4, we can make the following assumption.

Corollary 6.35. *If u, v is a bad pair, then without loss of generality either $u_3 = v_3, u_4 = v_4$ or $u_3 = v_3, u_4 = v_9$.*

Lemma 6.36. *If u, v is a bad pair, then we can assume that $u_3 = v_3, u_4 = v_4$.*

Proof. Let $u_3 = v_3, u_4 = v_9$. u_1 and v_1 have u_3 as unique common out-neighbour, so by Theorem 6.29 $u_4 \in O(v_1)$, whereas there is a 2-path from v_1 to u_4. □

Theorem 6.37. *There are no bad pairs.*

Proof. $u, v \notin T(u_1) - \{u_1\} = T(v_1) - \{v_1\}$, so $O(u) = \{v, v_1, x\}, O(v) = \{u, u_1, x\}$ for some vertex x. By the Neighbourhood Lemma

$$O(u_1) \cup O(u_2) = \{u_2, v_1, u_3, u_4\} \cup N^+(x) \text{ and } O(v_1) \cup O(u_2) = \{u_2, u_1, u_3, u_4\} \cup N^+(x).$$

As u_1 can reach u_3 and u_4, we have $u_3, u_4 \in O(u_2)$. Applying Lemma 6.22 to u_1 and v_1, we see that $u_1 \in O(v_1), v_1 \in O(u_1), u_3 \in O(u_4), u_4 \in O(u_3)$. Therefore

$$O(u_1) = \{u_2, v_1, x_1\}, O(u_2) = \{u_3, u_4, x_2\}, O(v_1) = \{u_2, u_1, x_1\},$$

where $N^+(x) = \{x_1, x_2\}$. Let $N^-(u_1) = \{u, u^-\}$ and $N^-(v_1) = \{v, v^-\}$. Obviously $|N^+(u) \cap N^+(u^-)| = |N^+(v) \cap N^+(v^-)| = 1$, so $u_2 \in O(u_1) \cap O(v_1) \cap O(u^-) \cap O(v^-)$. $u^-, v^- \notin \{u_1, v_1\}$, so it follows that $u^- = v^-$ and $N^+(u^-) = \{u_1, v_1\}$. As $N^+(u_1) = N^+(v_1)$, this contradicts 3-geodecity. □

Theorem 6.37 shows that we can assume that $v_1, v_4 \in O(u)$ and $u_1, u_4 \in O(v)$. The next step is to show that u has exactly one outlier in $N^+(v_1)$ and v has exactly one outlier in $N^+(u_1)$.

Lemma 6.38. *Either $O(u) \neq T_1(v_1)$ or $O(v) \neq T_1(u_1)$.*

Proof. Let $O(u) = \{v_1, v_3, v_4\}$ and $O(v) = \{u_1, u_3, u_4\}$. Applying the Neighbourhood Lemma to u and v yields $N^+(O(u)) = \{v_3, v_4, v_7, v_8, v_9, v_{10}\} = O(u_1) \cup O(u_2)$ and

$N^+(O(v)) = \{u_3, u_4, u_7, u_8, u_9, u_{10}\} = O(v_1) \cup O(u_2)$. If $u_3 \in O(u_2)$, then $u_3 \in \{v_3, v_4, v_7, v_8, v_9, v_{10}\}$, contradicting $u_3 \in O(v)$. Similarly $u_4, v_3, v_4 \notin O(u_2)$. We can thus assume that

$$O(u_1) = \{v_3, v_4, v_7\}, O(u_2) = \{u_8, u_9, u_{10}\} = \{v_8, v_9, v_{10}\}, O(v_1) = \{u_3, u_4, u_7\}.$$

As $v \notin O(u)$, $v \in N^2(u_1)$. $\{u_8, u_9, u_{10}\} = \{v_8, v_9, v_{10}\}$ implies that $v = u_7$. Likewise $u = v_7$. Therefore $N^3(u_2) = \{u, u_1, u_3, u_4, u_7 = v, v_1, v_3, v_4\}$. u and v have a common out-neighbour, so we can set $u_{11} \to u, u_{13} \to v$. We have $u \to u_1$, so $u_1 \in N^2(u_6)$. If $u_{13} \to u_1$, then u_{13} would have two ≤ 3-paths to v, so $u_{14} \to u_1$ and similarly $u_{12} \to v_1$. $v_1 \in N^2(u_5)$ implies that $v_3, v_4 \in N^2(u_6)$. u_{13} can already reach v_3 and v_4 by 3-paths via v, so we are forced to conclude that $N^+(u_{14}) = \{v_3, v_4\}$, contradicting $u_{14} \to u_1$. □

Lemma 6.39. *$O(u) \neq T_1(v_1)$ and $O(v) \neq T_1(u_1)$.*

Proof. By the preceding lemma at least one of these inequalities is valid. Let $O(u) = \{v_1, v_3, v_4\}$ and $u_1, u_3 \in O(v)$ but $u_4 \notin O(v)$. u_4 must lie in $N^2(u_1)$, say $u_4 = v_7$. We have $\{v, v_8, v_9, v_{10}\} \subseteq \{u, u_7, u_8, u_9, u_{10}\}$. As $u_4 = v_7$, $N^+(u_4) \cap \{v_8, v_9, v_{10}\} = \emptyset$, so $u_4 \to v$, say $u_9 = v$, and $\{v_8, v_9, v_{10}\} = \{u, u_7, u_8\}$. If $v_8 = u$, then v_3 would have two distinct ≤ 3-paths to u_4; hence we can set $u = v_9, u_7 = v_8, u_8 = v_{10}$. As u_1 and v_3 have unique common out-neighbour u_4, from Theorem 6.29 it follows that $u_7 \in O(u_1)$, which is plainly false. □

By Theorem 6.37 $O(u)$ contains v_1 and at least one vertex of $N^+(v_1)$, but Lemma 6.39 shows that $O(u) \neq \{v_1\} \cup N^+(v_1)$, so that we must have $|O(u) \cap N^+(v_1)| = 1$, with a similar result for v.

Corollary 6.40. *$|O(u) \cap N^+(v_1)| = |O(v) \cap N^+(u_1)| = 1$.*

Without loss of generality, we can assume that $u_3 \in T_3(v)$, $v_3 \in T_3(u)$, $u_4 \in O(v)$ and $v_4 \in O(u)$. There are now two possibilities, depending upon the distance from v to u_3: either $u_3 = v_3$ or we can put $u_3 = v_9, v_3 = u_9$.

Case 1: $u_3 = v_3$

We can define the vertex x by $O(u) = \{v_1, v_4, x\}$. Also $u_1, u_4 \in O(v)$. Let $N^+(x) = \{x_1, x_2\}$. As $v, v_9, v_{10} \notin \{v_1, v_4\}$, there are three essentially different possibilities: a) $x \notin \{v, v_9, v_{10}\}$, b) $x = v$ and c) $x = v_9$.

Case 1.a): $x \notin \{v, v_9, v_{10}\}$

In this case $O(u) = \{v_1, v_4, x\}, O(v) = \{u_1, u_4, x\}$. u can reach each of v, v_9, v_{10}, so $\{v, v_9, v_{10}\} = \{u, u_9, u_{10}\}$. We can assume that $u = v_9, v = u_9$ and $u_{10} = v_{10}$. It is obvious that $u_3, u_{10} \in O(u_2)$. u_1 and v_1 have the single out-neighbour u_3 in common, so $v_4, u \in O(u_1), u_4, v \in O(v_1)$. Applying the Neighbourhood Lemma to u and v, $N^+(O(u)) = O(u_1) \cup O(u_2) = \{u_3, v_4, u, u_{10}, x_1, x_2\}$, and $N^+(O(v)) = O(v_1) \cup O(u_2) = \{u_3, u_4, v, u_{10}, x_1, x_2\}$, so without loss of generality $O(u_1) = \{u, v_4, x_1\}, O(u_2) = \{u_3, u_{10}, x_2\}$ and $O(v_1) = \{u_4, v, x_1\}$. Now, $u^+ \in O(u) = \{v_1, v_4, x\}$ and by 3-geodecity $u^+ \neq v_1, v_4$, so that $u^+ = x$. Similarly $v^+ = x$, so by 3-geodecity applied to u^- and v^-, $x_2 \in T(u_2)$, contradicting $x_2 \in O(u_2)$.

Case 1.b): $x = v$

Now $O(u) = \{v, v_1, v_4\}$. v_9 and v_{10} are not outliers of u, so $N^+(u_4) \cap N^+(v_4) \neq \emptyset$. By Theorem 6.29, $u^+ \in O(u) = \{v, v_1, v_4\}$, so that u^- has distinct ≤ 3-paths to either u_3 or a vertex in $N^+(u_4) \cap N^+(v_4)$.

Case 1.c): $x = v_9$

In this case $O(u) = \{v_1, v_4, v_9\}$. As $v_{10} \notin O(u)$, without loss of generality, either i) $v_{10} = u$ or ii) $v_{10} = u_{10}$.

Case 1.c)i): $x = v_9, v_{10} = u$

Without loss of generality $v = u_{10}$, so that $O(v) = \{u_1, u_4, u_9\}$. Evidently $u_3 \in O(u_2)$. u_1 and v_1 have a single common out-neighbour, so $v_4 \in O(u_1), u_4 \in O(v_1)$ and $|O(u_1) \cap \{v_9, u\}| = |O(v_1) \cap \{u_9, v\}| = 1$. Applying the Neighbourhood Lemma, $N^+(O(u)) = O(u_1) \cup O(u_2) = \{u_3, v_4, v_9, u\} \cup N^+(v_9)$ and $N^+(O(v)) = O(v_1) \cup O(u_2) = \{u_3, u_4, u_9, v\} \cup N^+(u_9)$. If $u \in O(u_2)$, then $u_9 \to u$ and there are distinct ≤ 3-paths from u_4 to u_2, so $u \in O(u_1)$. Similarly $v \in O(v_1)$. Hence $d(u_1, v_9) = d(v_1, u_9) = 3$. If $v_9 \in N^2(u_3)$, then there are two ≤ 3-paths from v_1 to v_9, so $u_9 \to v_9$ and, by the same reasoning $v_9 \to u_9$, so that G would contain a digon.

Case 1.c)ii): $x = v_9, v_{10} = u_{10}$

Now $u_9 = v, O(v) = \{u, u_1, u_4\}$ and $u_3, u_{10} \in O(u_2)$. From $N^+(u_1) \cap N^+(v_1) = \{u_3\}$,

it follows that $v_4, v_9 \in O(u_1), u_4, v \in O(v_1)$. The Neighbourhood Lemma yields $N^+(O(u)) = O(u_1) \cup O(u_2) = \{u_3, v_4, v_9, u_{10}\} \cup N^+(v_9)$ and $N^+(O(v)) = O(v_1) \cup O(u_2) = \{u_1, u_2, u_3, u_4, v, u_{10}\}$. As $u_2 \notin O(u_2)$, the second equation implies that $O(v_1) = \{u_4, v, u_2\}, O(u_2) = \{u_1, u_3, u_{10}\}$ and $O(u_1) = \{v_4, v_9, y\}$, where $N^+(v_9) = \{u_1, y\}$. $u^+ \in O(u) = \{v_1, v_4, v_9\}$. This implies the existence of distinct ≤ 3-paths from u^- to u_3, u_{10} or u_1.

Case 2: $u_3 = v_9, v_3 = u_9$

Write $O(u) = \{v_1, v_4, x\}, O(v) = \{u_1, u_4, y\}$. By 3-geodecity, v_7, v_8 and v_{10} do not lie in $\{u_3, v_3, u_7, u_8\}$, so $\{v_7, v_8, v_{10}\} = \{u, u_{10}, x\}$. Likewise $\{u_7, u_8, u_{10}\} = \{v, v_{10}, y\}$. $u \neq v_{10}$ and $v \neq u_{10}$, so without loss of generality $u = v_7, v = u_7$ and $\{v_8, v_{10}\} = \{u_{10}, x\}, \{u_8, u_{10}\} = \{v_{10}, y\}$. Suppose that $u_{10} \neq v_{10}$. Then $u_{10} = v_8 = y$ and $v_{10} = u_8 = x$, so that $u_8 \in O(u)$, which is absurd. It follows that $u_{10} = v_{10}$, $v_8 = x$ and $u_8 = y$, so that $O(u) = \{v_1, v_4, v_8\}, O(v) = \{u_1, u_4, u_8\}$. By the Neighbourhood Lemma, $N^+(O(u)) = O(u_1) \cup O(u_2) = \{v_3, v_4, u_3, u_{10}\} \cup N^+(v_8)$ and $N^+(O(v)) = O(v_1) \cup O(u_2) = \{u_3, u_4, v_3, u_{10}\} \cup N^+(u_8)$. u_1 can reach v_3, u_3 and u_{10}, so $O(u_1) = \{v_4\} \cup N^+(v_8), O(u_2) = \{u_3, v_3, u_{10}\}$ and $O(v_1) = \{u_4\} \cup N^+(u_8)$. Thus $N^3(u_2) = \{u, u_1, u_4, u_8, v, v_1, v_4, v_8\}$. We can set $u_{11} \to u$, $u_{12} \to v_1$, $u_{13} \to v$ and $u_{14} \to u_1$. However, wherever u_4 lies in $N^3(u_2)$ we have a violation of 3-geodecity. In conclusion, we have the following theorem.

Theorem 6.41. *There are no diregular* $(2, 3; +3)$*-digraphs.*

Note that Theorem 6.41 does not immediately tell us that $\epsilon(2, 3) \geq 4$, as there could be a non-diregular $(2, 3; +3)$-digraph. We determine the true value of $\epsilon(2, 3)$ in Section 9.5.

Chapter 7

The degree/geodecity problem for mixed graphs

7.1 Mixed Moore graphs

It is often of practical interest to consider networks that include both undirected edges and directed arcs. For example, the road network of a city typically contains both two-way and one-way streets. Such networks are represented mathematically by mixed graphs. Mixed graphs are used in job scheduling, with nodes representing tasks that need to be completed, edges connect jobs that are incompatible in the sense that they cannot be processed simultaneously and there is an arc from task a to task b if task a must be completed before task b is begun [125]. Mixed graphs also have applications in the study of Bayesian inference; undirected links model correlation and directed arcs represent causation [49].

We remind the reader of the following notational conventions for a mixed graph G from Subsection 1.1.2. The set of undirected neighbours of a vertex u is denoted by $U(u) = \{v \in V(G) : u \sim v\}$ and the number of undirected neighbours of u is the *undirected degree* $d(u)$ of u. The *directed out-neighbourhood* of u is $Z^+(u) = \{v \in V(G) : u \to v\}$ and the *directed in-neighbourhood* of u is $Z^-(u) = \{v \in V(G) : v \to u\}$. The *directed out-degree* and *directed in-degree* of u are given by $d^+(u) = |Z^+(u)|$ and $d^-(u) = |Z^-(u)|$ respectively. Finally we set $N^+(u) = U(u) \cup Z^+(u)$ and $N^-(u) = U(u) \cup Z^-(u)$.

The degree/diameter problem can also be studied for mixed graphs. A survey of this problem is given in [121].

Problem 7.1 (Degree/diameter problem for mixed graphs)**.** *What is the largest possible order of a mixed graph with maximum undirected degree r, maximum directed out-degree z and diameter k?*

A *mixed Moore graph* is an out-regular mixed graph G such that for every pair of vertices u, v of G there is a unique mixed path of length $\leq k$ form u to v. We can

draw a *mixed Moore tree* to deduce an upper bound on the order of a mixed graph G with maximum undirected degree r, maximum directed out-degree z and diameter k. Fix a vertex u and call this root vertex Level 0 of the tree. Draw edges from Level 0 to Level 1 from u to all of the undirected neighbours of u and arcs from Level 0 to all of the directed out-neighbours of u. In general, once we have added all vertices at Level t, where $0 \leq t \leq k-1$, we add the next level to the tree by the following rule for each vertex u_i in Level t:

- Draw arcs from Level t to Level $t+1$ from u_i to all directed out-neighbours of u_i.
- If u_i appears in Level t as the terminal vertex of an arc from Level $t-1$ then draw edges from Level t to Level $t+1$ from u_i to all undirected neighbours of u_i.
- If u_i appears in Level t as the endpoint of an edge from a vertex u_j in Level $t-1$, then below u_i in the Moore tree draw an edge from u_i to all undirected neighbours of u_i apart from u_j.

We continue this process until we have a tree of depth k. As G has diameter k all vertices of G are contained in the mixed Moore tree. An example for a mixed graph with maximum undirected degree $r = 3$, maximum directed out-degree $z = 3$ and diameter $k = 2$ is shown in Figure 7.1. For each t in the range $0 \leq t \leq k-1$ each vertex u_i at Level t has at most z directed out-neighbours below it at Level $t+1$, r undirected neighbours below it at Level $t+1$ if u_i appears in the tree as the terminal vertex of an arc from level $t-1$ and $r-1$ undirected neighbours beneath it at Level $t+1$ if u_i appears in the Moore tree as the endpoint of an edge from Level $t-1$.

This reasoning was first employed to give the upper bound on the order of such a mixed graph in [120]. However, the argument in [120] actually overestimates the number of vertices in the Moore tree. An exact expression for the Moore bound for mixed graphs was derived in [37] using recurrence relations.

Theorem 7.2 ([37]). *[Mixed Moore bound] The order of a mixed graph with maximum undirected degree r, maximum out-degree z and diameter k is bounded above by*

$$M(r,z,k) = A\frac{u_1^{k+1}-1}{u_1-1} + B\frac{u_2^{k+1}-1}{u_2-1},$$

where

$$v = (z+r)^2 + 2(z-r) + 1, u_1 = \frac{z+r-1-\sqrt{v}}{2}, u_2 = \frac{z+r-1+\sqrt{v}}{2}$$

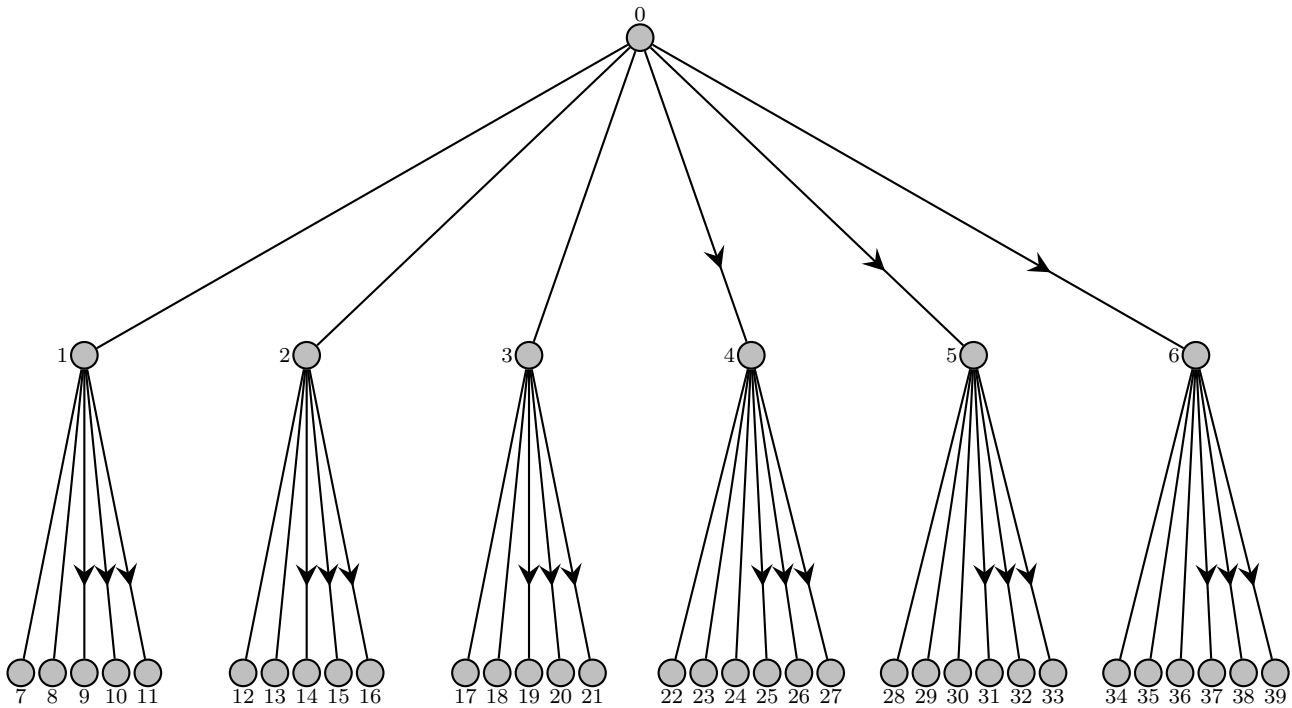

Figure 7.1: The Moore tree for $r = 3, z = 3, k = 2$

and

$$A = \frac{\sqrt{v} - (z + r + 1)}{2\sqrt{v}}, B = \frac{\sqrt{v} + (z + r + 1)}{2\sqrt{v}}.$$

If $r = 0$ or $z = 0$ then this expression reduces to the undirected and directed Moore bounds respectively. We record separately the special case of the mixed Moore bound for diameter $k = 2$.

Corollary 7.3. *The mixed Moore bound for mixed graphs with maximum undirected degree r, maximum directed out-degree z and diameter two is given by*

$$M(r, z, 2) = (r + z)^2 + z + 1.$$

A graph that meets the mixed Moore bound is called a *mixed Moore graph.* Recall that a mixed graph G is k-geodetic if and only if for any pair u, v of vertices of G there is at most one mixed path (i.e. non-backtracking mixed walk) of length $\leq k$ from u to v in G. It is easily seen that a mixed graph is Moore if and only if it satisfies the following conditions.

Theorem 7.4. *A mixed graph G is Moore if and only if*

- *G is totally regular with undirected degree r and directed degree z,*
- *the diameter of G is k, and*

Undirected degree r	Directed degree z	Order n
1	any	r^2+2r+3
3	1	18
	3	40
	4	54
	6	88
	7	108
	...	...
7	2	84
	5	150
	7	204
	...	...
13	4	294
	6	368
	...	...
21	1	486
	...	...
...	...	...

Table 7.1: Values of r and z not covered by Theorem 7.5

- *G is k-geodetic.*

Mixed Moore graphs with diameter $k = 2$ were first investigated by Bosák in the seventies [30, 31, 32]. In [32] he proved that any mixed Moore graph is totally regular and used spectral methods to prove that the undirected degree r and directed out-degree z of a mixed Moore graph with diameter two satisfy a very special condition.

Theorem 7.5 ([32])**.** *Apart from trivial cases, if there exists a mixed Moore graph with diameter two, undirected degree r and directed out-degree z, then there exists a positive odd integer c such that $c|(4z-3)(4z+5)$ and $c^2+3=4r$.*

However, Theorem 7.5 leaves an infinite number of pairs r, z for which the existence of a mixed Moore graph with undirected degree r, directed out-degree z and diameter two is undecided. The smallest orders not covered by Theorem 7.5 are displayed in Table 7.1.

There is one known infinite family of mixed Moore graphs with diameter two, formed by collapsing all digons in the Kautz digraph $K(d,k)$ discussed in Subsection 2.3.3 into edges. This mixed graph can be described quite easily. Take an alphabet Ω of size $z+2$. For the vertex set of the mixed graph we take the words ab, where $a, b \in \Omega$ and $a \neq b$. For all $a, b, c \in \Omega$ with $a \neq b$ and $b \neq c$ we introduce an arc $ab \to bc$ when $c \neq a$ and an edge $ab \sim ba$. It is easily verified that this yields a mixed Moore graph with undirected degree $r = 1$, directed out-degree z and diameter $k = 2$. In fact it shown in [78] using spectral techniques that these are the unique mixed Moore graphs

with these parameters.

Theorem 7.6 ([78]). *For all $z \geq 1$ there is a unique mixed Moore graph with undirected degree $r = 1$, directed out-degree z and diameter $k = 2$.*

In [32] Bosák identified a further mixed Moore graph with undirected degree $r = 3$, directed out-degree $z = 1$, diameter $k = 2$ and order $M(3, 1, 2) = 18$. The uniqueness of this graph was proven in [121].

One method of searching for mixed Moore graphs is to restrict the search space to Cayley mixed graphs. By carrying out a computer search for Cayley mixed graphs that meet the Moore bound Jørgensen found two Cayley mixed Moore graphs with undirected degree $r = 3$, directed out-degree $z = 7$, diameter $k = 2$ and order $n = 108$ [97]. However, it has been shown that there are no further Cayley mixed Moore graphs with diameter two and order ≤ 485 [66, 107]. A search using a SAT solver has also completely ruled out the existence of mixed Moore graphs with diameter two and orders $40, 54$ or 84 [105].

It is natural to ask whether there exist any mixed Moore graphs with diameter greater than two? It was shown by a counting argument in [121] that the answer to this question is negative, except in trivial cases. We will extend this style of argument to give better bounds on the order of mixed graphs in the next two chapters.

Theorem 7.7 ([121]). *There are no mixed Moore graphs with diameter $k \geq 3$, except for undirected and directed cycles.*

Whilst there remain an infinite number of open cases, it is evident that it is very difficult for a mixed graph to meet the mixed Moore bound. In general the mixed Moore tree of depth k will either not contain all vertices of G (in which case the diameter of G is larger than k) or there will be vertices repeated in the Moore tree (in which case G is not k-geodetic). It is therefore of interest to study the structure of mixed graphs with order close to the mixed Moore bound. To this end in the conditions in Theorem 7.4 we can either relax the requirement that all of the vertices in the Moore tree be distinct or the requirement that the Moore tree contains all of the vertices of G. This motivates the following definitions.

Definition 7.8.

- A mixed graph with maximum undirected degree r, maximum directed out-degree z, diameter k and order $M(r, z, k) - \delta$ is an $(r, z, k; -\delta)$*-graph* and has *defect* δ. A mixed graph with defect one is an *almost mixed Moore graph*.

- A k-geodetic mixed graph with minimum undirected degree r, minimum directed out-degree z and order $M(r,z,k)+\epsilon$ is an $(r,z,k;+\epsilon)$-*graph* and has *excess* ϵ. The smallest possible value of ϵ such that there exists an $(r,z,k;+\epsilon)$-graph will be written $\epsilon(r,z,k)$. We set $N(r,z,k) = M(r,z,k)+\epsilon(r,z,k)$.

7.2 Mixed graphs with positive defect

The degree/diameter problem for mixed graphs is equivalent to finding the smallest possible defect of an $(r,z,k;-\delta)$-graph for all $r,z \geq 0$ and $k \geq 2$. If $z=0$ then this becomes the undirected degree/diameter problem and if $r=0$ we recover the directed degree/diameter problem; hence the mixed degree/diameter problem is a generalisation of both the undirected and directed degree/diameter problems.

The mixed Moore tree rooted at a vertex u of an out-regular $(r,z,k;-\delta)$-graph will contain δ repeated vertices. Let $R(u)$ be the multiset of repeated vertices in the Moore tree rooted at u, i.e. any vertex that features t times in the Moore tree appears $t-1$ times in the multiset $R(u)$. With a slight abuse of notation, we call $R(u)$ the *repeat set* of u.

It is easily shown that any $(r,z,k;-1)$-graph is out-regular. For defect $\delta=1$ instead of the repeat set we have a *repeat function* $r: V(G) \to V(G)$. Hence for any vertex u of an $(r,z,k;-1)$-graph the vertex $r(u)$ is the unique vertex that appears twice in the Moore tree of depth k rooted at u; we call $r(u)$ the *repeat* of u. For any subset $W \subseteq V(G)$ we let $r(W) = \{r(w) : w \in W\}$. For almost mixed Moore graphs with diameter two it is shown in [104] that the repeat function of an $(r,z,2;-1)$-graph G is an automorphism if and only if G is totally regular.

Relatively little is known about mixed graphs with small defect. The only known non-trivial almost mixed Moore graph with diameter two is shown in Figure 7.2. This mixed graph has degree parameters $r=2, z=1$, diameter $k=2$ and order $n=10$. In [38] it is proven that this is the unique almost mixed Moore graph with these parameters. A simple parity argument also shows that there are no almost mixed Moore graphs with diameter two and odd undirected degree r [104].

López and Miret used spectral theory to derive the following necessary condition for the existence of a totally regular almost mixed Moore graph with diameter $k=2$ in [104].

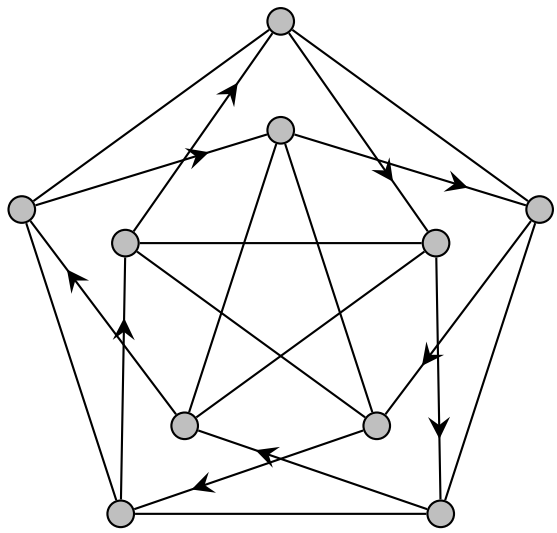

Figure 7.2: An almost mixed Moore graph

Theorem 7.9 ([104]). *Let G be a totally regular $(r, z, 2; -1)$-graph. Then r is even and one of the following three possibilities holds:*
i) $r = 2$,
ii) there exists an odd integer c such that $c^2 = 4r + 1$ and $c|(4z + 1)(4z - 7)$, or
iii) there exists an odd integer c such that $c^2 = 4r - 7$ and $c|(16z^2 + 40z - 23)$.

The analysis in [104] does not cover the case of almost mixed Moore graphs that are not totally regular. In the same paper López and Miret pose the following question.

Question 7.10 ([104]). *Are all almost mixed Moore graphs with diameter two totally regular?*

We answer this question in the affirmative in Chapter 8. We will also show that all $(1, 1, k; -1)$-graphs with $k \geq 3$ are totally regular.

In [51] Dalfó et al. use counting arguments to derive a lower bound for the defect of a totally regular $(r, z, k; -\delta)$-graph for $k \geq 3$.

Theorem 7.11 ([51]). *For $r, z \geq 1$ and diameter $k \geq 3$, the defect of a totally regular $(r, z, k; -\delta)$-graph satisfies*

$$\delta \geq r.$$

Note however that Theorem 7.11 does not give us a bound for the smallest possible defect of an $(r, z, k; -\delta)$-graph, as there could potentially be non-totally-regular mixed graphs that are closer to the Moore bound than the largest totally regular $(r, z, k; -\delta)$-graph. We will revisit this problem in Chapter 8.

The bound in Theorem 7.11 is tight; in [51] the authors show that there are exactly three totally regular $(1, 1, 3; -1)$-graphs. In Chapter 9 we will improve their bound in the case $r = z = 1$.

7.3 The mixed degree/geodecity problem: cages and monotonicity

In the previous section we described one approach to studying the structure of mixed graphs with order close to the Moore bound. If instead of allowing repeats in the Moore tree we preserve the k-geodecity condition in Theorem 7.4, then we obtain the mixed degree/geodecity problem.

Problem 7.12 (Degree/geodecity problem for mixed graphs)**.** *For $r, z \geq 1$ and $k \geq 2$ what is the smallest possible order of a k-geodetic mixed graph with minimum undirected degree r and minimum directed out-degree z?*

Again we will be particularly interested in the structure of the extremal mixed graphs.

Definition 7.13. A smallest possible k-geodetic mixed graph with minimum undirected degree r and minimum directed out-degree z is an (r, z, k)-cage or *mixed geodetic cage.*

With the caveat that the term *mixed cage* is also used in the mixed degree/girth problem [6] we will, as with the directed geodetic cages, simply speak of mixed cages here. The mixed degree/girth problem, which has seen some recent interesting progress in [5], bears much the same relation to the mixed degree/geodecity problem as the directed degree/girth problem does to the directed degree/geodecity problem.

We begin our discussion of the mixed degree/geodecity problem by proving the existence of mixed geodetic cages for all values of $r, z \geq 1$ and $k \geq 2$.

Theorem 7.14. *There exists a mixed geodetic (r, z, k)-cage for all $r, z \geq 1$ and $k \geq 2$. Their order satisfies*

$$N(r, z, k) \leq \min\{N(r, 0; k)N(0, N(r, 0; k)z; k), N(0, z; k)N(N(0, z; k)r, 0; k)\}.$$

Proof. We employ a truncation argument. Let H be an undirected cage with degree r, girth $g = 2k + 1$ and order n (which exists by the result of [126]). Let H' be a directed geodetic cage with geodetic girth k and directed out-degree nz (H' exists by Lemma 3.19). We form a mixed graph G by identifying each vertex u of H' with an

isomorphic copy H_u of H and connecting the copies of H by arcs in accordance with the topology of H'; specifically, for each vertex u of H' partition the nz arcs from u in H' into n sets $A_1, A_2, \ldots, A_n$ of z arcs and assign a set A_i of arcs to each of the n vertices in H_u, such that if an arc in A_i goes to a vertex v in H', then in G it is directed to any vertex of H_v. The resulting mixed graph G obviously has geodetic girth k. A similar construction starting with directed cages substituted for vertices of an undirected cage establishes the other part of the theorem. □

As in the undirected degree/girth problem, the bounds given in Theorem 7.14 are much too large to be of any practical help. We also note that by using regular graphs with girth $2k+1$ (which exist by the result of [126]) and diregular k-geodetic digraphs (we can use the permutation digraphs), the truncation argument in Theorem 7.14 also shows the existence of a smallest totally regular k-geodetic mixed graph with undirected degree r and directed degree z.

Corollary 7.15. *For all $r, z \geq 1$ and $k \geq 2$ there exists a smallest totally regular k-geodetic mixed graph with undirected degree r and directed degree z.*

Now that the existence of mixed geodetic cages has been established, the question of monotonicity arises. Intuition suggests that the order of a cage should grow strictly with increasing r, z and k. Recall that monotonicity of the order of cages in the undirected degree/girth problem was proven by Fu, Huang and Rodger [73] and degree monotonicity of undirected cages was discussed in [150], but appears to be a difficult problem. We combine the method of [73] with our proof of Theorem 3.26 to prove strict monotonicity of the order of mixed cages in the geodetic girth k.

Theorem 7.16. *$N(r, z, k) < N(r, z, k+1)$ for all $k \geq 2$.*

Proof. Let G be an $(r, z, k+1)$-cage. Suppose that there exists a vertex u of G with even undirected degree $d(u)$. Write $U(u) = \{u_1, u_2, \ldots, u_{2r-1}, u_{2s}\}$. Define the graph G' as follows: delete u from G, join u_{2i-1} to u_{2i} by an undirected edge for $1 \leq i \leq s$ and for every vertex u^- in $Z^-(u)$ insert an arc from u^- to some vertex u^+ in $Z^+(u)$. This construction is shown in Figure 7.3, with the new arcs and edges in red. Call the added arcs and edges *new elements*.

Suppose that G' is not k-geodetic; let w and w' be vertices of G' with distinct mixed paths P and Q of length $\leq k$ from w to w'. As each new element in G' can be extended to a walk of length two in G whilst preserving the non-backtracking property and G is $(k+1)$-geodetic, we can assume that the mixed path P contains at

least two new elements. Examining a mixed path with length $\leq k-2$ between consecutive new elements in P (i.e. there is no third new element between these two new elements in P), we see that there exists a non-backtracking closed walk of length $\leq k$ through u in G, which is impossible. Thus G is at least k-geodetic and, having order smaller than the $(r, z, k+1)$-cage G, its geodetic girth must be exactly k.

Thus we can assume that every vertex of G has odd undirected degree. Let $u \sim v$ be an undirected edge of G. Let $U(u) = \{v, u_1, u_2, \ldots, u_{2s}\}$ and $U(v) = \{u, v_1, v_2, \ldots, v_{2t}\}$. Form a new graph G'' by deleting u and v and matching up the remaining neighbours of u and v by new elements as in the previous construction, i.e. setting $u_{2i-1} \sim u_{2i}$ for $1 \leq i \leq s$, $v_{2j-1} \sim v_{2j}$ for $1 \leq j \leq t$ and inserting an arc from each vertex of $Z^-(u)$ to $Z^+(u)$ and an arc from each vertex of $Z^-(v)$ to $Z^+(v)$. Assuming $k \geq 2$, notice that the sets $U(u) - \{v\}$, $U(v) - \{u\}$, $Z^-(u)$, $Z^+(u)$, $Z^-(v)$ and $Z^+(v)$ are pairwise disjoint.

If G'' has geodetic girth $\leq k-1$, with two distinct mixed paths P and Q from a vertex w to a vertex w', then as before we can assume that P contains two new elements.

Consider consecutive new elements in P. By the preceding argument these new elements cannot be associated with same vertex in G, for example a new edge between undirected neighbours of u and an arc from $Z^-(u)$ to $Z^+(u)$ would yield a contradiction as above. By symmetry we can assume that the first element is associated with u and the second with v; for example, these elements could be a new arc from $Z^-(u)$ to $Z^+(u)$ followed by a new edge in $U(v)$. Looking at the mixed subpath of P between these consecutive new elements, we see that in G there is a mixed path of length $\leq k-2$ from $N^+(u)$ to $N^-(v)$; it follows that there are distinct mixed paths of length $\leq k$ from u to v in G, a contradiction, so G'' is k-geodetic. □

Applying the procedure of Theorem 7.16 to a smallest totally regular k-geodetic mixed graph with given undirected and directed degrees (which we know to exist by Corollary 7.15) by joining vertices of $Z^-(u)$ to $Z^+(u)$ by arcs in a one-to-one fashion, we see that strict monotonicity in the geodetic girth k also holds for the order of smallest possible totally regular k-geodetic mixed graphs. Monotonicity in the directed out-degree is simple to demonstrate.

Theorem 7.17. *$N(r, z, k) \leq N(r, z+1, k)$. If $r = 0$, then strict inequality holds.*

Proof. Let G be an $(r, z+1, k)$-cage. Delete an arc from every vertex; the resulting graph has minimum undirected degree r, minimum directed out-degree z and, as a

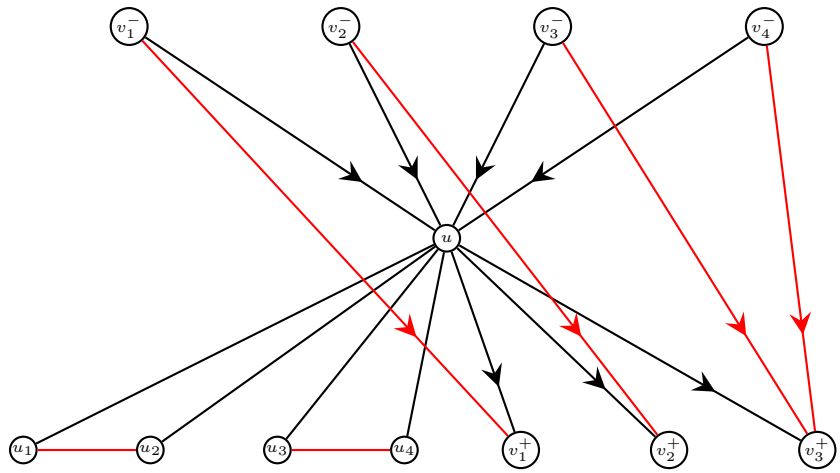

Figure 7.3: The construction in Theorem 7.16

subgraph of G, is obviously still k-geodetic. The statement for $r = 0$ is a result of the proof of Theorem 3.26. □

We note that by adapting the spectral method of [104] from the case of $(r, z, 2; -1)$-graphs to $(r, z, 2; +1)$-graphs we also have a strong restriction on the possible combinations of values of r and z for which a totally regular 2-geodetic mixed graph with excess one can exist. We omit the proof, as it is a relatively straightforward application of the reasoning of [104] combined with the results of [116].

Theorem 7.18. *Let G be a totally regular $(r, z, 2; +1)$-graph. Then either*

- $r = 2$,
- $4r + 1 = c^2$ *for some* $c \in \mathbb{N}$ *and* $c|(16z^2 - 24z + 25)$, *or*
- $4r - 7 = c^2$ *for some* $c \in \mathbb{N}$ *and* $c|(16z^2 + 40z + 9)$.

Finally we make the following conjecture that generalises Conjecture 5.1.

Conjecture 7.19. *All mixed geodetic cages are totally regular.*

We present several mixed geodetic cages in Chapter 9, all of which are totally regular, thereby adding some weight to Conjecture 7.19.

Chapter 8

Total regularity of mixed graphs with order close to the Moore bound

8.1 Introduction

In Chapter 5 we saw that it is difficult to analyse the structure of digraphs with order close to the Moore bound that are not diregular. A similar phenomenon occurs for mixed graphs. Recall that a mixed graph is totally regular if its undirected subgraph G^U is a regular graph and its directed subgraph G^Z is diregular; for other notation, see Section 1.1.2.

For an example of the problems caused by the issue of total regularity, consider Theorem 7.9 due to López and Miret [104], cited in Chapter 7, which gave very strong necessary conditions on the degree parameters r and z for the existence of an almost mixed Moore graph with diameter two; however, this analysis depends on the assumption of total regularity. Previously there was no information at all on almost mixed Moore graphs that are not totally regular. Therefore López and Miret posed the following question in [104]:

Question 8.1. *Are almost mixed Moore graphs with diameter two totally regular?*

In Section 8.2 we answer this question affirmatively. The problem of the total regularity of almost mixed Moore graphs with diameters greater than two is more difficult; in Section 8.3 we use counting arguments to show total regularity for the special case of $r = z = 1$ and diameters $k \geq 3$. Starting in Section 8.4 we apply these methods to the 'mirror image' problem of 2-geodetic mixed graphs with excess one; this turns out to be a simpler problem than the total regularity of almost mixed Moore graphs. In Section 8.5 we also prove that all mixed graphs with excess one and directed out-degree $z = 1$ are totally regular; this will prove to be a valuable result in the analysis contained in the next chapter.

For a mixed graph G with sufficiently small excess or defect it is trivial to show that G is out-regular; in the context of our investigation it is almost always safe to assume

out-regularity (we will have to be slightly more careful in the proof of Theorem 9.9).

Lemma 8.2. *If G is an $(r, z, k; -\delta)$- or $(r, z, k; +\epsilon)$-graph with defect/excess strictly less than $M(r, z, k-1)$, then the directed subgraph G^Z of G is out-regular. Furthermore, if δ or ϵ satisfies*

$$\delta, \epsilon < \sum_{t=1}^{k} (-1)^{t+1} M(r, z, k-t),$$

then G is out-regular.

Proof. We prove the result for mixed graphs with small excess; the case of small defect is very similar. Let G be an $(r, z, k; +\epsilon)$-graph with $\epsilon < M(r, z, k-1)$. If there is a vertex u of G with directed out-degree $d^+(u) \geq z+1$, then the mixed Moore tree of depth k rooted at u contains an extra directed branch, which contains at least $M(r, z, k-1)$ vertices, a contradiction.

Now we show that the undirected subgraph G^U is regular. Let $\mu(r, z, t)$ be the number of vertices contained in an undirected branch of the mixed Moore tree of depth $t+1$ of an out-regular $(r, z, t+1; +\epsilon)$-graph. For example, $\mu(r, z, 2)$ is the number of vertices in an undirected branch of the Moore tree of depth 3 of an out-regular $(r, z, 3; +\epsilon)$-graph; thus

$$\mu(r, z, 2) = (r+z)^2 - r + 1 = M(r, z, 2) - (r+z) = M(r, z, 2) - \mu(r, z, 1).$$

An undirected branch of depth t of a Moore tree of depth $t+1$ is has the same structure as a Moore tree of depth t with one undirected branch of depth $t-1$ deleted; therefore we have the recurrence relation $\mu(r, z, t) = M(r, z, t) - \mu(r, z, t-1)$. If a vertex u of G has undirected degree $d(u) \geq r+1$, then the Moore tree rooted at u has at least one extra undirected branch and G has excess at least $\mu(r, z, k-1)$. Expanding this expression using the recurrence relation gives the alternating sum in the statement of the lemma. □

By analogy with our notation in Chapter 5, we define the sets with 'too small' in-degree and 'too large' in-degree as follows for a given $(r, z, k; +\epsilon)$- or $(r, z, k; -\delta)$-graph

$$S = \{v \in V(G) : d^-(v) < z\}; \quad S' = \{v' \in V(G) : d^-(v') > z\}.$$

8.2 $(r, z, 2; -1)$-graphs are totally regular

We will now proceed to answer the question of López and Miret by showing that any $(r, z, 2; -1)$-graph is totally regular. Suppose that G is an $(r, z, 2; -1)$-graph that is not totally regular, where $r, z \geq 1$. Recall from Section 7.2 that the repeat $r(u)$ of a vertex u of G is the unique vertex of G such that there are two distinct non-backtracking mixed walks with length ≤ 2 from u to $r(u)$ in G. Our strategy is to use a purely combinatorial argument to deduce structural information about G and then apply spectral theory to obtain a contradiction. First we show that G must be out-regular.

Lemma 8.3. *G is out-regular with undirected degree r and directed out-degree z.*

Proof. It follows from Lemma 8.2 that if G is not out-regular, then it has defect at least $M(r, z, 1) - M(r, z, 0) = r + z \geq 2$. □

We now prove two fundamental lemmas that show the relationship between the sets S, S', out-neighbourhoods and repeats in G; these are generalisations of Lemmas 5.5 and 5.6 from Chapter 5 to mixed graphs. The result that the repeat function is an automorphism for totally regular almost mixed Moore graphs with diameter two [104] can again be viewed as a 'limiting case' of these results.

Lemma 8.4. *If $v \in S$, then $d^-(v) = z - 1$ and for all $u \in V(G)$ we have $S \subseteq N^+(r(u))$.*

Proof. Let $v \in S$ and $u \in V(G)$. Consider the Moore tree rooted at u. Suppose that $d(u, v) = 2$. As each vertex of $N^+(u)$ can reach v by paths of length ≤ 2, each branch of the Moore tree must contain an element of $N^-(v)$. However, there are $r + z$ branches, whereas v has $\leq r + z - 1$ in-neighbours, so at least one in-neighbour must be repeated in the tree. Hence v is an out-neighbour of $r(v)$. Evidently $d^-(v) = z - 1$, for otherwise more than one in-neighbour of v would be repeated and the defect of G would be at least two. The cases $u \sim v, u \to v$ and $u = v$ can be dealt with similarly. □

Corollary 8.5. $\sum_{v' \in S'} (d^-(v') - z) = \sum_{v \in S} (z - d^-(v)) = |S|$.

Proof. By Lemma 8.3, the average directed in-degree must be z. The final equality follows from Lemma 8.4. □

Lemma 8.6. *For all $u \in V(G)$ we have $S' \subseteq r(N^+(u))$.*

Proof. Let $v' \in S', u \in V(G)$. Suppose that $d(u, v') = 2$. Then $u \notin N^-(v')$. There are $r + z$ branches of the Moore tree at u, but v' has $\geq r + z + 1$ in-neighbours, so at least one branch contains more than one in-neighbour of v', so that $v' \in r(N^+(u))$. The remaining cases are similar. □

Lemmas 8.4 and 8.6 not only yield important information on the structure of G, but also show that the order of both sets S, S' is bounded above by $r + z$. A counting argument will now allow us to ascertain the exact size of S.

Lemma 8.7. $|S| = r + z$.

Proof. Let $v \in S$. By Lemma 8.4 we have $d^-(v) = z - 1$. We obtain an upper bound on the number of vertices that are initial points of paths of length ≤ 2 that terminate at v by assuming that $S' \subseteq N^-(v)$. As G has diameter two, this yields by Corollary 8.5

$$n \leq 1 + r + (z - 1) + r(r + z - 1) + (z - 1)(r + z) + |S|.$$

Rearranging, $|S| \geq r + z$. Combined with the result of Lemma 8.4, we see that $|S| = r + z$. □

As $S \subseteq N^+(r(u))$ for each $u \in V(G)$ and both sets have size $r + z$, we must have equality.

Corollary 8.8. $S = N^+(r(u))$ *for all* $u \in V(G)$.

We say that a vertex w is a *repeat* in G if there exists a vertex u such that $r(u) = w$. The preceding corollary allows us to determine both the value of the undirected degree r and the number of distinct repeats in G.

Lemma 8.9. $r = 2$ *and there are exactly two repeats in* G.

Proof. Suppose that there is only one repeat, call it R. As R is the only repeat, we must have $r(R) = R$. It is easily seen that there must be $u \in N^+(R)$ such that $R \to u \to R$. But u now lies in a 2-cycle and hence is a repeat, contradicting our hypothesis. Hence G has at least two repeats, call them R_1 and R_2.

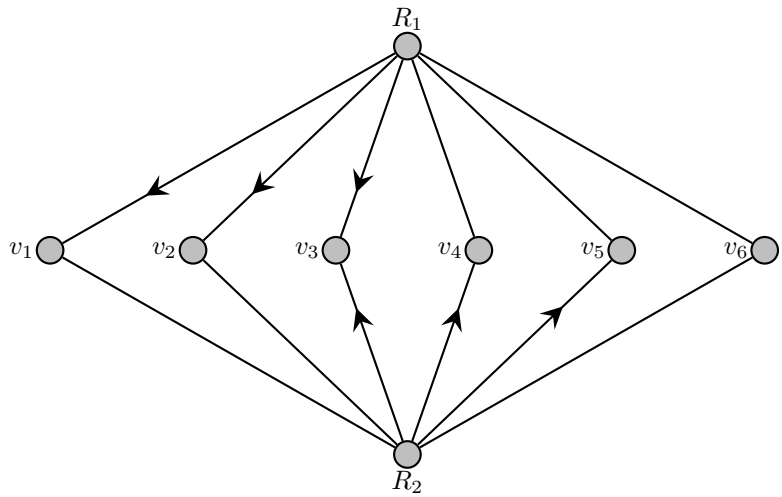

Figure 8.1: If $r \geq 3$

If $r = 1$, then G contains a perfect matching, so that G must have even order, whereas $|V(G)| = z^2 + 3z + 1$ would be odd. Suppose that $r \geq 3$. By Corollary 8.8, $N^+(R_1) = N^+(R_2) = S$. R_1 thus has at least $r \geq 3$ paths of length two to R_2, as shown in Figure 8.1, contradicting $\delta = 1$. Therefore $r = 2$. By the foregoing reasoning, $r(R_1) = R_2$ and $r(R_2) = R_1$. If there were a third repeat R_3, this argument could be repeated with R_3 in place of R_2 to give $r(R_1) = R_3$, so that $R_2 = R_3$, a contradiction. Therefore there are exactly two repeats R_1 and R_2. □

This provides us with all of the structural information necessary to complete our proof. We now adopt a spectral approach.

Theorem 8.10. *Almost mixed Moore graphs with diameter two are totally regular.*

Proof. Suppose that there are m_1 vertices with repeat R_1 and m_2 vertices with repeat R_2; we shall call vertices with repeat R_i *Type i*. Let us label the vertices of G $u_1, u_2, \ldots, u_n$, so that $u_1 = R_1, u_2 = R_2$, u_{2+s} is Type 2 for $1 \leq s \leq m_2 - 1$ and u_{1+m_2+t} is Type 1 for $1 \leq t \leq m_1 - 1$. If A is the adjacency matrix of G, then by Theorem 1.3 the (i, j)-entry of the sum $I + A + A^2$ is the number of distinct walks of length ≤ 2 from vertex u_i to vertex u_j. Hence

$$I + A + A^2 = J + 2I + P,$$

where I is the $n \times n$ identity matrix, J is the $n \times n$ all-one matrix and P is the matrix

with entries given by

$$P_{ij} = \begin{cases} 1, & \text{if } r(u_i) = u_j, \\ 0, & \text{otherwise.} \end{cases} \tag{8.1}$$

Observe that all non-zero entries of P occur in the first two columns. Inspection shows that the matrix $J + P$ has the following eigenvalues:

i) eigenvalue $n + 1$ with multiplicity one.
   Corresponding eigenvector: all-one vector of length n.
ii) eigenvalue -1 with multiplicity one.
   Corresponding eigenvector:

$$f(u_j) = \begin{cases} 1, & \text{if } u_j \text{ is Type 1,} \\ -(m_1 + 1)/(m_2 + 1), & \text{if } u_j \text{ is Type 2.} \end{cases} \tag{8.2}$$

iii) eigenvalue 0 with multiplicity $n - 2$.
   Corresponding eigenvectors:

$$f_i(u_j) = \begin{cases} 1, & \text{if } j = i + 2, \\ -1, & \text{if } j = n, \\ 0, & \text{otherwise.} \end{cases} \tag{8.3}$$

   for $1 \leq i \leq n - 3$ and

$$g(u_j) = \begin{cases} 1, & \text{if } j = 1 \text{ or } 2, \\ -3, & \text{if } j = n, \\ 0, & \text{otherwise.} \end{cases} \tag{8.4}$$

It follows that $I + A + A^2$ has spectrum $\{n + 3, 1, 2^{(n-2)}\}$, so that G must have spectrum $\sigma(G) = \{\lambda_1, \ldots, \lambda_n\}$, where

- λ_1 is a solution of $\lambda^2 + \lambda - (n + 2) = 0$,
- λ_2 is a solution of $\lambda^2 + \lambda = 0$, and
- λ_i is a solution of $\lambda^2 + \lambda - 1 = 0$ for $3 \leq i \leq n$.

The solutions of the first equation are $\lambda_1 = \frac{-1 \pm \sqrt{4n+9}}{2}$. As the undirected degree is $r = 2$ by Lemma 8.9, it follows from the Moore bound given in Corollary 7.3 for diameter two that the order of G is $n = z^2 + 5z + 4$, so

$4n+9 = 4z^2+20z+25 = (2z+5)^2$, yielding $\lambda_1 = z+2$ or $-z-3$. Trivially $\lambda_2 = 0$ or -1. Finally the third equation has solutions $\frac{-1\pm\sqrt{5}}{2}$.

G has no loops, so the trace of its adjacency matrix is $\mathrm{Tr}(A) = 0$. It follows that the sum of the eigenvalues of G is also zero. In order that this sum be rational, one half of the eigenvalues $\lambda_3, \ldots, \lambda_n$ must take the plus sign and half the negative sign. The sum of the eigenvalues $\lambda_3, \ldots, \lambda_n$ is thus $-(n/2)+1$. Depending upon the values of λ_1, λ_2, this leaves us with four possibilities for the sum of the eigenvalues, namely $z+3-(n/2)$, $z+2-(n/2)$, $-z-2-(n/2)$ and $-z-3-(n/2)$. The final two are clearly strictly negative, whilst the first two yield no feasible solutions for $z > 0$. □

8.3 Total regularity of $(1,1,k;-1)$-graphs for $k \geq 3$

The problem of the total regularity of almost mixed Moore graphs with diameter $k \geq 3$ is difficult and we consider it here only in the case $r = z = 1$. Let G be a $(1,1,k;-1)$-graph that is not totally regular. If a vertex u of G has undirected degree $d(u) = 0$, then the order of G is at most $M(r,z,k-1)+1$, which is too small for $k \geq 3$; similarly, if a vertex u has directed out-degree $d^+(u) = 0$, then the order of G is at most $M(r,z,k) - M(r,z,k-1)$, which again is too small. Therefore, G is out-regular, so that every vertex u has a unique undirected neighbour, which we will denote by u^*, and a unique directed out-neighbour, which will be written u^+. For these parameters $S = \{v \in V(G) : d^-(v) = 0\}$, $S' = \{v' \in V(G) : d^-(v') \geq 2\}$; hence vertices in S have no directed in-neighbours, i.e. $Z^-(v) = \emptyset$ for $v \in S$.

Let $F_0 = F_1 = 1, F_2 = 2, F_3 = 3, F_4 = 5\ldots$ be the sequence of Fibonacci numbers. It is easily verified that G has order $n = F_{k+3} - 3$. Since the order of G must be even, no almost mixed Moore graph exists with these parameters for $k \equiv 2 \pmod 3$. We will draw a Moore tree rooted at a vertex u as shown in Figure 8.2 for $k = 5$. In general, for $0 \leq \ell \leq k-1$ the children in level $\ell+1$ of a vertex at level ℓ of the tree are drawn below it, with the undirected neighbour (if the vertex has its undirected neighbour at level $\ell+1$ and not $\ell-1$) to the left and the directed out-neighbour on the right, where vertices are labelled $u_0, u_1 \ldots$ etc. in increasing order from top to bottom and left to right. This process is continued until the tree reaches depth k.

We begin with an elementary consideration on the length of the paths from a vertex to its repeat.

Lemma 8.11. *If there are two distinct mixed paths P_1, P_2 from x to y of length $\leq k$, then at least one of them has length k.*

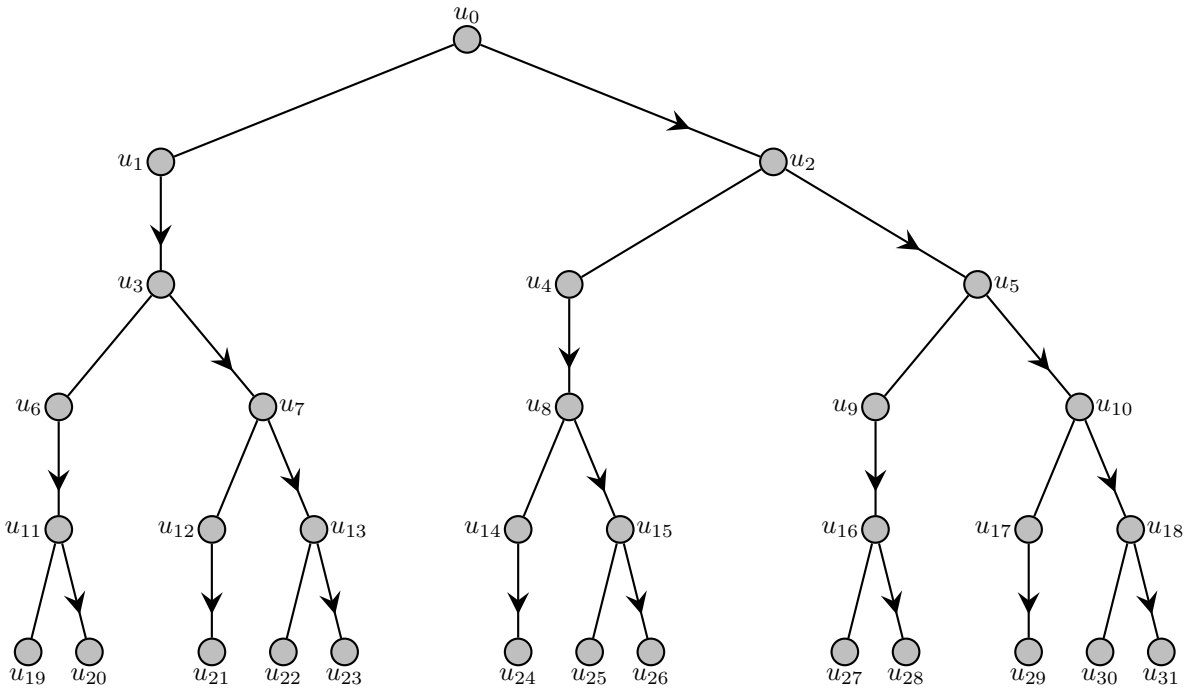

Figure 8.2: The Moore tree for $r = z = 1$ and $k = 5$

Proof. Suppose that there are mixed paths $P_1 \neq P_2$ from x to y and that both paths have length $\leq k - 1$. Draw the Moore tree of depth k rooted at x. y appears twice in this tree, as does y^+, so that the defect would be at least two. □

Colloquially, there cannot be two 'short' mixed paths between any pair of vertices.

Corollary 8.12. *No $v \in S$ is a repeat and S is an independent set.*

Proof. Let $v \in S$. Suppose that there exists a vertex u such that $v = r(u)$. If $u \neq v$, then u must have two paths of length $\leq k - 1$ to v^*, contradicting Lemma 8.11. If $u = v$, then v is contained in a mixed cycle of length $\leq k$, so that there are again two short paths from v to v^*.

By definition no arc can have both endpoints in S. If there are $v, w \in S$ such that $v \sim w$, then no other vertex of G would be able to reach v or w. Hence S is independent. □

We next deduce the relationship between repeats and the undirected neighbours of elements of S.

Lemma 8.13. *For every vertex u of G and $v \in S$, either $v^* = r(u)$ or $v^* = r(u^*)$.*

Proof. Draw the Moore tree rooted at u. As $u_2 = u^+$ has a directed in-neighbour,

obviously $u_2 \notin S$. G has diameter k and so, since u_2 can reach v only through v^*, we have $d(u_2, v^*) \leq k-1$. If $u = v$, then $u_1 = v^*$, so that v^* occurs in both branches and $v^* = r(u)$. If v belongs to the u_1-branch, then either v^* also lies in that branch or $u = v^*$, so that again $v^* = r(u)$. We may thus assume that v occurs only in the u_2-branch.

Suppose that $d(u_2, v) = k-1$. Then u_1 cannot reach v through u and so v^* occurs in both branches of the Moore tree. Finally assume that $d(u_2, v) \leq k-2$, so that $d(u_2, v^*) \leq k-3$. As $d(u_3, v) \leq k$, it follows that $d(u_3, v^*) \leq k-1$, so that $u_1 = u^*$ has two mixed paths to v^* with length $\leq k$, one through u_3 and the other through u and u_2, so that $v^* = r(u^*)$. □

This yields an upper bound on the size of S.

Corollary 8.14. $|S| \leq 2$.

Proof. Obviously $|S| \leq |\{v^* : v \in S\}|$. Fix a vertex u. By Lemma 8.13, $\{v^* : v \in S\} \subseteq \{r(u), r(u^*)\}$. □

As the average directed in-degree of vertices in G is one, Corollary 8.14 shows that there are three possible situations:

i) $S = \{v\}$, $S' = \{v'\}$, $d^-(v') = 2$;
ii) $S = \{v, w\}$, $S' = \{v'\}$, $d^-(v') = 3$;
iii) $S = \{v, w\}$, $S' = \{v', w'\}$, $d^-(v') = d^-(w') = 2$.

We complete the proof of the theorem by examining these cases in turn. Observe that in the final two cases, $v^* \neq w^*$, $\{v^*, w^*\} \cap \{v, w\} = \emptyset$ by Corollary 8.12 and $r(u) \in \{v^*, w^*\}$ for all $u \in V(G)$ by Lemma 8.13.

Theorem 8.15. *For $k \geq 3$, $(1,1,k;-1)$-graphs are totally regular.*

Proof. We refer the reader to Figure 8.2 for clarity. Suppose that option i) holds. By Corollary 8.12 each vertex has a unique mixed path of length $\leq k$ to v. We therefore obtain an upper bound on the order of G by assuming that $v' \sim v$ and counting the vertices with paths of length $\leq k$ to v. There are $M(1,1,k-2) = F_{k+1} - 3$ vertices that can reach each of the directed in-neighbours of v' by paths of length $\leq k-2$, so, counting also v and v', the maximum possible order of G would be $2(F_{k+1} - 3) + 2 = 2F_{k+1} - 4$, which is too small for $k \geq 3$.

Now let us examine option ii). We can see that v' is a repeat as follows. Draw the Moore tree rooted at v'. We can assume that $r(v') \neq v'$, so that all directed in-neighbours of v' lie at distance k from v'. One branch of the Moore tree must contain two elements of $Z^-(v')$, so that v' is the repeat of a vertex in $N^+(v')$.

As all repeats lie in $\{v^*, w^*\}$, we can set $v' = v^*$. Hence $d^-(w^*) = 1$. If $k = 3$, then w has a unique in-neighbour w^*, which in turn has a unique directed in-neighbour; hence at most 7 vertices can reach w by paths of length ≤ 3, this bound being achieved when $v' \in N^-(w^*)$, whereas $M(1,1,3) - 1 = 10$. Thus $k \geq 4$. Draw the Moore tree rooted at v. Then $v_1 = v'$. Neither v_3 nor v_7 is equal to v', or there would be a cycle of length ≤ 2 through v', contradicting Lemma 8.11. Hence, since v_2 can reach both of these vertices by paths of length $\leq k$, but all vertices in $N^-(v_3) = \{v_1, v_6\}$ and $N^-(v_7) = \{v_3, v_{12}\}$ already appear in the v_1-branch, $r(v)$ must occur in both $N^-(v_3)$ and $N^-(v_7)$, so that $v_1 = v'$ has two short paths to $r(v)$ in violation of Lemma 8.11.

Finally assume that iii) holds. As in ii), we can show that both v' and w' are repeats, so we can take $v^* = v'$ and $w^* = w'$. If $k = 3$, counting initial vertices of paths of length ≤ 3 to v shows that the order of G is at most 9, whereas $|G| = 10$. Similarly, if $k = 4$ the order is at most 16, whereas $|G| = 18$. Assume that $k \geq 5$ and let u be an arbitrary vertex. Consider u_3, u_7, u_{11} and u_{13}. A directed in-neighbour and the undirected neighbour of each of these vertices already occur in the u_1-branch. However, u_2 can reach all of these vertices by paths of length $\leq k$. Therefore

- if $u_3 \notin S'$, then $r(u) \in \{u_1, u_6\}$;
- if $u_7 \notin S'$, then $r(u) \in \{u_3, u_{12}\}$;
- if $u_{11} \notin S'$, then $r(u) \in \{u_6, u_{19}\}$;
- if $u_{13} \notin S'$, then $r(u) \in \{u_7, u_{22}\}$.

By Lemma 8.11 the above sets are disjoint, with the exception of $\{u_1, u_6\}$ and $\{u_6, u_{19}\}$. Hence the five sets $\{u_3, u_7\}, \{u_3, u_{13}\}, \{u_7, u_{11}\}, \{u_7, u_{13}\}$ and $\{u_{11}, u_{13}\}$ intersect S'. These vertices are distinct and $|S'| = 2$, so the only solution is $S' = \{u_7, u_{13}\}$, $u_3, u_{11} \notin S'$. Thus $r(u) \in \{u_1, u_6\} \cap \{u_6, u_{19}\}$, so $r(u) = u_6$. All repeats lie in $\{v^*, w^*\} = S' = \{u_7, u_{13}\}$, so $u_6 \in \{u_7, u_{13}\}$, contradicting Lemma 8.11 □

8.4 Total regularity of 2-geodetic mixed graphs with excess one

We turn now to the question of the total regularity of mixed graphs with small excess. Recall that a mixed graph is an $(r, z, k; +\epsilon)$-graph if it has minimum undirected degree r, minimum directed out-degree z, is k-geodetic and has order equal to $M(r, z, k) + \epsilon$;

ϵ is the *excess* of G. We will show that $(r, z, 2; +1)$-graphs are totally regular.

Let G be an $(r, z, 2; +1)$-graph that is not totally regular. The graph G has order $(r+z)^2 + z + 2$ and it follows from Lemma 8.2 that G is out-regular. Therefore for every vertex u of G there is a unique vertex $o(u)$ that cannot be reached by a path of length ≤ 2 from u. We call $o(u)$ the *outlier* of u. The proof of the next lemma is similar to that of Lemma 8.4 and hence is omitted.

Lemma 8.16. *$S \subseteq \bigcap_{u \in V(G)} o(N^+(u))$, $S' \subseteq \bigcap_{u \in V(G)} N^+(o(u))$ and $d^-(v') = z + 1$ for all $v' \in S'$.*

Lemma 8.17. *$S' = N^+(o(u))$ for all $u \in V(G)$ and $S \subseteq N^-(v')$ for all $v' \in S'$.*

Proof. Fix $v' \in S'$. By 2-geodecity, every vertex has at most one path of length ≤ 2 to v'. By Lemma 8.16, S' is contained in the out-neighbourhood of any outlier, so by 2-geodecity v' is not an outlier and $V(G) = T_{-2}(v')$. Each vertex of S that lies in $N^-(v')$ reduces the number of vertices in $N^{-2}(v')$; by Lemma 8.16 each vertex in S' has directed in-degree $z + 1$, so that

$$\Sigma_{v \in S}(z - d^-(v)) = |S'|,$$

so it follows that the vertices of S in $N^-(v')$ can reduce the number of vertices in $N^{-2}(v')$ by at most $|S'|$. Hence we obtain a lower bound for the order of G by assuming that $S \subseteq N^-(v')$ and counting paths of length ≤ 2 to v', yielding

$$|V(G)| \geq 1 + r + z + 1 + r(r - 1 + z) + (z + 1)(r + z) - |S'|. \tag{8.5}$$

Rearranging, we obtain $|S'| \geq r + z$. By Lemma 8.16, $r + z$ is also an upper bound on the size of S', so we must have $|S'| = r + z$. Since $S' \subseteq N^+(o(u))$ for any vertex u by Lemma 8.16 and $|N^+(o(u))| = r + z$, it follows that $S' = N^+(o(u))$ for all $u \in V(G)$. As we have equality in Equation 8.5, every vertex of S must be contained in $N^-(v')$, implying the second half of the result. □

Theorem 8.18. *All $(r, z, 2; +1)$-graphs are totally regular.*

Proof. As no vertex is its own outlier, G contains at least two distinct outliers o_1 and o_2. If G is not totally regular, then by Lemma 8.17, $N^+(o_1) = N^+(o_2)\,(= S')$. Suppose that $r \geq 2$; then there are two distinct paths of length two from o_1 to o_2, contradicting 2-geodecity. Therefore $r = 1$. However, this implies that G contains a

perfect matching and hence has even order, whereas the order $z^2 + 3z + 3$ is odd. Therefore G must be totally regular. □

8.5 Total regularity of $(r, 1, k; +1)$-graphs for $k \geq 3$

As in the case of almost mixed Moore graphs, showing total regularity of k-geodetic mixed graphs with excess one for $k \geq 3$ is a more difficult problem. We solve it for directed out-degree $z = 1$. Let G be an $(r, 1, k; +1)$-graph that is not totally regular, where $k \geq 3$. By Lemma 8.2 G is out-regular. As before, for any vertex u the unique directed out-neighbour of u will be written u^+. We first make an observation concerning the relationship between the position of vertices in the Moore tree rooted at u and the outlier of the vertex u^+.

Lemma 8.19. *Draw the Moore tree of depth k for an arbitrary vertex u. Let w be such that $d(u, w) \leq k - 1$ and the mixed path from u to w does not begin with a directed arc (this includes the possibility $w = u$). Then if either*
i) $w \in S$ or
ii) $w \notin S'$ and w appears in the Moore tree as the endpoint of an arc,
then $w = o(u^+)$.

Proof. Condition ii) is illustrated in Figure 8.3, where dotted rectangles represent trees of depth $k - 1 \geq 2$. We suppose that $w \notin S'$; in-neighbours of w are shown in black. If w satisfies either of these conditions i) or ii), then, as in Figure 8.3, every vertex of $N^-(w)$ appears in the undirected branches of the tree. In particular, if $w = u \in S$, then u has no in-neighbours apart from those in $U(u) = N^+(u) - \{u^+\}$. Therefore by k-geodecity there are no in-neighbours of w within distance $k - 1$ of u^+, so that $d(u^+, w) > k$. □

Corollary 8.20. *$o(v^+) = v$ for all $v \in S$.*

Proof. As $v \in S$, all of the in-neighbours of v are contained in undirected branches of the Moore tree rooted at v. Therefore by Lemma 8.19 the outlier of v^+ must be v itself. □

We may now deduce the relative size of the sets S and S' and restrict the existence of edges and arcs in $S \cup S'$.

Lemma 8.21. *$|S| = |S'|$ and $o(v') \in Z^-(v')$ for all $v' \in S'$.*

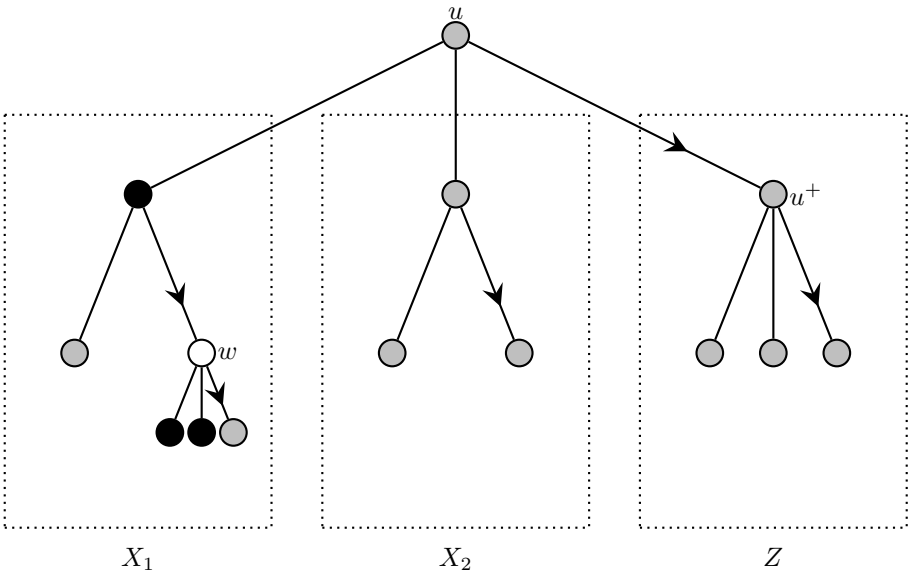

Figure 8.3: Diagram for Lemma 8.19

Proof. Every vertex in S has directed in-degree zero. Let v' be a vertex in S' and consider the Moore tree of depth k rooted at v'. By k-geodecity, none of the $r+1$ branches of the tree can contain more than one in-neighbour of v', so it follows that $d^-(v') = 2$ and $o(v')$ lies in $Z^-(v')$. As the average directed in-degree of G is one, S and S' must have the same size. □

Lemma 8.22. *S is an independent set. For each $v \in S$ we have $v^+ \in S'$.*

Proof. By definition S contains no arc. Suppose that $v \sim w$, where $v, w \in S$. Draw the Moore tree of depth k rooted at v. By Corollary 8.20, $o(v^+) = v$. But as $w \in S$ is at distance $\leq k-1$ from u and lies in an undirected branch, Lemma 8.19 implies that w would also be an outlier of v^+, so that $v = w$, which is impossible. Suppose now that $v \to w$, where $v \in S$ and $d^-(w) = 1$. Let $u \in U(v)$, so that there is a path $u \sim v \to w$. Applying Lemma 8.19 to u shows that both v and w would be outliers of u^+, again a contradiction. Thus $v^+ \in S'$ for all $v \in S$. □

These lemmas allow us to readily deduce the total regularity of $(r, 1, k; +1)$-graphs for $k \geq 4$.

Theorem 8.23. *$(r, 1, k; +1)$-graphs are totally regular for $k \geq 4$.*

Proof. Let $v \in S$. We know from Lemma 8.22 that v has no out-neighbours in S and that $v^+ \in S'$. We now show that in fact all out-neighbours of v lie in S'. Suppose for a contradiction that there is an edge $v \sim w$, where $d^-(w) = 1$. Choose a path $x \sim y \to w$. Applying Lemma 8.19 to the Moore tree rooted at x shows that v and w

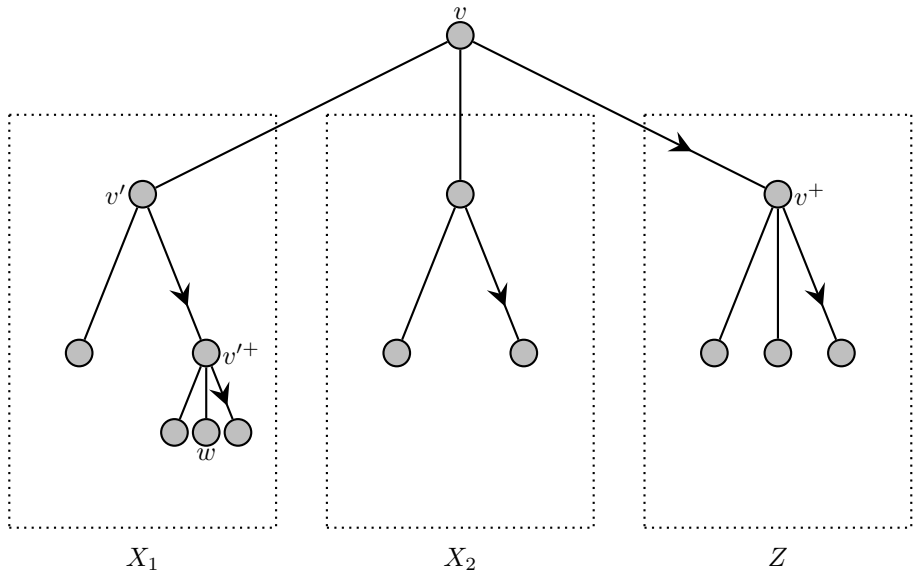

Figure 8.4: Diagram for Theorem 8.23 for $k \geq 4$

would both be outliers of x^+, an impossibility. Hence there can be no such edge and so $U(v) \subseteq S'$ for all $v \in S$. S and S' have the same size by Lemma 8.21, so we also have $U(v') \subseteq S$ for all $v' \in S'$.

Let $v \in S$ and draw the Moore tree of depth k rooted at v. Recall that $o(v^+) = v$. Let $v' \in S' \cap U(v)$. $(v')^+$ appears as the endpoint of an arc in an undirected branch of the tree, so by Lemma 8.19 $(v')^+$ must be in S', or it would be another outlier of v^+. Hence $U((v')^+) \subseteq S$, so $(v')^+$ has an undirected neighbour w in S at level three of the tree. This situation is depicted in Figure 8.4. By Lemma 8.19, w must be the outlier of v^+, so $w = v$, in violation of k-geodecity. Therefore G must be totally regular. □

The case $k = 3$ is more challenging. For the remainder of this section, assume G to be an $(r, 1, 3; +1)$-graph that is not totally regular. We first establish an upper bound on the size of the sets S and S'.

Lemma 8.24. $|S| = |S'| \leq r + 2$.

Proof. Fix $v \in S$. Drawing a Moore tree rooted at v^+ and applying Lemma 8.19, we see that at most one element of S is contained in $N^+(v^+)$, for any such vertex in $U(v^+)$ would be an outlier of $(v^+)^+$. Now considering the Moore tree rooted at v, we see from Lemma 8.19 that any element of S lying in an undirected branch of the tree lying at distance ≤ 2 from v would be an outlier of v^+, whereas we already know from Corollary 8.20 that $o(v^+) = v$; it follows by 3-geodecity that there can be at most 2 vertices of S at distance ≤ 2 from v, including v itself.

Now let w be a vertex of S that lies at distance ≥ 3 from v. There are more branches in the Moore tree rooted at v than there are in-neighbours of w, so there must be an out-neighbour x of v such that the branch of the Moore tree associated with x contains no in-neighbour of w, yielding $o(x) = w$. Since $o(v^+) = v$, we can in fact say that $x \in U(v)$. Therefore $\{w \in S : d(v, w) \geq 3\} \subseteq \{o(x) : x \in S\}$. It follows that there are at most r vertices of S lying at distance ≥ 3 from v. In total, there are thus at most $r + 2$ vertices in S. □

Lemma 8.25. $r = 2$.

Proof. Draw the Moore tree of depth 3 rooted at some $v \in S$, numbering vertices in accordance with our convention. Suppose that $r = 1$. As v_3 is not the outlier of $v_2 = v^+$, we must have $v_3 \in S'$ by Lemma 8.19. By Lemma 8.21, $o(v_3) \neq v$, for otherwise there would be an arc from v to v_3, so that v_3 can reach v by a mixed path of length ≤ 3. As v_1 is the only in-neighbour of v, it follows that there would be a ≤ 3-cycle through v_1. Hence $r \geq 2$.

There are exactly r vertices that v can reach by paths of length two consisting of an edge followed by an arc, each of which must lie in S', as none are outliers of v^+. Examine the r vertices that v^+ can reach by paths of this form; any of these vertices which do not lie in S' must be an outlier of $(v^+)^+$, so at least $r - 1$ of them belong to S'. Along with v^+, we have thus identified at least $1 + r + (r - 1) = 2r$ elements of S' in the tree. By Lemma 8.24, it follows that $2r \leq r + 2$. □

Theorem 8.26. $(r, 1, 3; +1)$*-graphs are totally regular.*

Proof. By Lemma 8.25, $r = 2$. By the argument of the preceding theorem, $|S| = |S'| = 4$ and each element v of S has four mixed paths of length ≤ 3 to S', namely an arc to v^+, a path of length three via v^+ and two paths of length two through the undirected neighbours of v. As $o(v^+) = v$ for $v \in S$, distinct elements of S have distinct directed out-neighbours in S', so there must be $v, w \in S$ and $v' \in S'$ such that there are paths $v \sim x \to v'$ and $w \sim y \to v'$ for some vertices x, y. It follows from Lemma 8.19 that $x \neq y$. Every vertex of S' has a directed in-neighbour in S and $d^-(v') = 2$, which implies that there is an edge in S, contradicting Lemma 8.22. □

Chapter 9

Bounds on the order of mixed graphs

As discussed in Chapter 7, it was shown by Nguyen et al. in [121] that there are no mixed Moore graphs with diameter $k \geq 3$. In this chapter we will extend their reasoning to give strong lower bounds on the excess of $(r, z, k; +\epsilon)$-graphs with $k \geq 3$ by a series of counting arguments using recurrence relations similar to those used to derive the mixed Moore bound [37].

In Section 9.1 we apply this method to totally regular mixed graphs and show that the outlier function of a mixed graph G with excess one is an automorphism if and only if G is totally regular. Section 9.2 extends this method to graphs that are not totally regular. In Section 9.3 we exploit these results to characterise $(2, 1, 2; +1)$-graphs. We then shift our attention to the degree/diameter problem for mixed graphs in Section 9.4, giving a lower bound on the excess of totally regular mixed graphs with given diameter, undirected degree $r = 1$ and directed out-degree $z = 1$. Finally in Section 9.5 we present the results of a computer search that identifies new mixed geodetic cages and, in cases in which geodetic cages have not yet been identified, establishes strong upper bounds on the excess of cages.

9.1 Bounds on totally regular mixed graphs with small excess

The proof of the non-existence of mixed Moore graphs [121] uses an argument that admits of very useful generalisations. We begin by proving a lemma that gives a counting principles that we will use throughout this chapter; we then immediately use this lemma to give a new bound on the order of totally regular $(r, z, k; \epsilon)$-graphs.

Definition 9.1. Let G be an out-regular mixed graph with undirected degree r and directed out-degree z. Fix a vertex $u \in V(G)$ and let $U(u) = \{u_1, u_2, \ldots, u_r\}$. Consider the Moore tree of depth k rooted at u. We call a position x in the Moore tree an *arrow vertex* (relative to the vertex u) if it satisfies the following three conditions:

- x lies in an undirected branch $T(u_i)$ of the Moore tree,
- x is at Level t of the Moore tree, where $2 \leq t \leq k - 1$, and
- x appears as the end-point of an arc from Level $t - 1$.

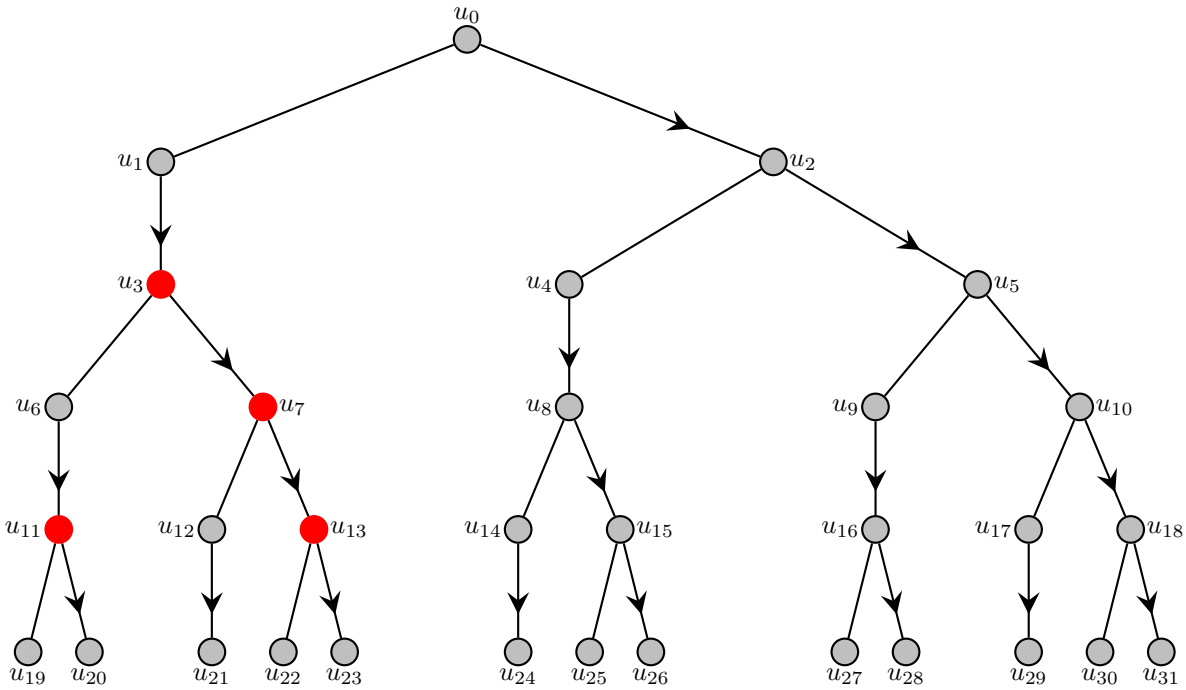

Figure 9.1: Arrow vertices in the Moore tree for $r = z = 1$ and $k = 5$

Notice that in general a vertex of G can appear several times in a Moore tree as an arrow vertex; however, if G is k-geodetic, then this issue does not arise.

For an illustration of Definition 9.1, see Figure 9.1; the vertices in red, namely u_3, u_7, u_{11} and u_{13}, are the arrow vertices of u_0 in this tree. Now we show how we will use the arrow vertices in our counting arguments.

Lemma 9.2. *Let u be a vertex of an out-regular k-geodetic mixed graph G with undirected degree r and directed out-degree z. Let x be an arrow vertex of u. Then either x has directed in-degree $d^-(x) \geq z + 1$, or else it is an outlier of at least $z - d^-(x) + 1$ vertices in $Z^+(u)$.*

Proof. Let x be an arrow vertex of u that lies at Level t of the Moore tree rooted at u, where $2 \leq t \leq k - 1$. As x is the end-point of an arc from Level $t - 1$ of the Moore tree, x has a directed in-neighbour at Level $t - 1$ of the tree inside an undirected branch. Furthermore, as x is at distance at most $k - 1$ from u, all vertices of $U(x)$ also appear at Level $t + 1$ of the tree in an undirected branch. Thus in total x has at least $r + 1$ members of $N^-(u)$ inside the undirected branches of the tree; hence there are at most $d^-(x) - 1$ vertices of $N^-(x)$ that can be contained in directed branches of the tree.

As G is k-geodetic, any in-neighbour of x that lies in a directed branch of the tree must lie at Level k; thus by k-geodecity each directed branch of the tree contains at

most one in-neighbour of x. Suppose that x has directed in-degree $d^-(x) \leq z$. Since at most $d^-(x) - 1$ vertices of $N^-(x)$ are contained in these branches, it follows that at least $z - d^-(x) + 1$ directed branches of the tree contain no in-neighbour of x, so that x is an outlier of at least $z - d^-(x) + 1$ vertices of $Z^+(u)$. □

Definition 9.3. The number of arrow vertices (counted by multiplicity) in the Moore tree of depth k of an out-regular mixed graph with undirected degree r and directed out-degree z will be denoted by $A(r, z, k)$.

We now count the arrow vertices to determine the function $A(r, z, k)$.

Lemma 9.4. *The number of arrow vertices in a Moore tree of depth k of an out-regular mixed graph with undirected degree r and directed out-degree z is given by*

$$A(r, z, k) = \frac{rz}{\phi}\Big[\frac{\lambda_1^{k-1} - 1}{\lambda_1 - 1} - \frac{\lambda_2^{k-1} - 1}{\lambda_2 - 1}\Big], \tag{9.1}$$

where

$$\phi = \sqrt{(r + z - 1)^2 + 4z},$$

$$\lambda_1 = \frac{1}{2}(r + z - 1 + \phi)$$

and

$$\lambda_2 = \frac{1}{2}(r + z - 1 - \phi).$$

Proof. Fix a vertex u of an out-regular mixed graph G with undirected degree r and directed out-degree z and consider the Moore tree of depth k rooted at u. For $1 \leq t \leq k - 1$, let Z_t be the number of vertices in the undirected branches at Level t in the Moore tree based at u that are end-points of arcs emanating from Level $t - 1$ and let U_t be the number of vertices in the undirected branches at Level t that are connected by an edge to Level $t - 1$. Obviously $U_1 = r, Z_1 = 0$ and $Z_1 = rz$. These numbers satisfy the recurrence relations

$$U_{t+1} = (r - 1)U_t + rZ_t, Z_{t+1} = zU_t + zZ_t$$

for $t \geq 1$. It follows that

$$Z_{t+2} = zU_{t+1} + zZ_{t+1} = z((r - 1)U_t + rZ_t) + zZ_{t+1}.$$

Substituting using the second relation,

$$Z_{t+2} = zZ_{t+1} + rzZ_t + z(r-1)(1/z)(Z_{t+1} - zZ_t) = (r+z-1)Z_{t+1} + zZ_t.$$

This second-order recurrence relation has characteristic equation

$$\lambda^2 - (r+z-1)\lambda - z = 0,$$

with solutions λ_1, λ_2 as given in the statement of the lemma. Observe that the discriminant $\phi^2 = (r+z-1)^2 + 4z$ is strictly positive, so that λ_1, λ_2 are real and distinct. It follows that

$$Z_t = A\lambda_1^t + B\lambda_2^t$$

for $t \geq 1$ and some constants A and B. Substituting $Z_1 = 0, Z_2 = rz$, we obtain

$$Z_t = \frac{rz}{\phi}(\lambda_1^{t-1} - \lambda_2^{t-1})$$

for $t \geq 1$. Summing, we find that there are

$$\sum_{i=0}^{k-2} \frac{rz}{\phi}(\lambda_1^i - \lambda_2^i) = \frac{rz}{\phi}\Big[\frac{\lambda_1^{k-1} - 1}{\lambda_1 - 1} - \frac{\lambda_2^{k-1} - 1}{\lambda_2 - 1}\Big]$$

arrow vertices. □

We now combine Lemmas 9.2 and 9.4 to give a strong bound on the excess of a totally regular k-geodetic mixed graph.

Theorem 9.5. *For $k \geq 3$, the excess ϵ of a totally regular $(r, z, k; +\epsilon)$-graph satisfies*

$$\epsilon \geq \frac{r}{\phi}\Big[\frac{\lambda_1^{k-1} - 1}{\lambda_1 - 1} - \frac{\lambda_2^{k-1} - 1}{\lambda_2 - 1}\Big],$$

where ϕ, λ_1 and λ_2 are as defined in Lemma 9.4.

Proof. Let G be a totally regular $(r, z, k; +\epsilon)$-graph. Fix a vertex u of G and consider the multiset

$$O(Z^+(u)) = \bigcup_{v \in Z^+(u)} O(v),$$

where vertices are counted by multiplicity. As each outlier set contains ϵ vertices, this multiset has size $z\epsilon$. By Lemma 9.2, each of the $A(r, z, k)$ arrow vertices of u is an

r/z	1	2	3	4	5	6
1	2	3	4	5	6	7
2	6	8	10	12	14	16
3	12	15	18	21	24	27
4	20	24	28	32	36	40
5	30	35	40	45	50	55
6	42	48	54	60	66	72
7	56	63	70	77	84	91
8	72	80	88	96	104	112
9	90	99	108	117	126	135
10	110	120	130	140	150	160
11	132	143	154	165	176	187
12	156	168	180	192	204	216
13	182	195	208	221	234	247
14	210	224	238	252	266	280
15	240	255	270	285	300	315

Table 9.1: Lower bound on the excess from Theorem 9.5 for $k = 4$

outlier of at least one vertex in $Z^+(u)$. It follows that

$$A(r, z, k) \leq z\epsilon.$$

Substituting using Equation 9.1 and dividing both sides by z yields the result. □

Some values of the lower bound in Theorem 9.5 for $k = 4$ are displayed in Table 9.1. We are not aware of any instance in which the bound of Theorem 9.5 is tight. However, as we shall now demonstrate, it does yield a powerful result on mixed graphs with excess one.

Corollary 9.6. *If G is a totally regular $(r, z, k; +1)$-graph with $k \geq 3$, then $r = 1$ and $k = 3$.*

Proof. If $k \geq 4$, then there are $> rz$ arrow vertices in the Moore tree of G, so that the bound of Theorem 9.5 shows that the excess of such a graph would be $\epsilon > \frac{rz}{z} = r$. We are assuming that G is mixed, so that $r \geq 1$ and ϵ would be strictly greater than one. Hence we can assume that $k = 3$, in which case Theorem 9.5 tells us that $\epsilon \geq r$, implying that for a totally regular $(r, z, 3; +1)$-graph we must have $r = 1$. □

Theorem 9.7. *There are no totally regular $(r, z, k; +1)$-graphs for $k \geq 3$.*

Proof. Let G be a totally regular $(1, z, 3; +1)$-graph. For any vertex $u \in V(G)$ write u^* for the undirected neighbour of u. Let the adjacency matrices of G, G^U and G^Z be A, A_U and A_Z respectively. Fix a vertex u and draw the Moore tree rooted at u.

Examination of the Moore tree shows that there are two walks of length ≤ 3 from u to itself (the trivial walk u of length zero and the walk $u \sim u^* \sim u$ of length two), two walks of length ≤ 3 from u to u^* ($u \sim u^*$ and $u \sim u^* \sim u \sim u^*$), three walks of length ≤ 3 from u to any directed out-neighbour v of u ($u \to v, u \sim u^* \sim u \to v$ and $u \to v \sim v^* \sim v$) and unique walks of length ≤ 3 from u to the vertices at distance two and three from u. It follows that

$$I + A + A^2 + A^3 = I + J + A + A_Z - P,$$

where I is the $n \times n$ identity matrix, J is the all-one matrix and $P_{vv'} = 1$ if $o(v) = v'$ and 0 otherwise. As G is totally regular, J commutes with the left-hand side, I and A_Z; therefore $JP = PJ$ and o is a permutation.

Take an edge uu^*. Lemma 9.2 and the fact that o is a permutation show that $o(Z^+(u)) = Z^+(u^*)$ and $o(Z^+(u^*)) = Z^+(u)$. Applying this result to an arbitrary directed in-neighbour v of u, we see that there is a path $v \sim v^* \to o(u)$. Let $w \in Z^+(o(u))$. A diagram of this situation is shown in Figure 9.2. There is a path of length three from v to w, so $d(u, w) \geq 3$; in fact, since o is a permutation, we have equality. Since only $r + z - 1$ in-neighbours of w lie in the Moore tree rooted at u, it follows that w must be the outlier of an out-neighbour of u. Examining the Moore tree of depth three based at v, we see that if w is an outlier of a vertex in $Z^+(u)$, then it would appear twice in the Moore tree rooted at v, once in the undirected v^*-branch and once in the u-branch in $Z^+(u^*)$, violating 3-geodecity. Therefore w is the outlier of u^*; as the excess is one, u^* has a unique outlier, so $z = 1$.

We can dispose of the case $r = z = 1, k = 3$ using Lemma 9.2. Let $u_8 \sim a, u_8 \to b, u_9 \to c, u_{10} \sim d, u_{10} \to e$; see Figure 9.3. Our argument shows that $o(u_2) = u_3$, so

$$\{a, b, c, d, e\} = \{u, u_1, u_6, u_7, u_{11}\},$$

where $u_{11} = o(u)$. As the undirected neighbours of u, u_1 and u_6 are accounted for, $\{b, c, e\} = \{u, u_1, u_6\}$ and $\{a, d\} = \{u_7, u_{11}\}$. We have $\{c, e\} \neq \{u, u_1\}$ or there would be a repeat in the Moore tree rooted at u_5. $u \neq b$ or else there would be paths $u_4 \sim u_2$ and $u_4 \to u_8 \to u \to u_2$, so $u \in \{c, e\}$. Thus $u_1 \notin \{c, e\}$, so $b = u_1$ and $\{c, e\} = \{u, u_6\}$. By 3-geodecity applied to u_8, $b = u_1$ implies that $a \neq u_7$, so $a = u_{11} = o(u)$ and hence $d = u_7$. $e \neq u_6$, or u_{10} would have two paths of length ≤ 3 to u_7. Therefore $c = u_6, e = u$.

Taking into account all adjacencies, it follows that there are three arcs from

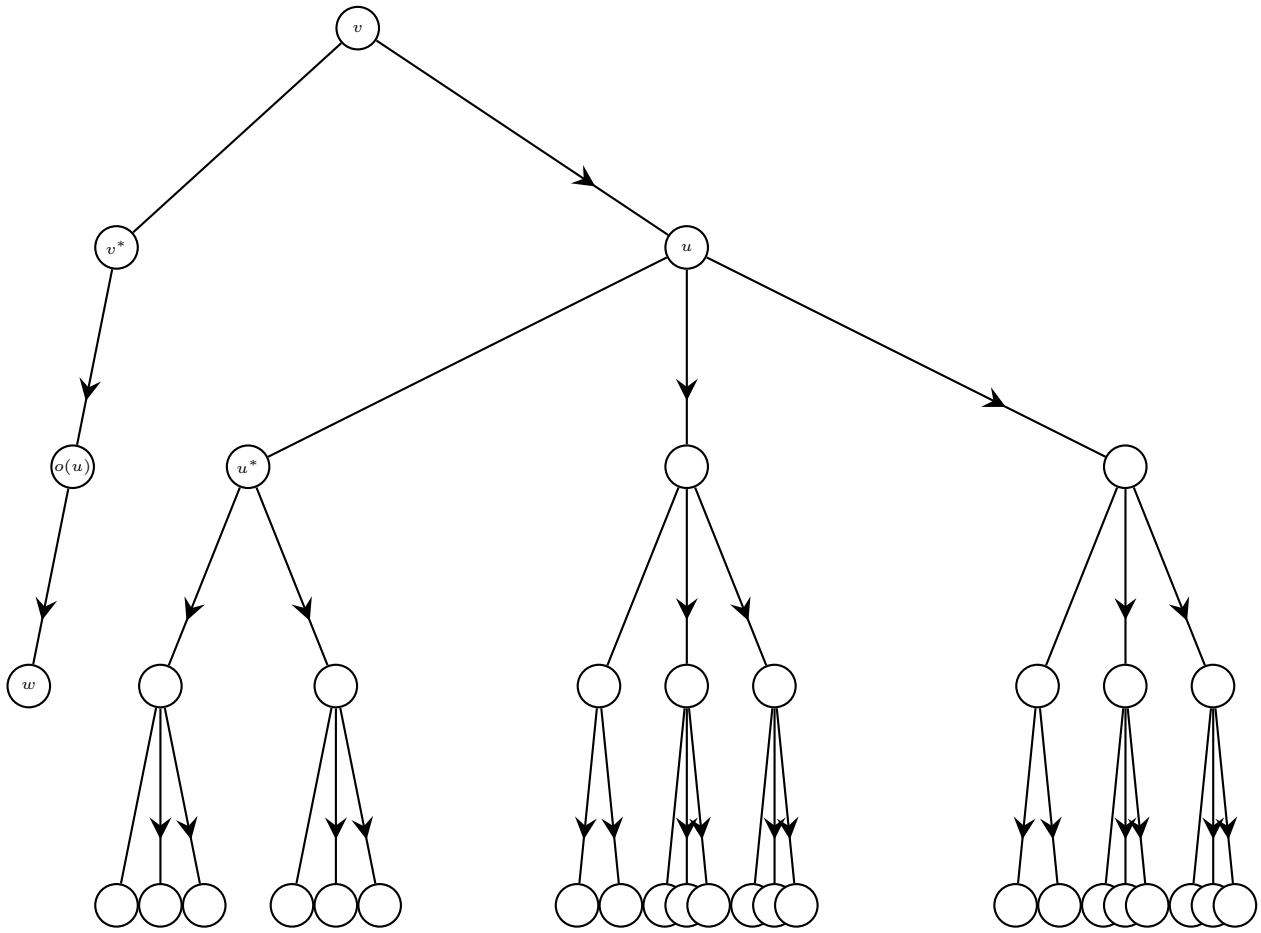

Figure 9.2: Configuration for Theorem 9.7 for $z = 2$

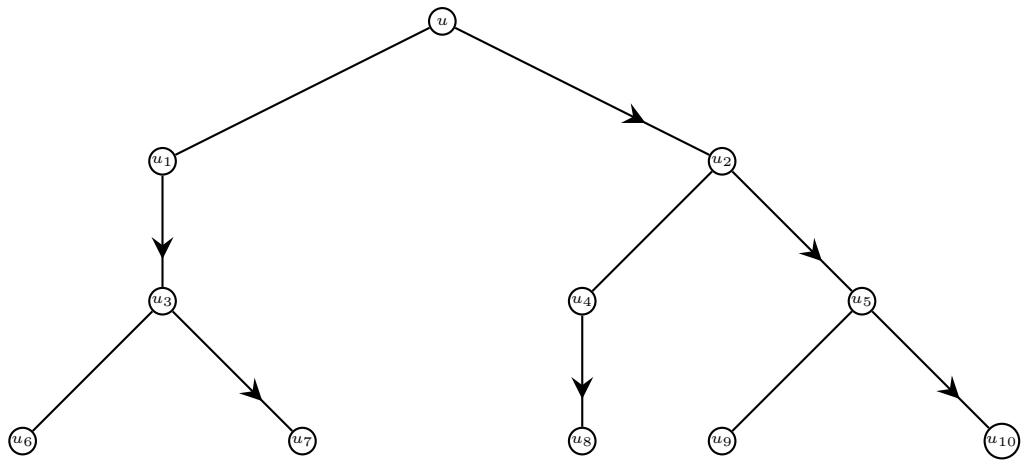

Figure 9.3: Moore tree for a 3-geodetic mixed graph with $r = z = 1$

$\{u_6, u_7, u_{11}\}$ to $\{u_4, u_9, u_{11}\}$. $u_{11} \not\to u_{11}$ and $u_{11} \not\to u_4$, or we would have $u_4 \to u_8 \sim u_{11} \to u_4$. Hence $u_{11} \to u_9$. $u_6 \not\to u_{11}$, or $u_9 \to u_6 \to u_{11} \to u_9$, so $u_6 \to u_4$ and $u_7 \to u_{11}$. But now there are paths $u_1 \sim u \to u_2 \sim u_4$ and $u_1 \to u_3 \sim u_6 \to u_4$, contradicting 3-geodecity. As G has even order, G has excess $\epsilon \geq 3$. □

It follows from Corollary 9.6, Theorem 9.7 and the results of Chapter 8 that any $(r, z, k; +1)$-graph is either totally regular with $k = 2$, satisfying the conditions in Theorem 7.18, or else $k \geq 3$, $z \geq 2$ and G is not totally regular.

We conclude this section with a result on the connection between outlier sets and automorphisms of mixed graphs with excess one. It is known that the outlier function of a $(d, k; +1)$-digraph G is an automorphism if and only if G is diregular [132]. The above results now allow us to extend this result to the more general mixed setting.

Theorem 9.8. *The outlier function of an $(r, z, k; +1)$-graph G is an automorphism if and only if G is totally regular.*

Proof. Suppose firstly that G is not totally regular; recall that G must be out-regular. Let $v' \in S'$. Suppose that o is an automorphism. It follows that $o(v') \in S'$. However, this implies that $o(v')$ has $> r + z$ in-neighbours distributed among the $r + z$ branches of the Moore tree based at v', so that some out-neighbour of v' has ≥ 2 mixed paths to $o(v')$ with length $\leq k$. Thus if o is an automorphism, then G is totally regular.

Now let G be totally regular. Let $k = 2$ and write A for the adjacency matrix of G. Then

$$I + A + A^2 = J + rI - P,$$

where I is the $n \times n$ identity matrix, J is the all-one matrix and $P_{uv} = 1$ if $o(u) = v$ and 0 otherwise. As G is totally regular, both I and J commute with A. Therefore P commutes with A, so that o is an automorphism. There are no totally regular mixed graphs with excess one for $k \geq 3$ by Theorem 9.7, so the proof is complete. □

9.2 Excess of mixed graphs that are not totally regular

We will now revisit the counting arguments used in the previous section to derive a bound in the more difficult context of mixed graphs that are not totally regular. We will see that a bound for all mixed graphs, totally regular or not, can be achieved by relaxing the bound in Theorem 9.5 by a factor of $\frac{z}{2r+3z}$. It was shown in Chapter 8 that any $(r, z, k; +1)$-graph must be totally regular if either $k = 2$ or $z = 1$. Using the new bound presented in Theorem 9.9 we will improve on this result.

Theorem 9.9. *The excess of any (r, z, k)-cage satisfies*

$$\epsilon \geq \frac{rz}{(2r+3z)\phi}\Big[\frac{\lambda_1^{k-1}-1}{\lambda_1-1} - \frac{\lambda_2^{k-1}-1}{\lambda_2-1}\Big],$$

where λ_1, λ_2 and ϕ are as defined in Lemma 9.4.

Proof. Let G be an (r, z, k)-cage. We can assume that the directed subgraph of G is out-regular, by deleting some arcs if necessary. Recall that the number of arrow vertices in the Moore tree of an out-regular $(r, z, k; +\epsilon)$-graph is $A(r, z, k)$. By Lemma 9.4 we know that

$$A(r, z, k) = \frac{rz}{\phi}\Big[\frac{\lambda_1^{k-1}-1}{\lambda_1-1} - \frac{\lambda_2^{k-1}-1}{\lambda_2-1}\Big].$$

We are therefore aiming to prove that

$$\epsilon \geq \frac{1}{2r+3z}A(r, z, k).$$

We have $\frac{A(k)}{2r+3z} < \frac{A(k)}{r}$. Now $\frac{A(k)}{r}$ is the number of arrow vertices of G in an undirected branch of the Moore tree, so the number of vertices in a branch is at least $\frac{A(k)}{r}$; in the notation of Lemma 8.2 this yields $\frac{A(k)}{r} < \mu(r, z, k-1)$, so that

$$\frac{A(k)}{2r+3z} < \frac{A(k)}{r} < \mu(r, z, k-1).$$

Therefore if G contains a vertex u with undirected degree $d(u) \geq r+1$, then the claimed bound holds. Thus we can assume that G is out-regular.

Let the deficiency $\sigma^-(v)$ of a vertex $v \in S$ be $z - d^-(v)$ and the surplus $\sigma^+(v')$ of a vertex $v' \in S'$ be $d^-(v') - z$. As G is out-regular we have for the total deficiency σ

$$\sigma = \sum_{v \in S} \sigma^-(v) = \sum_{v' \in S'} \sigma^+(v').$$

As each vertex in S' contributes at least one to σ, we have $\sigma \geq |S'|$. We will now find an upper bound for σ in terms of r, z and ϵ.

Fix a vertex u of G and draw the Moore tree of depth k rooted at u. Write $U(u) = \{u_1, u_2, \ldots, u_r\}$. Let $v \in S$ have deficiency $\sigma^-(v) = s$. Suppose firstly that $d(u, v) \geq k$ (i.e. either v lies at the bottom of the tree or $v \in O(u)$). Then v can have in-neighbours in at most $r + z - s$ branches of the Moore tree and so lies in the outlier sets of at least s members of $N^+(u)$.

Now suppose that either $u = v$ or $d(u, v) \leq k - 1$ and v lies in an undirected branch of the tree. At most $z - s$ directed branches of the tree can contain in-neighbours of v (in fact $z - s - 1$ branches if v is an arrow vertex), so again v occurs at least s times in the multiset $O(Z^+(u))$.

Lastly we must consider the case that v lies in a directed branch of the tree and $d(u, v) \leq k - 1$. Consider the Moore tree based at any $u_i \in U(u)$, say u_1. v lies in an undirected branch of this tree and so by our previous analysis v occurs at least s times in $O(N^+(u_1))$.

We have now dealt with all members of S. Summing their deficiencies to find σ we find that the elements of S appear at least σ times in the multiset $O(N^+(u)) \cup O(N^+(u_1))$. As this multiset contains $(2r + 2z)\epsilon$ elements, we conclude that

$$\sigma \leq (2r + 2z)\epsilon.$$

We now estimate the size of the set S'. Again we consider the Moore tree rooted at u. If an arrow vertex x relative to u lies in $V(G) - S'$, then x cannot have an in-neighbour in every directed branch of the tree and so must be an outlier of at least one directed out-neighbour of u. There are $z\epsilon$ elements in $O(Z^+(u))$, so it follows that at least $A(r, z, k) - z\epsilon$ of the arrow vertices must lie in S'. Therefore

$$(2r + 2z)\epsilon \geq \sigma \geq |S'| \geq A(r, z, k) - z\epsilon.$$

Rearranging we derive the inequality

$$\epsilon \geq \frac{1}{2r+3z} A(r,z,k).$$

This proves the theorem. □

This result now enables us to rule out the existence of mixed graphs with excess one for $k \geq 4$ and 'most' values of r and z for $k = 3$.

Theorem 9.10. *There are no $(r,z,k;+1)$-graphs for $k \geq 4$ or for $k = 3$, $r \geq 4$ and $z > \frac{2r}{r-3}$.*

Proof. Setting $\epsilon = 1$ in Theorem 9.9 shows that if $A(r,z,k) > 2r+3z$, then no $(r,z,k;+1)$-graph can exist. If $k \geq 5$, then

$$A(r,z,k) \geq A(r,z,5) = rz^3 + 2r^2z^2 + r^3z - r^2z + rz.$$

If $z \geq 2$, then this expression obviously exceeds $2r+3z$, so let $z = 1$. By Theorem 8.23 G must be totally regular; however, no such graphs exist by Theorem 9.7.

Let $k = 4$. We have $A(r,z,4) = rz^2 + zr^2$. If $r \geq 2$ and $z \geq 2$, then $rz^2 + zr^2 \geq 4r + 4z > 2r + 3z$. The result follows for $z = 1$ by Theorem 8.23 and Theorem 9.7, so we can assume that $r = 1$. We want to show that $z^2 + z > 3z + 2$, i.e. $z^2 - 2z - 2 > 0$. This inequality holds for $z \geq 3$, so this leaves only the pair $(r,z) = (1,2)$ to deal with. However in this case the Moore bound $M(1,2,4)$ is even, so that G must have odd order. However, $r = 1$ implies that G has a perfect matching, so this is impossible.

Finally let $k = 3$. We have $A(r,z,3) = rz$, so $A(r,z,3) > 2r+3z$ if and only if $r \geq 4$ and $z > \frac{2r}{r-3}$. □

For $k = 3$ this leaves open the cases $r = 1,2,3$, $r = 4$ and $2 \leq z \leq 8$, $r = 5$ and $2 \leq z \leq 5$, $r = 6$ and $2 \leq z \leq 4$, $r = 7,8$ and 9 and $2 \leq z \leq 3$ and $r \geq 10$ and $z = 2$. We can deal with the majority of these cases by a slightly more sophisticated method.

Lemma 9.11. *If G is an $(r,z,k;+1)$-graph that is not totally regular, then every vertex $v' \in S'$ has directed in-degree $z+1$. Therefore $\sigma = |S'|$.*

Proof. Consider the Moore tree rooted at $v' \in S'$. Each branch of the tree can contain at most one in-neighbour of v' by k-geodecity. Therefore, as v' has at least $r+z+1$

in-neighbours we conclude that each branch contains exactly one in-neighbour of v' and $o(v') \in Z^-(v')$. Hence v' has exactly $r + z + 1$ in-neighbours. □

Lemma 9.12. *No $v' \in S'$ is an outlier.*

Proof. Assume for a contradiction that G is an $(r, z, k; +1)$-graph in which $o(u) = v'$ for some $u \in V(G)$ and $v' \in S'$. As v' is the outlier of u, no in-neighbour of v' can lie at distance less than k from u. By k-geodecity, we conclude that every branch of the Moore tree rooted at u contains a unique in-neighbour of v' at distance k from u. Therefore we must have $o(u) \in N^-(v')$ to account for the final in-neighbour of v'. As $v' = o(u)$, this contradicts k-geodecity. □

Lemma 9.13. *For $k = 3$, if an $(r, z, 3; +1)$-graph exists, then $z^2 + z + r \geq \sigma \geq z + r$.*

Proof. Let G be an $(r, z, 3; +1)$-graph. The Moore bound for $k = 3$ is

$$M(r, z, 3) = r^3 + z^3 + 3rz^2 + 3r^2z - r^2 + z^2 + r + z + 1.$$

The order of G is $n = M(r, z, 3) + 1$. The Moore bound for $k = 2$ is

$$M(r, z, 2) = r^2 + z^2 + 2rz + z + 1.$$

Fix some $v' \in S'$. By Lemma 9.12, every vertex of G can reach v' by a mixed path of length ≤ 3. We achieve a lower bound for the number of these vertices by assuming that $S \subseteq N^-(v')$. Taking into account that v' has exactly one extra directed in-neighbour by Lemma 9.11 and since all vertices of $T_{-3}(v')$ are distinct by 3-geodecity we obtain the following inequality:

$$n = M(r, z, 3) + 1 \geq M(r, z, 3) + M(r, z, 2) - \sigma(1 + r + z).$$

Rearranging,

$$\sigma(1 + r + z) \geq M(r, z, 2) - 1 = r^2 + z^2 + 2rz + z.$$

Multiplying out, it is easily seen that $\sigma \geq r + z$. Now we turn to the upper bound. Fix a vertex u and draw the Moore tree based at u. By the argument of Theorem 9.9, we see that any vertex v in S that lies in $\{u, o(u)\} \cup N^k(u)$ or any of the undirected branches of the tree must be an outlier of at least $\sigma^-(v)$ vertices in $N^+(u)$. Therefore these vertices between them contribute at most $r + z$ to the total σ.

Fix a directed out-neighbour u^+ of u and consider the vertices in the Moore tree rooted at u^+ at distance ≤ 1 from u^+. Any vertex $v \in S$ belonging to this set will be an outlier of at least $\sigma^-(v)$ vertices in $Z^+(u^+)$. Between them such vertices can therefore contribute at most z^2 to the total σ. Since we have now considered all vertices in G, the conclusion follows. □

Theorem 9.14. *There are no $(r, z, 3; +1)$-graphs with $r \geq 2$.*

Proof. Suppose that G is an $(r, z, 3; +1)$-graph with $r > 1$. We know from Lemma 9.13 that $z^2 + r + z \geq \sigma \geq r + z$, so we can write $\sigma = z^2 + r + z - \alpha$, where $0 \leq \alpha \leq z^2$. Fix an arbitrary vertex u of G and draw the Moore tree rooted at u. There are rz arrow vertices in the tree relative to u, i.e. rz vertices in the set $Z^+(U(u))$. If any of the arrow vertices does not belong to S', then it will be an outlier of a vertex in $Z^+(u)$. It follows that at least $(r-1)z$ of the arrow vertices belong to S'. Repeating this reasoning for each vertex in $N^+(u)$ and taking into account that the vertices of $Z^+(u)$ are arrow vertices relative to any vertex in $U(u)$, we see that there are at least

$$(r-1)z + (r-1)z + (r-1)(r-2)z + z^2(r-1) = (r-1)(z^2 + rz)$$

vertices of S' in the tree. In fact, if we take u to be an element of S', a valid assumption by Theorem 9.7, then we can actually deduce that

$$\sigma = z^2 + r + z - \alpha = |S'| \geq (r-1)(z^2 + rz) + 1.$$

Rearranging, we see that α must satisfy

$$\alpha \leq z^2 + r + z - rz^2 - r^2z + z^2 + rz - 1 = -zr^2 - (z^2 - z - 1)r + (2z^2 + z - 1).$$

If $r \geq 2$ and $z \geq 2$, then

$$\alpha \leq -zr^2 - (z^2 - z - 1)r + (2z^2 + z - 1) \leq -4z - 2(z^2 - z - 1) + (2z^2 + z - 1) = -z + 1 < 0,$$

so it follows that we must have $r = 1$ and, considering the parity of the Moore bound, z must be odd. □

By Theorems 9.10 and 9.14 the only remaining open case left for $k \geq 3$ is the question of the existence of a non-totally regular $(1, z, 3; +1)$-graph. We finally settle this outstanding problem.

Theorem 9.15. *If G is an $(r, z, k; +1)$-graph with $r, z \geq 1$, then $k = 2$ and G is totally regular.*

Proof. Suppose that G is an $(r, z, k; +1)$-graph with $k \geq 3$. Then by Theorems 9.10 and 9.14 we have $r = 1$, $k = 3$ and z is odd. Also G is not totally regular by Theorem 9.7, which rules out $z = 1$ by Theorem 8.26. Fix a vertex u of G. Let u^* be the undirected neighbour of u and $\{u_1, u_2, \ldots, u_z\}$ be the set $Z^+(u)$ of directed out-neighbours of u. Draw the Moore tree of depth 3 rooted at u.

By counting the in-neighbours of a vertex $v \in S$ that are available to lie in the directed branches of the tree, it can be seen that v will be the outlier of at least $\sigma^-(v)$ vertices of $N^+(u)$ unless v lies in $U(Z^+(u))$, i.e. unless v is the undirected neighbour of a directed out-neighbour of u. For example, if $v \in Z^+(u)$, then the vertices u^* and v can reach v by mixed paths of length $\leq k$ and v has two in-neighbours already appearing in the tree (one is u and the other is v^* at Level 2), so that v has at most $z - \sigma^-(v) - 1$ further in-neighbours that can lie in the remaining $z - 1$ directed branches, so that v is the outlier of at least $\sigma^-(v)$ vertices in $N^+(u)$. Repeating this analysis for each position in the Moore tree implies the result.

However, if v lies in $U(Z^+(u))$, then we can only say that it will be the outlier of at least $\sigma^-(v) - 1$ vertices of $N^+(u)$ (it can be reached by two vertices of $N^+(u)$ by $\leq k$-paths and has a further $z - \sigma^-(v)$ in-neighbours available for the remaining $z - 1$ directed branches). Observe also that if an arrow vertex in the Moore tree lies in S, then this vertex v will be an outlier of at least $\sigma^-(v) + 1$ vertices of $Z^+(u)$.

Summing the deficiencies of all the vertices in S to get the total deficiency σ, we conclude that there are at most $2z + 1$ vertices of S, for at most z vertices of S can lie in $U(Z^+(u))$ and every other vertex v of S is an outlier of at least $\sigma^-(v)$ vertices in $N^+(u)$ and hence appears at least $\sigma^-(v)$ times in $o(N^+(u))$, which is a multiset with size $z + 1$. We now make this estimate more precise. For any vertex u of G define $\rho(u) = |S \cap U(Z^+(u))|$. Also let $\rho_{\min} = \min\{\rho(u) : u \in V(G)\}$. If u is a vertex at which this minimum value $\rho_{\min}$ is achieved, then as there are exactly $\rho_{\min}$ undirected neighbours of $Z^+(u)$ that lie in S, the total deficiency satisfies $\sigma \leq z + \rho_{\min} + 1$.

Suppose that $\rho_{\min} \geq 1$. For any vertex u, the sets $U(Z^+(u))$, $U(Z^+(u^*))$ and $U(Z^+(u_i))$ for $1 \leq i \leq z$ are mutually disjoint and each contain at least $\rho_{\min}$ vertices of S, which are distinct by 3-geodecity. Thus

$$(z + 2)\rho_{\min} \leq |S| \leq \sigma \leq z + \rho_{\min} + 1. \tag{9.2}$$

Rearranging, we see that either $\rho_{\min} = 0$ or $\rho_{\min} = 1$. Suppose that $\rho_{\min} = 1$; then we have equality in Equation 9.2, which implies that $|S| = z + 2$ and $\rho(u^*) = \rho(u_i) = 1$

for $1 \leq i \leq z$. Then as $\rho(u) = 1$, there is a directed out-neighbour of u (say u_1) such that $u_1^* \in S$. Applying the same reasoning to u_1, we conclude that each of the $z+2$ sets $U(Z^+(u_1))$, $U(Z^+(u_1^*))$ and $U(Z^+(u'))$, where u' is any directed out-neighbour of u_1, each contain one element of S; however, including u_1^*, we see that there would be at least $z+3$ elements of S in the Moore tree of depth three rooted at u_1, a contradiction.

Thus $\rho_{\min} = 0$. Hence by Lemma 9.13 we have $\sigma = z+1$. As no vertices of S lie in $U(Z^+(u))$, each of the elements $v \in S$ is an outlier of at least $\sigma^-(v)$ vertices of $N^+(u)$, so that we must have $o(N^+(u)) = S$ as multisets, where $v \in S$ appears $\sigma^-(v)$ times on the right-hand side. If any arrow vertex v in the Moore tree rooted at u (i.e. any vertex of $Z^+(u^*)$) belongs to S, then this vertex would contribute at least $\sigma^-(v)+1$ times to the set $o(Z^+(u))$, so that as $\sigma \geq z+1$, in total there would be $\geq z+2$ vertices in $o(N^+(u))$, which is impossible. Furthermore, if an arrow vertex lies in $V(G) - (S \cup S')$, then this vertex would be an outlier of a vertex in $Z^+(u)$, contradicting $o(N^+(u)) = S$. Thus all arrow vertices in the tree belong to S'.

Applying the same reasoning to the vertices in $N^+(u)$, we see that if some $w \in N^+(u)$ has $\rho(w) = 0$, then all vertices of $Z^+(w^*)$ would lie in S', so that the Moore tree of depth three rooted at u would contain at least $2z$ vertices of S', which is strictly greater than σ for $z \geq 3$. Thus $U(Z^+(w))$ contains at least one vertex of S for each $w \in N^+(u)$; it follows that each branch of the Moore tree rooted at u contains at least one vertex of S at distance three from u. As $|S| \leq \sigma = z+1$, we must have $|S| = z+1$ and each vertex in S has directed in-degree $z-1$.

There are only $z+1$ vertices in S, so we conclude that $\rho(w) = 1$ for each $w \in N^+(u)$. As there is only one vertex of S' not contained in $Z^+(u^*)$, there must be a directed out-neighbour of u, say u_1, such that $S' \cap Z^+(u_1^*) = \emptyset$. Since the $z+1$ vertices of S are contained in $U(Z^+(N^+(u)))$, we also have $S \cap Z^+(u_1^*) = \emptyset$, so that $Z^+(u_1^*) \subseteq V(G) - (S \cup S')$. It follows that $Z^+(u_1^*) = o(Z^+(u_1))$. However, as just one vertex of S is contained in $U(Z^+(u_1))$, at least z vertices in $N^+(u_1)$ must have outliers in S, implying that $z = 1$, a contradiction. □

This completes our classification of k-geodetic mixed graphs with excess one for $k \geq 3$.

9.3 The unique $(2, 1, 2; +1)$-graph

In [38] it is proven that there is a unique almost mixed Moore graph with diameter $k = 2$ and degree parameters $r = 2, z = 1$. At the time it was unknown whether such a graph must be totally regular. Using our total regularity result in Theorem 8.18, we will now prove that there is a unique 2-geodetic mixed graph with the same degree parameters $r = 2, z = 1$ and excess $\epsilon = 1$.

Let $D_{12} = \langle x, y : x^6 = y^2 = e, yxy^{-1} = x^{-1} \rangle$ be the dihedral group with order 12. It is easily verified that the Cayley graph on D_{12} with generating set $\{x^2, y, xy\}$, where the generator x^2 is associated with arcs and the involutions y, xy with edges, is a $(2, 1, 2; +1)$-graph. It is displayed in Figure 9.4. We proceed to show that up to isomorphism this graph is the unique $(2, 1, 2; +1)$-graph. Hence let G stand for an arbitrary graph with these parameters.

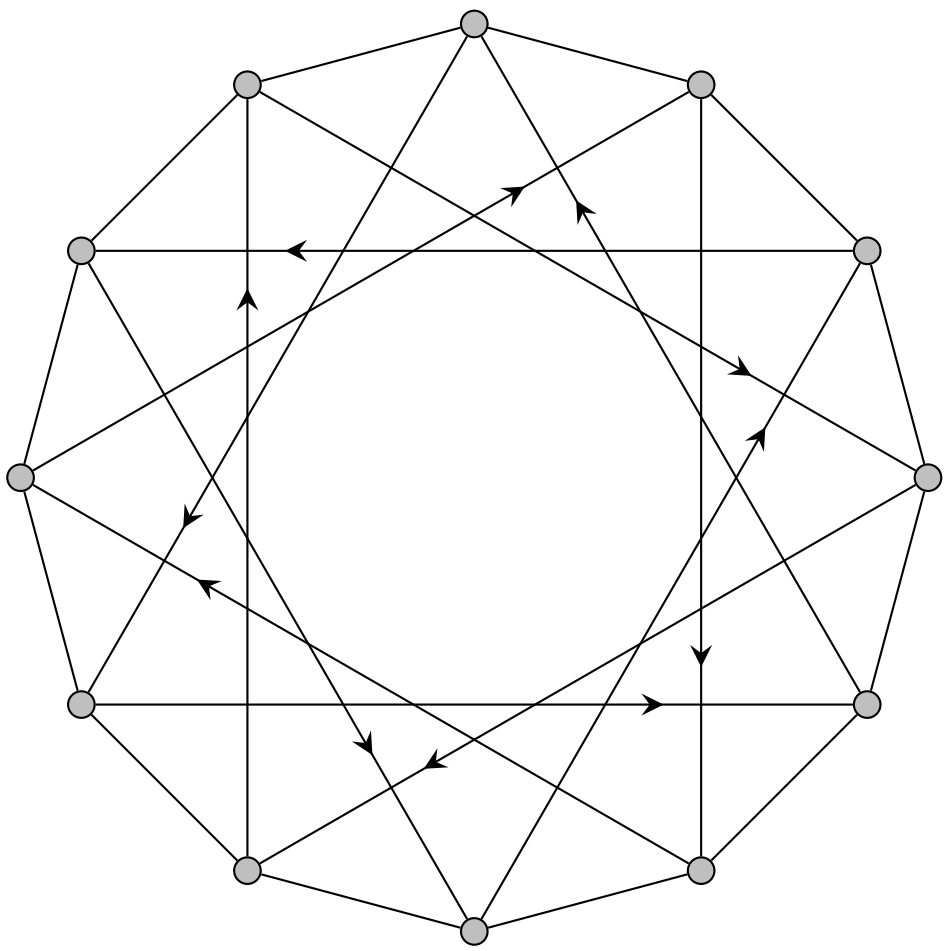

Figure 9.4: The unique 2-geodetic mixed graph with $r = 2, z = 1$ and excess $\epsilon = 1$

By Theorem 8.18, G^U is 2-regular and G^Z is diregular with degree $z = 1$. By 2-geodecity, G^U cannot contain any cycle of length ≤ 4. Hence there are three

possibilities: i) $G^U \cong C_5 \cup C_7$, ii) $G^U \cong 2C_6$ and iii) $G^U \cong C_{12}$.

Lemma 9.16. *If $d_U(u,v) \leq 3$, then u and v are independent in G^Z.*

Proof. The result is trivial if $d_U(u,v) = 1$. If $d_U(u,v) = 2$, then any arc between u and v would violate 2-geodecity. Similarly, if $d_U(u,v) = 3$ and $u \to v$, there is a path $u \sim u_1 \sim u_2 \sim v$, so that there are paths $u_1 \sim u \to v$ and $u_1 \sim u_2 \sim v$, which again is impossible. □

Lemma 9.17. $G^U \cong C_{12}$.

Proof. Suppose that $G^U \cong C_5 \cup C_7$. By Theorem 8.18, there must be an arc with both endpoints in C_7. However, these endpoints are at distance at most three in G^U, contradicting Lemma 9.16.

Now let $G^U \cong 2C_6$. We shall label the vertices of G (i,r), where $i \in \mathbb{Z}_6$ and $r = 0,1$, so that $(i,r) \sim (i \pm 1, r)$, where addition is carried out modulo 6. By Lemma 9.16, any arc must have its initial and terminal points in different cycles and by Theorem 8.18 arcs that begin at distinct vertices of one cycle have distinct endpoints. Without loss of generality, $(0,0) \to (3,1)$. As $(0,0)$ can already reach the vertices $(1,0),(2,0),(5,0)$ and $(4,0)$ by paths in G^U of length ≤ 2, by 2-geodecity we must have $(3,1) \to (3,0)$. Continuing in this manner, we deduce the existence of the 4-cycle $(0,0) \to (3,1) \to (3,0) \to (0,1) \to (0,0)$. Now $(0,0)$ can reach the vertices $(3,1),(2,1)$ and $(4,1)$ by paths of length ≤ 2, so either $(1,0) \to (1,1)$ or $(1,0) \to (5,1)$; by symmetry, we can set $(1,0) \to (5,1)$. We now deduce the existence of the cycle $(1,0) \to (5,1) \to (4,0) \to (2,1) \to (1,0)$. But now $(5,0) \not\to (4,1)$, or we would have $(0,0) \to (3,1) \sim (4,1)$ and $(0,0) \sim (5,0) \to (4,1)$, and likewise $(5,0) \not\to (1,1)$, or else $(4,0) \to (2,1) \sim (1,1)$ and $(4,0) \sim (5,0) \to (1,1)$. It follows that G^U is a twelve-cycle. □

Theorem 9.18. *The graph in Figure 9.4 is the unique $(2,1,2;+1)$-graph up to isomorphism.*

Proof. By Lemma 9.17, G^U is a 12-cycle. We will label its vertices by the elements of $\mathbb{Z}_{12}$, so that $i \sim i \pm 1$ for $i \in \mathbb{Z}_{12}$, where addition is modulo 12. By Lemma 9.16, for each $i \in \mathbb{Z}_{12}$ we have $i \to i + r$, where $4 \leq r \leq 8$. Suppose that for some i we have $i \to i + 6$, say $0 \to 6$. Then 6 is not adjacent to any vertex in $\{3,4,5,6,7,8,9\}$ by Lemma 9.16. Also 0 can already reach every vertex in $\{10,11,0,1,2\}$ by undirected paths of length ≤ 2, so by 2-geodecity the arc from 6 also cannot terminate in this set. Thus $i \not\to i + 6$ for all $i \in \mathbb{Z}_{12}$.

Suppose now that there are vertices u, v such that $d_U(u, v) = 5$ and $u \to v$; without loss of generality, let $0 \to 5$. By 2-geodecity, $5 \not\to 10, 11, 0, 1$ or 2 and by Lemma 9.16 $5 \not\to 3, 4, 5, 6, 7$ or 8. Thus $5 \to 9$. Consider the vertices that could be the directed in-neighbour of 0. By Lemma 9.16 none of the vertices $9, 10, 11, 1, 2$ or 3 can have an arc to 0. The vertices $4, 6$ and 7 can already reach 5 by undirected paths of length ≤ 2, so, as $0 \to 5$, none of these vertices has an arc to 0. Therefore $8 \to 0$. Finally we turn to the vertex 1. By Lemma 9.16 1 cannot have an arc to any of $10, 11, 2, 3$ or 4. If $1 \to 8$, then 1 would have two paths $1 \sim 0$ and $1 \to 8 \to 0$ to 0. Similarly, if $1 \to 6$ then 1 would have two paths to 5. Thus $1 \to 7$. However, $7 = 1 + 6$, contradicting our previous result.

Therefore for each $i \in \mathbb{Z}_{12}$ we have $i \to i \pm 4$. By symmetry we can take $0 \to 4$, so that we have the 3-cycle $0 \to 4 \to 8 \to 0$. We cannot have $1 \to 5$, or there would be two paths from 0 to 5 of length two. Therefore $1 \to 9 \to 5 \to 1$. Applying the same reasoning to the vertices 2 and 3, we deduce that G^Z contains cycles $2 \to 6 \to 10 \to 2$ and $3 \to 11 \to 7 \to 3$. By Theorem 8.18 we have accounted for all edges and arcs, so it follows that G is isomorphic to the graph in Figure 9.4. □

This reasoning can be extended to the open case of $(2, z, 2; +1)$-graphs in Theorem 7.18. Let G be any $(2, z, 2; +1)$-graph. We know by the results of Chapter 8 that G is totally regular and by Theorem 9.8 that the outlier function o is an automorphism of G. Let G^U and G^Z be respectively the undirected and directed subgraphs of G. G^U is a disjoint union of cycles of length ≥ 5, so we can characterise G^U by giving the lengths of the cycles in G^U. We will say that an s-cycle in G^U is *unique* if it is the only cycle of that length in G^U. We will also say that a cycle of G^U is *empty* if it induces an independent set in G^Z.

Lemma 9.19. *If u lies in a cycle of length s in G^U, then $o(u)$ also belongs to a cycle of length s. In particular, if C is a unique cycle, then o acts on C as a rotation.*

Proof. The first part of the statement follows from the fact that o is an automorphism of G and hence of G^U. Thus if C is the only cycle of length s in G^U, then o is a symmetry of C, so that o acts on C either as a rotation or a reflection. However o can have no fixed points and also contains no transpositions (u, v) where $u \sim v$ in G, so o must act on C as a rotation. □

Corollary 9.20. *There are no unique 5-cycles in G^U.*

Proof. By Lemma 9.3 if C is a unique 5-cycle an $u \in V(C)$, then $o(u)$ also lies in C; however u can reach every vertex of C by paths of length ≤ 2 in G^U. □

Lemma 9.21. *Any cycle in G^U of length ≤ 7 is empty. Any unique cycle of length 8 is empty.*

Proof. Let C be a cycle of length s. We will identify its vertex set with $\mathbb{Z}_s$. Suppose that there is a directed chord in C; without loss of generality we can assume that this arc is $0 \to i$. By 2-geodecity $i \notin \{-3,-2,-1,0,1,2,3\}$, so it follows instantly that $s \geq 8$. If $s = 8$ and C is unique, then we must have $o(0) \in \{3,4,5\}$ and by the previous reasoning we have $i = 4$; however, this means that 0 has a mixed path of length ≤ 2 to each of $3, 4$ and 5, a contradiction. □

Lemma 9.22. *Let C be a non-empty unique cycle of length $s \geq 8$ and identify its vertex set with $\mathbb{Z}_s$. Then o acts on $V(C)$ as $o(i) = i + r$, where $r \notin \{-2,-1,0,1,2\}$ and the gcd of r and s satisfies $(r,s) > 1$.*

Proof. The form of o follows immediately from Lemma 9.3. Suppose that $(r,s) = 1$ and that $0 \to t$. Applying the automorphism o repeatedly to this arc we deduce that $r \to t + r$, $2r \to t + 2r$ and in general $jr \to t + jr$ for $0 \leq j \leq s - 1$. However, as $(r,s) = 1$, we conclude that for every vertex i in C we have an arc $i \to i + t$. It follows that we would have mixed paths $0 \to t \sim t + 1$ and $0 \sim 1 \to t + 1$, violating 2-geodecity. □

The condition $(r,s) > 1$ is clearly not satisfied if s is prime.

Corollary 9.23. *Any unique cycle of prime length is empty.*

Corollary 9.24. *G^U does not consist of two empty cycles of different lengths; in particular, the cycle lengths cannot be (p,q), where p and q are prime.*

Proof. Suppose that G^U is the union of two empty cycles C and D with lengths s and t respectively. Then by total regularity each vertex in C has two arcs to D and each vertex of D has two arcs from D, so we must have $2s = 2t$. The final statement follows from Corollary 9.23. □

It follows by Corollaries 9.20 and 9.24 that the possible cycle-lengths in the undirected subgraph G^U of a $(2,2,2;+1)$-graph are i) $(5,5,5,5)$, ii) $(10,5,5)$, iii) $(8,6,6)$, iv) $(7,7,6)$, v) $(14,6)$, vi) $(12,8)$, vii) $(10,10)$ and viii) (20). This fact can be

used to show non-existence of $(2,2,2;+1)$-graphs by a case analysis; however, the proof is long. The computer search presented in Section 9.5 shows that $(2,2,2)$-cages have excess $\epsilon = 2$ (see also [144]).

9.4 Bounds on totally regular mixed graphs with small defect

We now return to the degree/diameter problem for mixed graphs and extend the counting arguments from the previous section to deal with totally regular mixed graphs with small defect. The first non-trivial bound for such graphs was derived in [51], where it is shown that for a totally regular $(r,z,k;-\delta)$-graph with $k \geq 3$ the defect is bounded below by the undirected degree r. There is equality for $k = 3$ and hence the bound is tight. We present a new upper bound on the order of totally regular $(1,1,k;-\delta)$-graphs that improves on the result of [51] for $k \geq 4$.

Let G be a totally regular mixed graph with undirected degree $r = 1$, directed degree $z = 1$ and diameter k. We will denote the unique undirected neighbour of a vertex v of G by v^*, the directed in-neighbour by v^- and the directed out-neighbour by v^+. Since $r = 1$, G contains a perfect matching and must have even order.

For any vertex v of G we make the further definition that $v^1 = (v^+)^*$, that is v^1 is the undirected neighbour of the directed out-neighbour of v. We extend this definition as follows. We set $v^0 = v$ and by iteration define $v^s = (v^{s-1})^1$ for $s \geq 2$. By analogy we specify that $v^{-1} = (v^*)^-$, so that v^- is the directed in-neighbour of the undirected neighbour of v. Again we set iteratively $v^{-s} = (v^{-(s-1)})^-$. Notice that $(v^1)^{-1} = (v^{-1})^1 = v$ for all $v \in V(G)$.

We draw the Moore tree of G of depth k based at a vertex u as indicated in Figure 9.5. In particular, if a vertex at Level $t \leq k-1$ of the tree has both an undirected neighbour and a directed out-neighbour at below it at Level $t+1$ of the tree, then we will place the undirected neighbour on the left and label the vertices accordingly. If $k \geq 3$, then there will be vertices repeated in the tree, so that a vertex of G can receive distinct labels in the Moore tree; nevertheless, for counting purposes we will still distinguish between the position labels in the tree. The left-hand side branch beginning at u_1 is the *undirected branch* and the right-hand side branch beginning at u_2 is the *directed branch*.

To reiterate, an arrow vertex in the Moore tree of G rooted at u is a vertex x at a Level t, $2 \leq t \leq k-1$, of the tree in the undirected branch such that x appears as the terminal vertex of an arc with its initial vertex at Level $t-1$. Unlike the k-geodetic

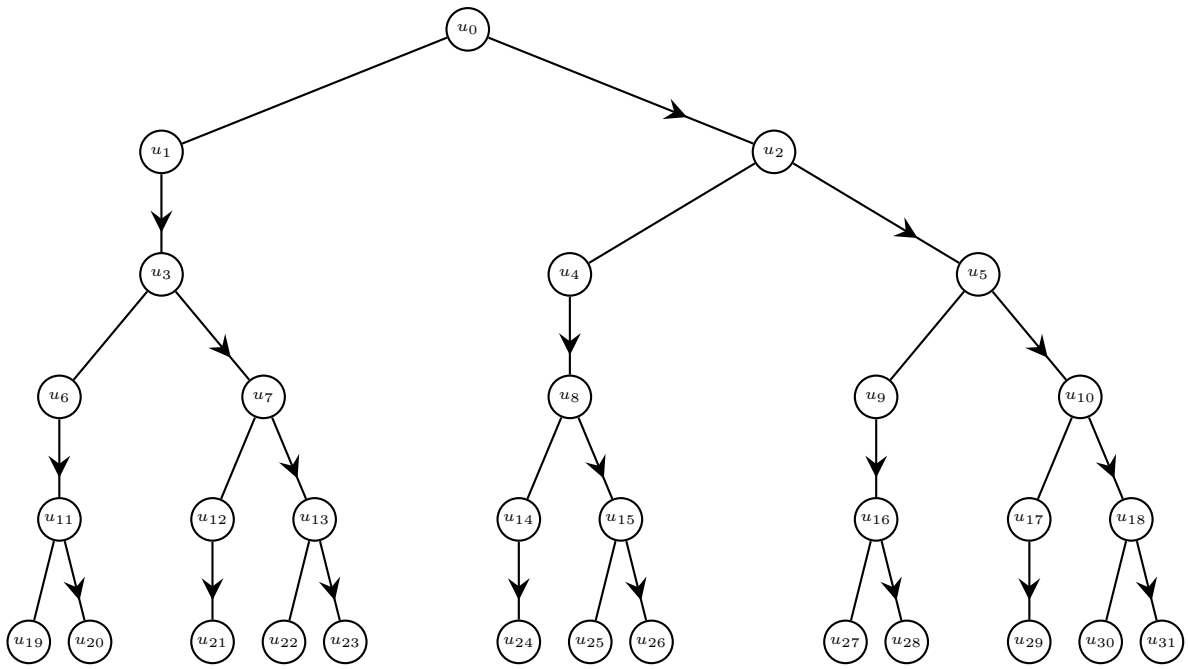

Figure 9.5: The Moore tree for $r = z = 1$ and $k = 5$.

case, arrow vertices can be equal in G or be equal to a vertex in the directed branch; therefore we will slightly abuse the term 'arrow vertex' by associating it, not with a vertex of G, but with a position or label in the tree.

Consider an arrow vertex x at Level t of the Moore tree. Its directed in-neighbour x^- appears at Level $t-1$ and its undirected neighbour x^* at Level $t+1$, so that the entire in-neighbourhood $N^-(x) = \{x^-, x^*\}$ is also contained in the undirected branch of the Moore tree. As G has diameter k, u_2 must be able to reach x by a mixed path of length $\leq k$, so it follows that at least one of x^-, x^* also appears in the directed branch of G. For every such occurrence there will be an additional repeat of u_0, so that we can bound the defect δ from below by counting the smallest possible number of positions in the undirected branch such that for every arrow vertex x either x^* or x^- lies in one of these positions. We will call such a set of positions a *transversal* of the undirected branch.

We will now focus on the undirected branch of the Moore tree. The undirected branch of a Moore tree of depth 8 is shown in Figure 9.6. For convenience we use a different labelling of the undirected branch; for example, vertex 1 corresponds to u_1 in Figure 9.5, 2 to u_3, 3 to u_6, 5 to u_{11}, etc. For the moment we ignore the complication that a vertex of G could appear multiple times as an arrow vertex in this tree. Under this assumption we will show that δ is bounded from below by the size of a minimum transversal of the Moore tree.

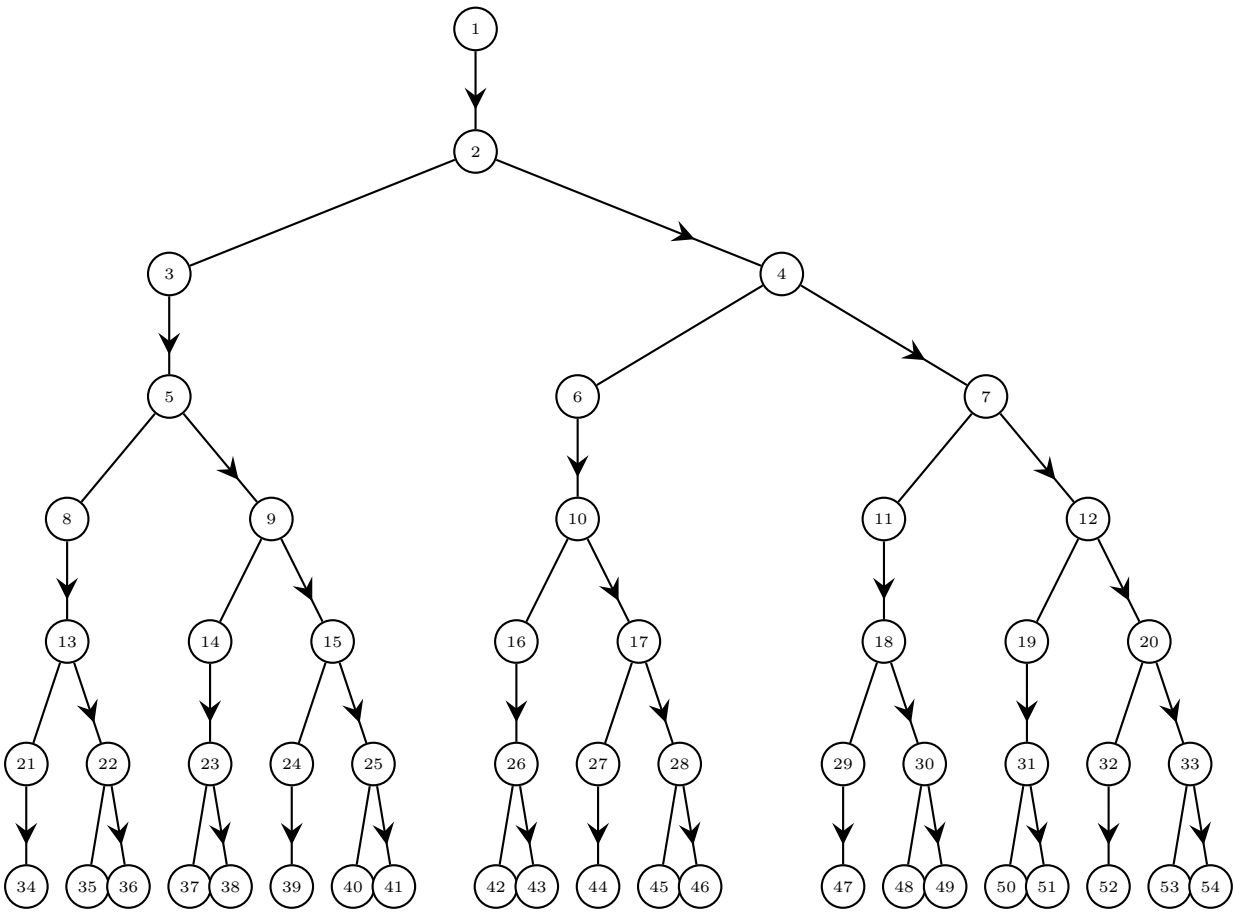

Figure 9.6: The undirected branch for $k = 8$

Consider an arrow vertex x at Level t of the tree, where $2 \leq t \leq k-1$. In the undirected branch shown in Figure 9.6 these are vertices 2, 4, 5, 7, 9, 10, 12, 13, 15, 17, 18, 20, 22, 23, 25, 26, 28, 30, 31 and 33. As already noted, either the undirected neighbour x^* or the directed in-neighbour x^- of x must occur in the directed branch of the Moore tree, and each such occurrence counts towards the number of repeats of the root vertex u of the tree. However, the in-neighbourhoods of the arrow vertices overlap; for example, the vertex 8 is an in-neighbour both of the vertex 5 and the vertex 13. We will partition the positions in the undirected branch of the Moore tree corresponding to vertices in the in-neighbourhoods of the arrow vertices into *chains*.

A chain is a maximal string of vertices in the undirected branch of the Moore tree of the form $v = v^0, v^1, v^2, v^3, \ldots$, where v is an in-neighbour of an arrow vertex. If v is at Level $t \leq k-2$, then v^2 is at Level $t+2$. For example $1, 3, 8, 21$ is a chain in Figure 9.6. Every in-neighbourhood of an arrow vertex is contained in a unique chain. Every arrow vertex at Level t, where $2 \leq t \leq k-2$, is the beginning of a chain, as is the vertex 1. Conversely, by iterating the $^-$ operation on an in-neighbour of an arrow vertex, i.e. considering the sequence of vertices $v, v^{-1}, v^{-2}, \ldots$, we see that every chain begins either at 1 or an arrow vertex at Level $t \leq k-2$. This decomposition is displayed for $k = 8$ in Figure 9.7.

We will call the number of vertices (i.e. positions in the Moore tree) in a chain $v, v^1, v^2, \ldots$ the *length* of the chain. For example, for $k = 8$ the chain $1, 3, 8, 21$ has length 4. Let C be a chain of length ℓ. Any pair of consecutive vertices in C is the in-neighbourhood of an arrow vertex, so at least one of them must appear in the directed branch of the Moore tree. As any vertex in C is contained in two pairs of consecutive vertices of the chain, it follows that the smallest transversal of C, i.e. the smallest number of vertices in the Moore tree that intersect every in-neighbourhood of arrow vertices that is contained in the chain, is $\lceil \frac{\ell}{3} \rceil$ (this follows from the domination number of the path [41]).

The number of chains beginning at Level t of the tree, where $2 \leq t \leq k-2$, is equal to the number of arrow vertices at Level t. From the calculation of Lemma 9.4 we know that this number is

$$Z_t = \frac{1}{2^{t-1}\sqrt{5}}((1+\sqrt{5})^{t-1} - (1-\sqrt{5})^{t-1}).$$

The first vertex 1 of the undirected branch is also the first vertex of a chain. We therefore define $Z'_t = 1$ for $t = 1$ and $Z'_t = Z_t$ for $2 \leq t \leq k-1$. The length of a chain beginning at Level t is $\ell(t) = 1 + \lfloor \frac{k-t}{2} \rfloor$. It follows from our argument that the

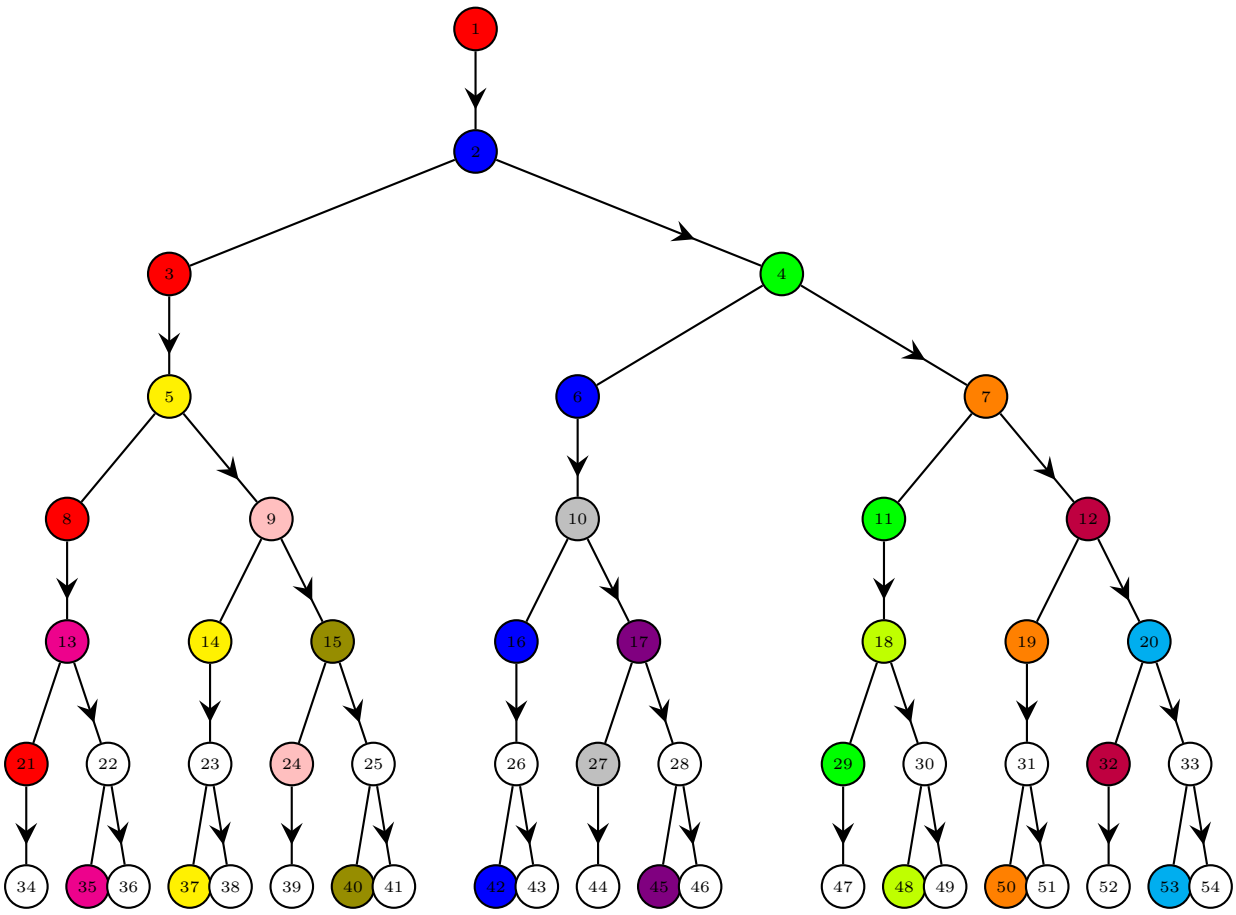

Figure 9.7: The chain decomposition for $k = 8$

smallest transversal of the undirected branch of the Moore tree has size

$$\sum_{t=1}^{k-2} Z'_t \left\lceil \frac{1}{3} + \frac{1}{3} \left\lfloor \frac{k-t}{2} \right\rfloor \right\rceil .$$

This expression gives a lower bound for the number of positions in the undirected branch of the Moore tree that are occupied by vertices that also appear in the directed branch. It could happen that these positions in the undirected branch are actually occupied by the same vertex, which would reduce the number of vertices that would have to be repeated in the directed branch.

However, it is easily seen that this does not affect our lower bound for the defect. Let T be the transversal of the undirected branch that is repeated in the directed branch of a largest $(r, z, k; -\delta)$-graph. If s positions of T are occupied by the same vertex v, then v occurs at least once in the directed branch of the Moore tree, but is also repeated at least $s - 1$ times in the undirected branch, so that this set of s positions nevertheless contributes at least s to the total defect δ. We therefore have proved the following theorem.

Theorem 9.25. *Any totally regular* $(1, 1, k; -\delta)$*-graph has defect*

$$\delta \geq \sum_{t=1}^{k-2} Z'_t \left\lceil \frac{1}{3} + \frac{1}{3} \left\lfloor \frac{k-t}{2} \right\rfloor \right\rceil$$

for $k \geq 3$.

9.5 Mixed geodetic cages and record graphs

In this section we present the results of a computer search due to Erskine that identifies new mixed geodetic cages and record graphs. We describe the search method only briefly and refer the reader to the paper [144] for more detail.

To identify geodetic cages, Erskine used a program in C to progressively add edges and arcs to a mixed Moore tree of depth k plus ϵ additional vertices, checking the geodetic girth at each step and backtracking whenever a violation was detected and increasing ϵ by one if no $(r, z, k; +\epsilon)$-graph exists. The results are summarised in Table 9.2. Mixed geodetic cages were classified for $(r, z, k) = (1, 1, 3)$ (shown in Figure 9.8) and $(r, z, k) = (1, 1, 4)$ (see Figure 9.9). The search also identified a geodetic cage for $(r, z, k) = (2, 2, 2)$ (see Figure 9.10), but has not yet completely classified these graphs.

r	z	k	M	n	ϵ	Comment
1	1	2	6	6	0	Kautz graph
1	1	3	11	16	5	Cages classified, Figure 9.8
1	1	4	19	30	11	Cages classified, Figure 9.9
1	1	5	32	54*	22*	No graphs of order less than 50
2	1	2	11	12	1	Cayley graph of D_{12}
2	1	3	28	48*	20*	No graphs of order less than 32
1	2	2	12	12	0	Kautz graph
3	1	2	18	18	0	Bosák graph
2	2	2	19	21	2	Figure 9.10, cages not classified
1	3	2	20	20	0	Kautz graph

Table 9.2: Smallest $(r, z, k; +\epsilon)$-graphs for given r, z and k (* = smallest known)

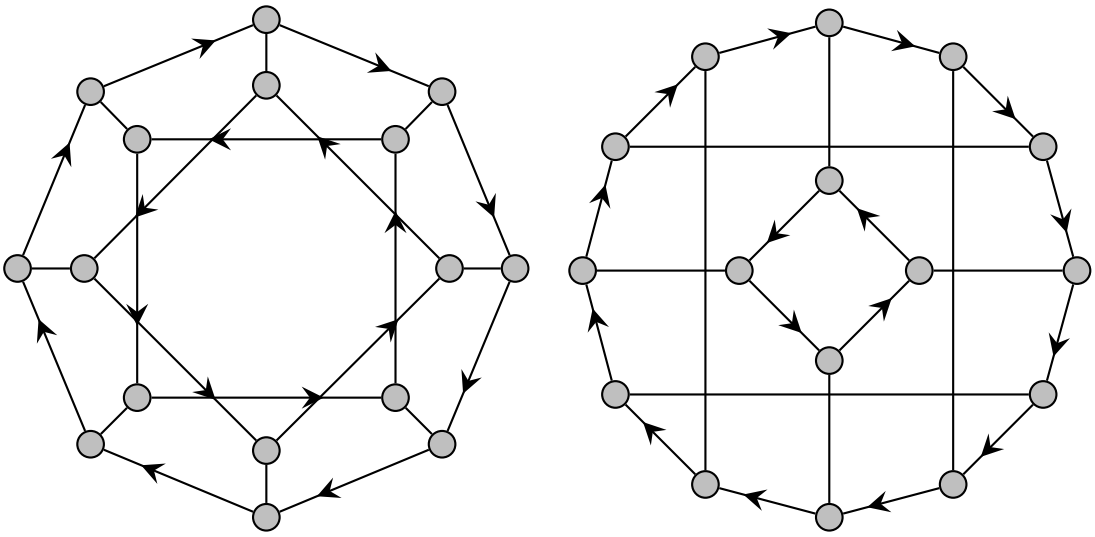

Figure 9.8: Two mixed graphs with $r = 1, z = 1, k = 3, \epsilon = 5$

This search was also run for purely directed graphs. This confirmed the two geodetic cages for $(d, k) = (2, 2)$ found in Chapter 6; for completeness, these are displayed in Figure 9.11. The search also classified $(2, 3)$-geodetic-cages (there are two cages up to isomorphism, shown in Figures 9.12 and 9.13, the second of which is a Cayley digraph) and $(3, 2)$-geodetic-cages (there is a unique $(3, 2)$-cage with excess $\epsilon = 3$, which is displayed in Figure 9.14). The results of the search for digraphs are summarised in Table 9.3.

d	k	M	n	ϵ	Comment
2	2	7	9	2	Figure 9.11
2	3	15	20	5	Figures 9.12 and 9.13
2	4	31	54*	23*	No graphs of order less than 34
3	2	13	16	3	Figure 9.14

Table 9.3: Smallest digraphs of given degree d and geodecity k (* = smallest known)

We saw in Section 7.1 that one useful technique for finding mixed graphs with order

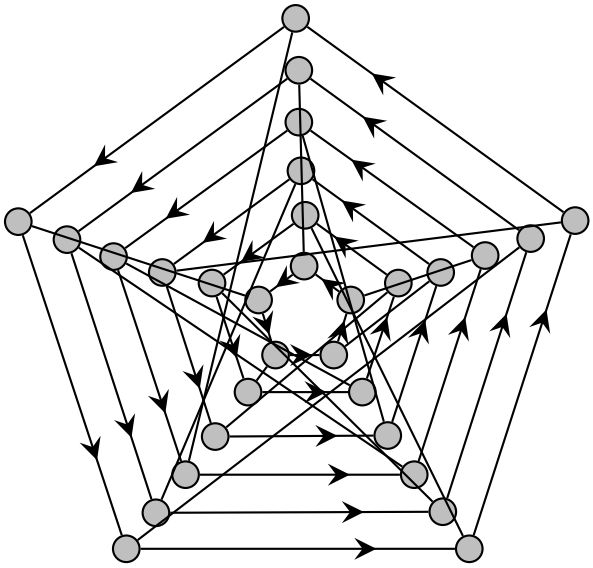

Figure 9.9: A mixed graph with $r = 1, z = 1, k = 4, \epsilon = 11$

close to the Moore bound is to restrict oneself to a search in the class of Cayley mixed graphs [66]. Erskine carried out a search for k-geodetic Cayley mixed graphs [144], the results of which are shown in Table 9.4. The orders of these graphs give upper bounds on the order of mixed cages.

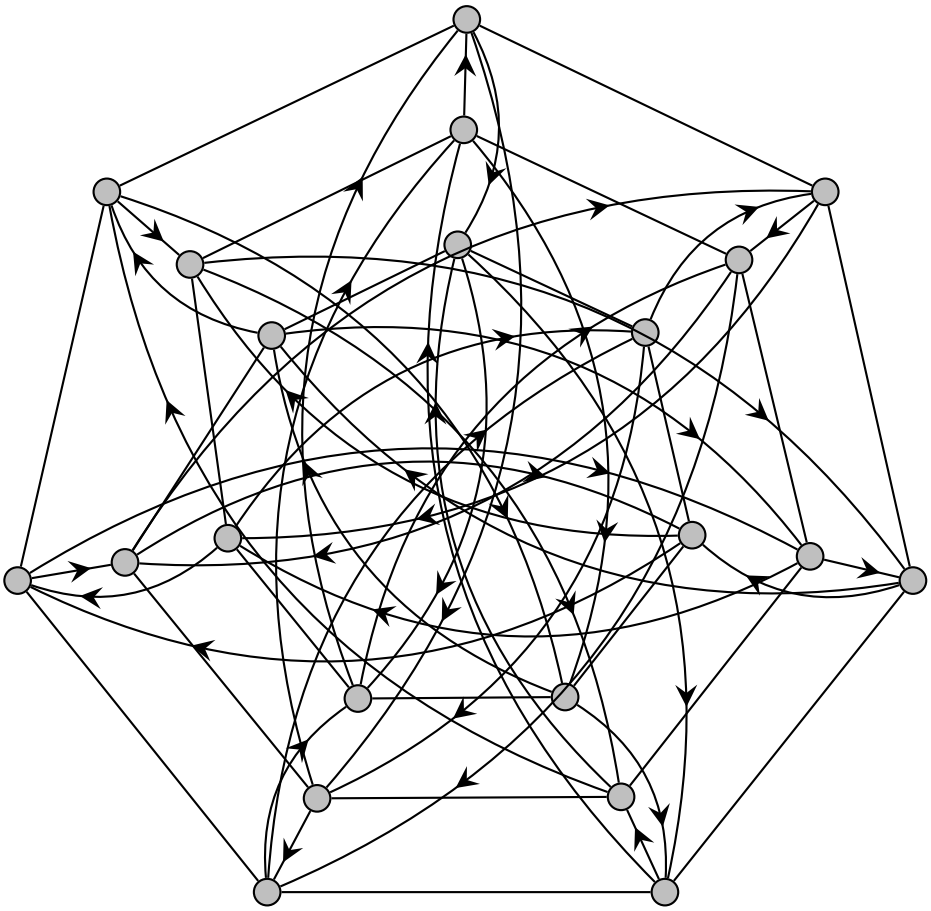

Figure 9.10: A mixed graph with $r = 2, z = 2, k = 2, \epsilon = 2$

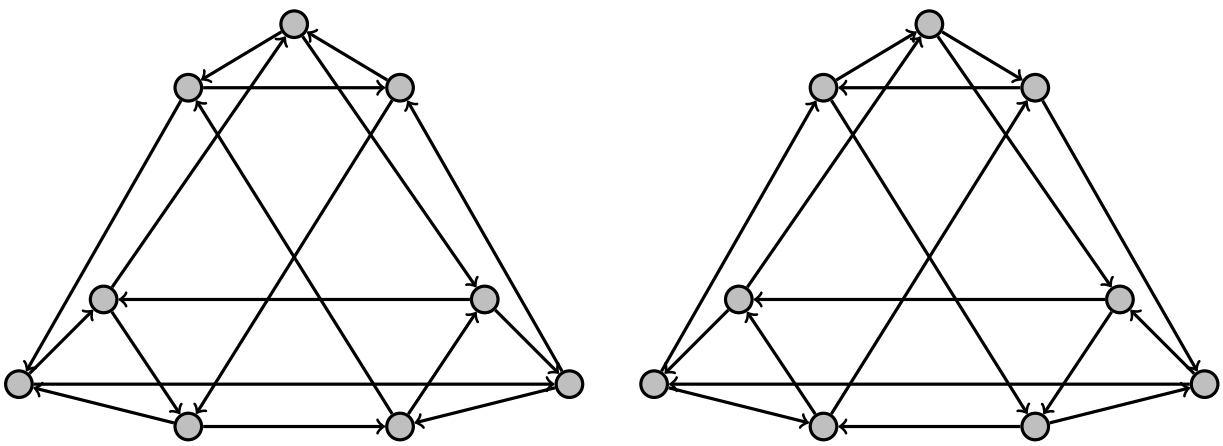

Figure 9.11: The two $(2, 2)$-geodetic-cages

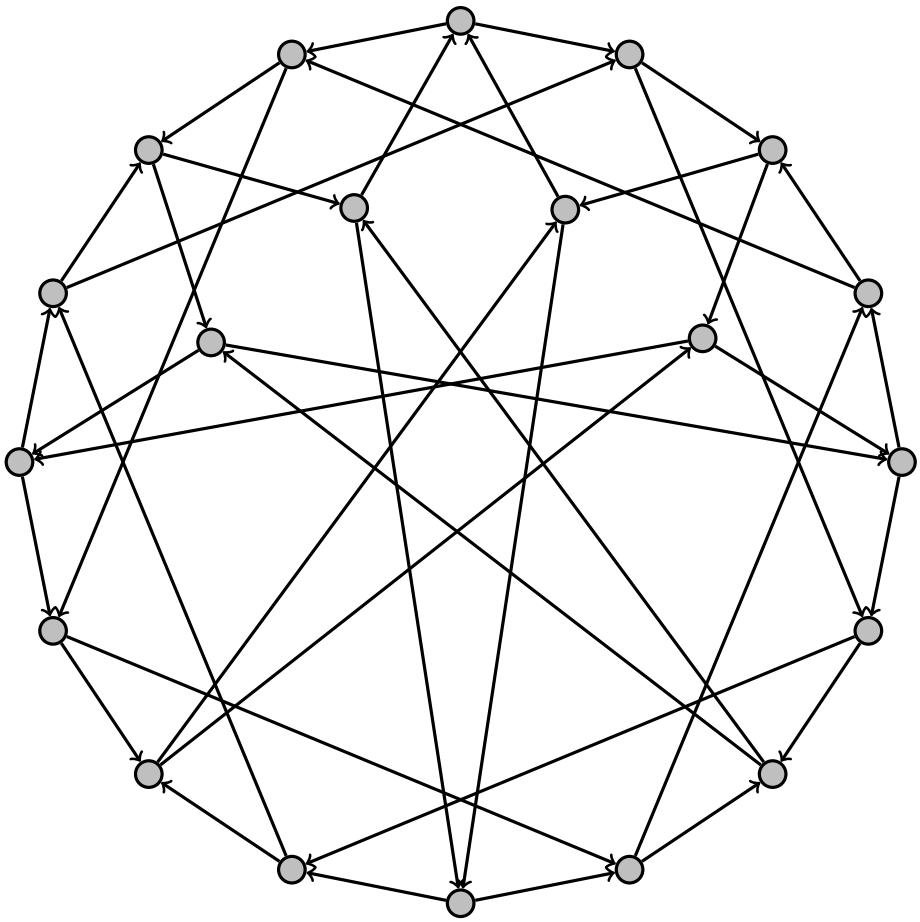

Figure 9.12: The first $(2, 3; +5)$-digraph

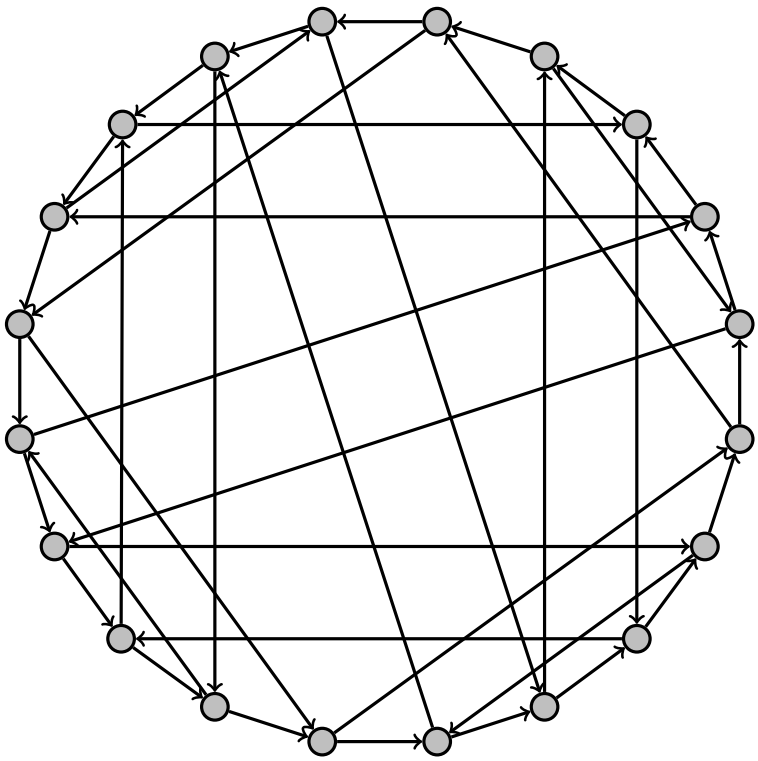

Figure 9.13: The second $(2, 3; +5)$-digraph

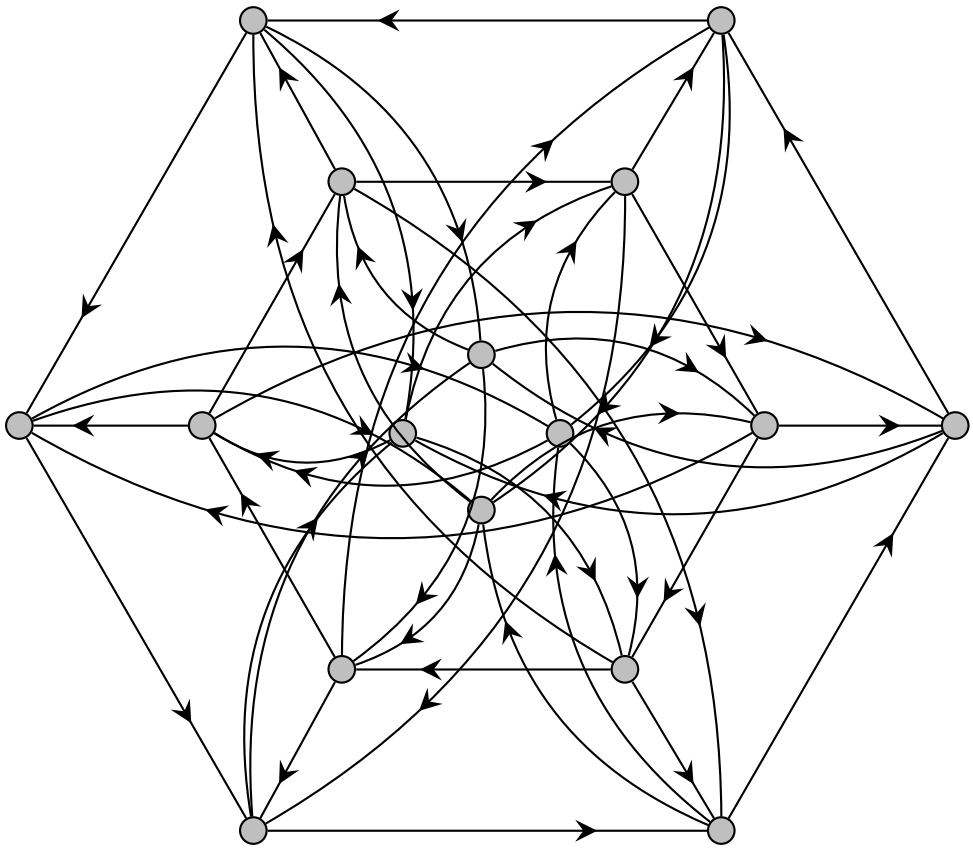

Figure 9.14: The unique extremal digraph $d = 3, k = 2, n = 16$

r	z	k	M	n	ϵ	Group
1	1	2	6	6	0	S_3
1	1	3	11	20	9	$\mathrm{AGL}(1,5)$
1	1	4	19	32	13	$(\mathbb{Z}_8 \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_2$
1	1	5	32	54	22	$(\mathbb{Z}_9 \rtimes \mathbb{Z}_3) \rtimes \mathbb{Z}_2$
2	1	2	11	12	1	D_{12}
2	1	3	28	48	20	$\mathbb{Z}_2 \times S_4$
1	2	2	12	12	0	A_4
1	2	3	34	64	30	$((\mathbb{Z}_8 \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_2$
3	1	2	18	18	0	$\mathbb{Z}_3 \times S_3$
2	2	2	19	24	5	$\mathrm{SL}(2,3)$
1	3	2	20	20	0	$\mathrm{AGL}(1,5)$
4	1	2	27	30	3	$\mathbb{Z}_5 \times S_3$
3	2	2	28	42	14	$\mathbb{Z}_7 \times S_3$
2	3	2	29	39	10	$\mathbb{Z}_{13} \times \mathbb{Z}_3$
1	4	2	30	42	12	$\mathrm{AGL}(1,7)$
5	1	2	38	48	10	D_{48}
4	2	2	39	48	9	$D_8 \times S_3$
3	3	2	40	52	12	$\mathbb{Z}_{13} \rtimes \mathbb{Z}_4$
2	4	2	41	54	13	$(\mathbb{Z}_3 \times \mathbb{Z}_3) \rtimes \mathbb{Z}_6$
1	5	2	42	42	0	$\mathrm{AGL}(1,7)$

Table 9.4: Smallest Cayley $(r, z, k; +\epsilon)$-graphs for given r, z and k

Chapter 10

Turán problems for k-geodetic directed graphs

10.1 Introduction

In this chapter we shall investigate an extension of the Turán problem of the largest possible size of a graph with order n and girth $\geq g$ to the setting of directed graphs. Recalling that the girth of a digraph G is the length of a shortest directed cycle in G, a natural first question is: what is the largest possible size of a digraph with order n and no directed cycles of length $< g$? In fact, as there exists an acyclic tournament for any order n, this is a trivial question and it is more interesting to restrict our attention to strongly connected digraphs. This problem was solved by Bermond et al. in [21] and is discussed independently in [152].

Theorem 10.1 ([21])**.** *Let D be a strong digraph of order n, size m and girth g. Let $k \geq 2$. Then if*

$$m \geq \frac{1}{2}(n^2 + (3-2k)n + k^2 - k),$$

we must have $g \leq k$.

A construction is also given in [21] that shows that this bound is best possible. Hence, in marked contrast to the undirected case, this result shows that, asymptotically speaking, an oriented graph can have 'almost all' arcs present and still have arbitrarily large girth, even if the digraph is strongly connected. This raises the question of the asymptotic behaviour of the largest possible size of a digraph with order n and geodetic girth k. This problem can be put into the form of a forbidden subgraph problem, as every violation of k-geodecity in G can be identified with the occurrence of a specific subdigraph of G; in [149] these subdigraphs are referred to as 'hooves' or 'commutative diagrams'. It has recently come to the author's attention that some related Turán problems forbidding 'hooves' of particular lengths have been investigated by Huang, Lyu, Qiao et al. [92, 93, 108].

Problem 10.2. *What is the largest possible size of a k-geodetic digraph with order n?*

In the papers [128, 149] Ustimenko et al. prove that, if $f(n,k)$ is the largest size of a diregular k-geodetic digraph with order n, then for fixed k we have $f(n,k) \sim n^{\frac{k+1}{k}}$. The digraphs used in [128, 149] to show that this bound is tight are exactly the permutation digraphs; recall that the permutation digraph $P(d,k)$ has as vertex set all permutations $x_0x_1\dots x_{k-1}$ of length k drawn from an alphabet of size $d+k$, with arcs of the form $x_0x_1\dots x_{k-1} \to x_1x_2\dots x_{k-1}x_k$, where $x_k \notin \{x_0, x_1, \dots, x_{k-1}\}$. We record this result as a separate theorem.

Theorem 10.3 ([128, 149])**.** *For fixed k, the largest possible size of a diregular k-geodetic digraph with order n is asymptotic to $n^{\frac{k+1}{k}}$ as $n \to \infty$. This bound is met asymptotically by the permutation digraphs $P(d,k)$.*

We will see in Section 10.5 that the permutation digraphs have other interesting extremal properties in Turán problems.

We can easily generalise the result of Ustimenko et al. to out-regular digraphs by appealing to the directed Moore bound. The following argument was suggested by Erskine and simplified by the author [146].

Theorem 10.4. *For $k \geq 2$, the largest size $\mathrm{ex}_{out}(n;k)$ of an out-regular k-geodetic digraph with order n satisfies $\mathrm{ex}_{out}(n;k) \sim n^{\frac{k+1}{k}}$ as $n \to \infty$.*

Proof. The order n of a k-geodetic digraph with minimum out-degree d is bounded below by the directed *Moore bound* $M(d,k) = 1 + d + d^2 + \cdots + d^k$. Hence $n \geq d^k$ and, rearranging, $d \leq n^{1/k}$. The size m of an out-regular k-geodetic digraph G with order n thus satisfies $m = nd \leq n^{\frac{k+1}{k}}$. □

What can we say about the maximum number of arcs in a k-geodetic digraph if we make no assumption of out-regularity? We make the following definition.

Definition 10.5. For $n, k \geq 2$, define $\mathrm{ex}(n;k)$ to be the largest possible size of a k-geodetic digraph on n vertices.

In contrast to the out-regular case, it is easy to provide a quadratic lower bound for the numbers $\mathrm{ex}(n;k)$. This observation is due to Erskine.

Observation 10.6. *[Erskine] For $n, k \geq 2$, we have $\mathrm{ex}(n;k) \geq \lfloor n^2/4 \rfloor$.*

Proof. Orienting all edges of the complete bipartite graph $K_{\lceil n/2 \rceil, \lfloor n/2 \rfloor}$ in the same direction yields a k-geodetic digraph. □

We now show that this lower bound is optimal. We offer two distinct proofs, the first being a simple inductive argument, whereas the second appeals to a standard result of Turán theory and also gives a classification of the underlying graphs of the extremal digraphs. For our inductive proof, observe that if a digraph G is k-geodetic, then every subdigraph of G must also be k-geodetic. This approach yields a simple upper bound for $\mathrm{ex}(n;k)$ in terms of $\mathrm{ex}(t;k)$ for $t < n$.

Lemma 10.7. *For any $2 \leq t \leq n-1$, we have $\mathrm{ex}(n;k) \leq \frac{n(n-1)}{t(t-1)}\mathrm{ex}(t;k)$.*

Proof. Let G be a k-geodetic digraph with order n and size $\mathrm{ex}(n;k)$. We count the pairs (F,e), where F is a subset of t vertices of G and e is an arc with both end-points in F. Let F be any subset of t vertices of G. In the corresponding induced subdigraph there can be at most $\mathrm{ex}(t;k)$ arcs. Therefore there are at most $\binom{n}{t}\mathrm{ex}(t;k)$ such pairs. For each arc e there are exactly $\binom{n-2}{t-2}$ subsets of size t containing the endpoints of e, so it follows that

$$\mathrm{ex}(n;k)\binom{n-2}{t-2} \leq \binom{n}{t}\mathrm{ex}(t;k).$$

Rearranging yields the result. □

Theorem 10.8. *For $n \geq 4$ and $k \geq 2$, we have $\mathrm{ex}(n;k) = \left\lfloor \frac{n^2}{4} \right\rfloor$.*

Proof. Let $k = 2$. The theorem is easily shown to be true for $n = 4$. Let $n \geq 5$ and assume that the theorem is true for $n-1$. Suppose that $n = 2r$ is even. Putting $t = n-1$ in Lemma 10.7 and using the induction hypothesis we have

$$\mathrm{ex}(2r;2) \leq \frac{2r(2r-1)}{(2r-1)(2r-2)}r(r-1) = r^2$$

as required. Now let $n = 2r+1$. Lemma 10.7 with $t = 2r$ gives

$$\mathrm{ex}(2r+1;2) \leq \frac{2r(2r+1)}{2r(2r-1)}r^2 = \frac{(2r+1)r^2}{2r-1} < r^2 + r + 1.$$

As $\mathrm{ex}(2r+1;2)$ is an integer the necessary inequality

$$\mathrm{ex}(2r+1;2) \leq r^2 + r = \left\lfloor \frac{(2r+1)^2}{4} \right\rfloor$$

follows. As a k-geodetic digraph is also 2-geodetic for $k \geq 2$, no k-geodetic digraph can have more than $\mathrm{ex}(n;2)$ arcs; at the same time, the digraph in Observation 10.6 is trivially k-geodetic for any $k \geq 2$. □

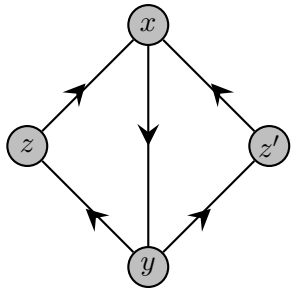

Figure 10.1: There is no 2-geodetic orientation of K_4^-

We now show how this result also follows from a forbidden-subgraph approach. The complete graph K_4 with one edge deleted is also known as the *diamond graph* and is denoted by K_4^-.

Lemma 10.9. *Every graph with a 2-geodetic orientation is K_4^--free.*

Proof. Suppose for a contradiction that a graph G contains two triangles x, y, z and x, y, z', where $z \neq z'$. The only 2-geodetic orientation of a triangle is a directed 3-cycle, so we can assume that $x \to y \to z \to x$ and $x \to y \to z' \to x$. This situation is shown in Figure 10.1. However there are now two distinct directed paths from y to x of length two, violating 2-geodecity. □

Theorem 10.10. *For $n \geq 4$ and $k \geq 2$ we have $\mathrm{ex}(n;k) = \left\lfloor \frac{n^2}{4} \right\rfloor$ and for $n \geq 7$ all extremal 2-geodetic digraphs are orientations of complete balanced bipartite graphs $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.*

Proof. As noted previously, it is sufficient to prove the upper bound for $k = 2$. A simple inductive argument shows the well-known result [56, 57] that for $n \geq 7$ any graph with order n and size $> \left\lfloor \frac{n^2}{4} \right\rfloor$ contains a copy of K_4^- and the unique K_4^--free graph with size $\left\lfloor \frac{n^2}{4} \right\rfloor$ is $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. The result therefore follows by Lemma 10.9. The graph in Figure 10.2 shows that $n \geq 7$ cannot be reduced. □

We now know that for $n \geq 7$ any 2-geodetic digraph with $\mathrm{ex}(n;2)$ arcs is an orientation of a complete bipartite graph $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. However, there are a large number of non-isomorphic orientations of $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$, not all of which are 2-geodetic. We now completely classify all extremal 2-geodetic digraphs. We will label one partite set of our bipartite graph X and the other Y. If X contains a source, then Y contains no sources and vice versa, so we can assume that any source of G lies in X. If X contains only sources, then Y consists only of sinks, in which case we recover the

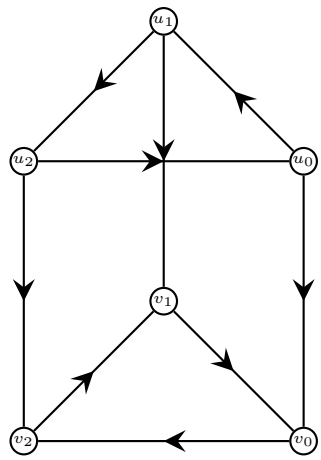

Figure 10.2: A 2-geodetic digraph with order 6 and size 9 containing a triangle

construction in Observation 10.6. We can therefore assume that X contains a vertex that is neither a source nor a sink.

Lemma 10.11. *Let K be a 2-geodetic orientation of a complete bipartite graph $K_{s,t}$ with partite sets X and Y, where $s \geq t \geq 2$. If x is any vertex of K that is neither a source nor a sink, then either $d^+(x) = 1$ or $d^-(x) = 1$.*

Proof. Let $x \in X$ be a vertex of K that is neither a source nor a sink. Suppose that $d^+(x) \geq 2$ and $d^-(x) \geq 2$. Let $y \in Y$ be an out-neighbour of x such that y is not a sink. Hence $y \to x'$ for some $x' \in X - x$. If any other out-neighbour y' of x has an arc to x', then we would have two 2-paths $x \to y \to x'$ and $x \to y' \to x'$, violating 2-geodecity, so it follows that x' has arcs to every vertex of $N^+(x) - \{y\}$. Any in-neighbour y^- of x can already reach every vertex of $N^+(x)$ by a 2-path via x. As x' has arcs to every vertex of $N^+(x) - \{y\}$, it follows that $x' \to y^-$ for every in-neighbour y^- of x. However, there are at least two such in-neighbours y_1^- and y_2^- by assumption, so there exist paths $x' \to y_1^- \to x$ and $x' \to y_2^- \to x$, a contradiction.

It follows that every out-neighbour of x in Y is a sink and similarly every in-neighbour of x is a source. Let $x^* \in X - \{x\}$. Then if $y^+ \in N^+(x), y^- \in N^-(x)$ we have two paths $y^- \to x \to y^+$ and $y^- \to x^* \to y^+$, which is impossible. Hence we must have either $d^+(x) = 1$ or $d^-(x) = 1$. □

Theorem 10.12. *Let K be a 2-geodetic orientation of a complete bipartite graph $K_{s,t}$, where $s \geq t \geq 2$. Then all of the arcs of K are oriented in the same direction, except for a matching (possibly of size zero) in the opposite direction.*

Proof. As K is 2-geodetic X cannot contain both sources and sinks; for example if $x_1 \in X$ is a source and $x_2 \in X$ is a sink, then if $y_1, y_2 \in Y$ we have paths

$x_1 \to y_1 \to x_2$ and $x_1 \to y_2 \to x_2$, which is impossible.

Note that if all vertices are neither a source nor a sink, then both partitions contain a vertex which is neither a source nor a sink. If $s = t = 2$, then by Lemma 10.11 we are done, so we may assume that $|Y| > 2$ and X contains a vertex which is neither a source nor a sink. By Lemma 10.11, any such vertex has either in-degree or out-degree one; without loss of generality, we assume that $N^+(x_1) = \{y_1\}$. Then X contains no vertex $x' \in X$, $d^+(x') > 1$, for otherwise there would be paths $x' \to y_2 \to x_1$ and $x' \to y_3 \to x_1$ if $y_2, y_3 \neq y_1$, a contradiction, or there is a vertex y' in Y such that we have $y' \to x$ and $y' \to x'$ which leads us also to a contradiction since there are two paths from y' to y_1. Applying Lemma 10.11, we have the desired result. □

Combining Theorems 10.10 and 10.12 immediately yields a classification of all 2-geodetic digraphs of order n and maximal size.

Theorem 10.13. *Let G be a 2-geodetic digraph with order n and maximal size. For $n \geq 7$, G is isomorphic to an orientation of $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ with all arcs oriented in the same direction, except for a matching that is oriented in the opposite direction. The number of isomorphism classes of extremal digraphs is $n+1$ for odd $n \geq 7$ and $\frac{n}{2}+1$ for even $n \geq 8$.*

10.2 The largest size of a strongly connected 2-geodetic digraph

For even n, if the matching mentioned in Theorem 10.13 is chosen to be a perfect matching, then the resulting digraph is strongly connected. Therefore for even n there is always a strongly connected 2-geodetic digraph with $\mathrm{ex}(n; 2)$ arcs. Such a digraph is shown in Figure 10.3. However, it is easily seen that if n is odd, then all of the 2-geodetic digraphs given in Theorem 10.13 contain either a source or a sink and so are not strongly connected. This leads us to make the following definition.

Definition 10.14. For $n \geq k+1$ and $k \geq 2$, $\mathrm{ex}^*(n; k)$ is the largest possible size of a strongly connected k-geodetic digraph with order n.

From the former observation we know that for $r \geq 4$ we have $\mathrm{ex}^*(2r; 2) = r^2$. We turn to the question of determining $\mathrm{ex}^*(2r+1; 2)$. Taking a strongly connected 2-geodetic digraph with order $2r$ and size r^2 and expanding one arc into a directed triangle shows that $\mathrm{ex}^*(2r+1; 2) \geq r^2 + 2$ (this construction is shown in Figure 10.4). We now show that this lower bound is optimal. In fact we prove slightly more: that any 2-geodetic

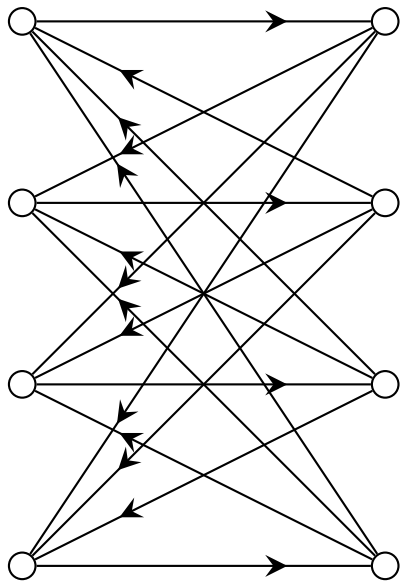

Figure 10.3: A strongly connected digraph with $n = 2r$ and $m = r^2$ (for $r = 4$)

digraph with larger size contains either a source or a sink. The approach of the proof in [146] is due to Salia; here we give the original argument due to the author.

Therefore let G be a 2-geodetic digraph with order $n = 2r + 1$ and largest possible size $r^2 + r - \epsilon$, where $1 \leq \epsilon \leq r - 2$, subject to G containing no sources or sinks. Let H be the underlying undirected graph of G and let H have minimum (resp. maximum) degree δ (Δ).

Lemma 10.15. *For $1 \leq \epsilon \leq r - 2$, either H is bipartite or else $\epsilon = r - 2$ and H contains a triangle.*

Proof. The stability result of [35] shows that any triangle-free graph with order $2r + 1$ and size $\geq r^2 + 2$ is bipartite. Therefore we need only show that H must be triangle-free for $1 \leq \epsilon \leq r - 3$.

Suppose that H has size $\geq r^2 + 3$ and contains a triangle T with vertices x, y, z. By Lemma 10.9, H is diamond-free, so the neighbours of x, y and z outside of T are all distinct. This implies that

$$d(x) + d(y) + d(z) \leq n + 3 = 2r + 4.$$

Consider the digraph $G' = G - \{x, y, z\}$ obtained by deleting T; G' has order $2(r - 1)$ and size $m' = r^2 + r - \epsilon - d(x) - d(y) - d(z) + 3$. Thus by Theorem 10.10

$$r^2 + r - \epsilon - d(x) - d(y) - d(z) + 3 \leq (r - 1)^2,$$

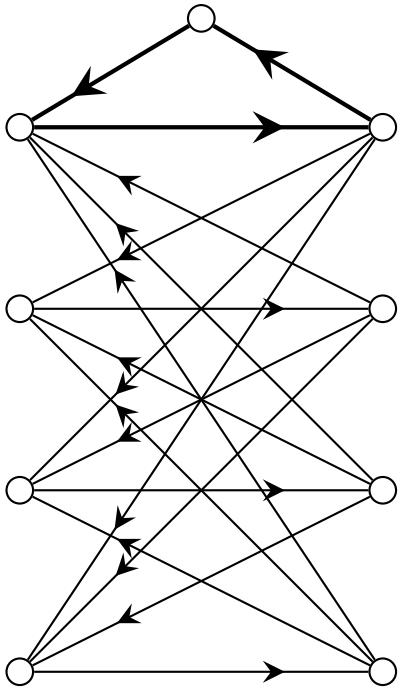

Figure 10.4: A strongly connected digraph with $n = 2r + 1$ and $m = r^2 + 2$ for $r = 4$ with the triangle in bold

yielding $d(x) + d(y) + d(z) \geq 3r + 2 - \epsilon$. These two inequalities together imply that $3r + 2 - \epsilon \leq 2r + 4$, so that $\epsilon \geq r - 2$, a contradiction. □

If $\epsilon = r - 2$, we have equality in the last part of the argument of Lemma 10.15, so if $\epsilon = r - 2$ and H contains a triangle T, then the subgraph of H obtained by deleting T must be a complete bipartite graph $K_{r-1,r-1}$ by Theorem 10.10 and every vertex of H is adjacent to a vertex of T. We will use this fact in Section 10.3 to classify the extremal digraphs.

Corollary 10.16. *If G is a strongly connected 2-geodetic digraph with order $2r + 1$ and size $r^2 + 2$ that contains a triangle T, then the underlying undirected graph H of G can be formed from a triangle T and a complete bipartite graph $K_{r-1,r-1}$ by joining each vertex of $K_{r-1,r-1}$ to a unique vertex of T.*

By Lemma 10.15, to prove that $\mathrm{ex}^*(2r + 1; 2) = r^2 + 2$ it is sufficient to show that H cannot be bipartite; this will also show that any strongly connected 2-geodetic digraph with order $n = 2r + 1$ and size $r^2 + 2$ contains a triangle, a case that we will take up in the next section. Therefore for the remainder of this section we assume that G is an orientation of a bipartite graph (i.e. that H is bipartite). Let the two partite sets in the bipartition of H be X and Y (as yet we make no assumption concerning their size). The maximum possible size of a bipartite graph with order

$2r+1$ is r^2+r; therefore to complete our proof it is sufficient to show that there are at least $r-2$ arcs missing in G between X and Y.

Lemma 10.17. *If G is bipartite and has size $r^2+r-\epsilon$, where $1 \leq \epsilon \leq r-2$, then for any vertex x of G we have the following bound for ϵ:*

$$\epsilon \geq \max\{|N^{+2}(x)|, |N^{-2}(x)|\}(\min\{d^+(x), d^-(x)\} - 1).$$

Proof. Fix a vertex x of G; without loss of generality, let $x \in X$. Let $N^+(x) = \{y_1, \ldots, y_z\}$ and consider a vertex $x' \in N^{+2}(x)$. We distinguish two situations: i) there is an arc from x' to $N^+(x)$ and ii) there is no arc from x' to $N^+(x)$.

Suppose firstly that there is an arc $x' \to y_i$ from x' to $N^+(x)$. Then by 2-geodecity there can be no arc from $N^-(x)$ to x', for if there is an arc $y \to x'$ for some in-neighbour y of x, then G would contain paths $y \to x' \to y_i$ and $y \to x \to y_i$. Furthermore x' can have at most one arc to $N^-(x)$; otherwise x' would have more than one 2-path to x. Thus there are at least $d^-(x)-1$ arcs missing between x' and Y.

On the other hand, if there is no arc from x' to $N^+(x)$, then, considering that there is a unique arc from $N^+(x)$ to x' by 2-geodecity, there are at least $d^+(x)-1$ arcs missing between x' and Y.

As there are $|N^{+2}(x)|$ vertices to which this argument can be applied, we conclude that there are at least $|N^{+2}(x)|(\min\{d^+(x), d^-(x)\} - 1)$ arcs missing between X and Y, which by our previous observation gives a lower bound for ϵ. A dual argument using vertices in $N^{-2}(x)$ completes the proof of the result. □

Lemma 10.17 shows that if a vertex has large out-degree, then it must have small in-degree, and vice versa.

Corollary 10.18. *If a vertex u of G satisfies $d^+(u) \geq \max\{d^-(u), r-1\}$, then $d^-(u) = 1$. If u has out-degree $d^+(u) \geq \max\{d^-(u), \frac{r-1}{2}\}$, then $d^-(u) \leq 2$.*

Proof. Suppose that u is a vertex of G with $d^+(u) \geq \max\{d^-(u), r-1\}$. Then if $d^-(u) \geq 2$, Lemma 10.17 shows that

$$r-2 \geq \epsilon \geq |N^{+2}(u)| \geq d^+(u) \geq r-1,$$

which is a contradiction. As G has no sources or sinks, it follows that $d^-(u) = 1$.

Similarly, if $d^+(u) \geq \max\{d^-(u), \frac{r-1}{2}\}$, but $d^-(u) \geq 3$, then Lemma 10.17 would again yield $\epsilon \geq r-1$. □

Let us now suppose that X is the larger of the two partite sets, i.e. $|X| > |Y|$.

Lemma 10.19. *The maximum degree of the underlying undirected graph H of G is less than or equal to r.*

Proof. Suppose that there exists a vertex u of G with degree $\geq r+1$; as $|Y| \leq r$, the vertex u must lie in Y. By taking the converse if necessary, we can assume that $d^+(u) \geq d^-(u)$. Then $d^+(u) \geq \frac{r+1}{2}$, so Corollary 10.18 tells us that $d^-(u) = 1$ or 2. In either case we must have $d^+(u) \geq r-1$, so by Corollary 10.18 we must have $d^-(u) = 1$ and $d^+(u) \geq r$. Thus $|N^{+2}(u)| \geq d^+(u) \geq r$. However, each vertex of $N^{+2}(u)$ must lie in Y, as H is bipartite. As u also lies in Y, this implies that $|Y| \geq r+1$, contradicting our choice $|X| > |Y|$. □

The bound in Lemma 10.17 is most helpful when applied to vertices with large degree. In fact, we can guarantee the existence of many vertices with degree r in H.

Lemma 10.20. *The underlying undirected graph H of G has maximum degree $\Delta = r$ and contains at least $r+5$ vertices with this degree.*

Proof. By Lemma 10.19, the maximum degree Δ of H is $\leq r$. Let H contain a vertices with degree r and b vertices with degree $\leq r-1$. Then $a+b = 2r+1$ and by the Handshaking Lemma the size m of H is bounded by

$$2(r^2 + r - \epsilon) = 2m \leq ar + b(r-1) = (a+b)r - b = 2r^2 + r - b.$$

Rearranging, we obtain $b \leq 2\epsilon - r \leq 2(r-2) - r = r-4$. Therefore $a \geq 2r + 1 - (r-4) = r+5$. □

Corollary 10.21. *The sizes of the partite sets X and Y are $|X| = r+1$ and $|Y| = r$ respectively.*

Proof. The size of Y is at most r, so by Lemma 10.20 there is a vertex in X with degree r; therefore the size of Y is exactly r. □

We can thus label the elements of X and Y as $X = \{x_1, x_2, \ldots, x_{r+1}\}$ and $Y = \{y_1, y_2, \ldots, y_r\}$.

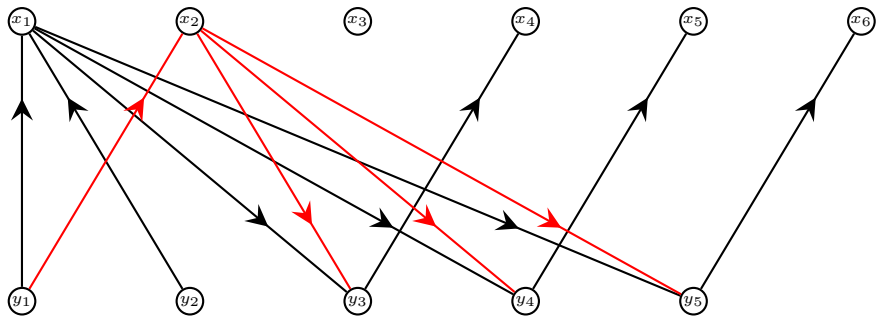

Figure 10.5: Illustration for Lemma 10.22

Lemma 10.22. *If a vertex u of H has degree r, then in G either $d^+(u) = r - 1$ and $d^-(u) = 1$ or $d^+(u) = 1$ and $d^-(u) = r - 1$.*

Proof. Let u have degree r in H. Let $d^+(u) \geq d^-(u)$, taking the converse of G if necessary. By Corollary 10.18, either $d^+(u) = r - 2$ and $d^-(u) = 2$, or else $d^+(u) = r - 1$ and $d^-(u) = 1$. Suppose that the former holds. We can assume that $u = x_1$; the argument for $u \in Y$ is the same.

Without loss of generality $N^-(x_1) = \{y_1, y_2\}$ and $N^+(x_1) = \{y_3, y_4, \ldots, y_r\}$. Each of $y_3, y_4, \ldots, y_r$ has at least one out-neighbour in X; let us set $y_i \to x_{i+1}$ for $3 \leq i \leq r$. Potentially there could also be arcs from $N^+(x_1)$ to $\{x_2, x_3\}$; however the argument of Lemma 10.17 shows that each member of $N^{+2}(x_1)$ has at least one arc missing to Y, so as $\epsilon \leq r - 2$ there can be no more than $r - 2$ vertices in $N^{+2}(x_1)$ and hence each vertex of $N^+(x_1)$ has out-degree exactly one.

Moreover, as each vertex in $N^{+2}(x_1)$ has at least one arc missing to Y, it follows that the vertices x_2 and x_3 are adjacent in H with every vertex of Y. As $N^{+2}(x_1) = \{x_4, x_5, \ldots, x_{r+1}\}$, there must be arcs from x_2 to every vertex in $N^+(x_1)$. Also x_2 cannot have arcs to both y_1 and y_2, or it would have distinct 2-paths to x_1, so we can assume that $y_1 \to x_2$. However, this implies the existence of paths $y_1 \to x_2 \to y_3$ and $y_1 \to x_1 \to y_3$, violating 2-geodecity. The resulting configuration is shown in Figure 10.5 with the arcs associated with x_2 in red. □

Theorem 10.23. *No strongly connected 2-geodetic digraph with order $n = 2r + 1$ and size $> r^2 + 2$ exists and any such digraph with size $r^2 + 2$ contains a triangle.*

Proof. By Lemma 10.20 there is a vertex with degree r in X; say that x_1 has degree r in H. Taking the converse of G if necessary, we can assume by Lemma 10.22 that $d^-(x_1) = 1$ and $d^+(x_1) = r - 1$. We can set $N^-(x_1) = \{y_1\}$ and $N^+(x_1) = \{y_2, y_3, \ldots, y_r\}$. Furthermore each y_i has an out-neighbour in X, so we can

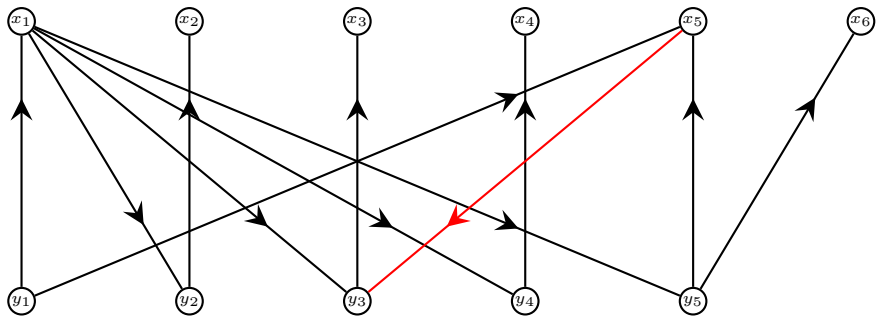

Figure 10.6: Illustration for Theorem 10.23: if an out-neighbour of x_1 has out-degree two

assume that $y_i \to x_i$ for $2 \leq i \leq r$. This accounts for $r-1$ vertices of $N^{+2}(x_1)$, so there can be at most one further element of $N^{+2}(x_1)$.

Suppose that an out-neighbour of x_1 has out-degree two in G, say $N^+(y_r) = \{x_r, x_{r+1}\}$. By 2-geodecity for $2 \leq i \leq r-1$ there are no arcs from y_i to x_r or x_{r+1} and there can be at most one arc from $\{x_r, x_{r+1}\}$ to y_i. This already accounts for $r-2$ missing arcs between X and Y; hence we have $\epsilon = r-2$ and all other possible edges between X and Y are present in H. Thus in H y_1 is adjacent to both x_r and x_{r+1}; we cannot have both of these arcs oriented toward y_1 in G, or else y_r would have distinct 2-paths to y_1, so we can assume that $y_1 \to x_r$. As y_1 can already reach every other vertex of Y by 2-paths via x_1, this implies that there are no arcs from x_r to $\{y_2, y_3, \ldots, y_{r-1}\}$; however, x_r is not a sink and so at least one of these arcs must exist, a contradiction. This situation is shown in Figure 10.6 for $r = 5$, with an impossible arc shown in red.

Thus we can take $N^+(y_i) = \{x_i\}$ for $2 \leq i \leq r$, as shown in Figure 10.7 for $r = 5$. Now the remaining vertex x_{r+1} has no arcs from $\{y_2, \ldots, y_r\}$, but as x_{r+1} is not a source we must have $y_1 \to x_{r+1}$. However x_{r+1} must also have an out-neighbour in Y, say y_r (this arc is shown in red in Figure 10.7), which means that there are paths $y_1 \to x_1 \to y_r$ and $y_1 \to x_{r+1} \to y_r$, violating 2-geodecity. This completes our proof that H cannot be bipartite; hence by Lemma 10.15 it follows that $\epsilon = r-2$ and H contains a triangle. □

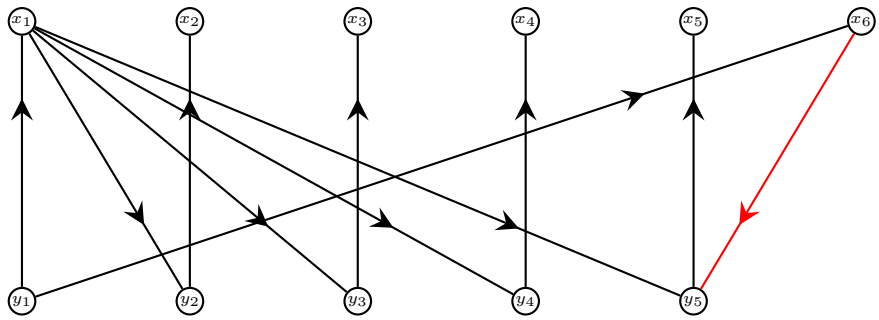

Figure 10.7: Illustration for Theorem 10.23: if all out-neighbours of x_1 have out-degree one

10.3 Classification of extremal 2-geodetic digraphs without sources and sinks

In the previous section it was shown that for $r \geq 1$ any strongly connected 2-geodetic digraph with order $n = 2r + 1$ has at most $\mathrm{ex}^*(2r + 1; 2) = r^2 + 2$ arcs. In this section we will classify the strongly connected 2-geodetic digraphs that achieve this bound. Our analysis will focus on the case $r \geq 5$, i.e. odd $n \geq 11$. Computer search shows that there is a unique extremal strongly connected 2-geodetic digraph with size $r^2 + 2$ for $r = 1$, 3 extremal digraphs for $r = 2$, 29 solutions for $r = 3$ and 19 solutions for $r = 4$; and any 2-geodetic digraphs with larger size contain either a source or a sink.

Let G be a 2-geodetic digraph with order $n = 2r + 1 \geq 11$, size $r^2 + 2$ and no sources or sinks and let H be the underlying undirected graph of G. By Theorem 10.23 H contains a triangle T with vertices x, y, z, which is oriented in G as $x \to y \to z \to x$ and each vertex in $H - T$ is adjacent to exactly one of x, y or z. Furthermore, $G - T$ must be one of the r orientations of $K_{r-1,r-1}$ given in Theorem 10.13. Let the bipartition of $K_{r-1,r-1}$ be X, Y, where $X = \{x_1, \ldots, x_{r-1}\}, Y = \{y_1, \ldots, y_{r-1}\}$. By Theorem 10.13 we can assume that $x_i \to y_i$ for $1 \leq i \leq r - 1 - s$ for some $0 \leq s \leq r - 1$, with all other edges oriented in the other direction. Obviously there are s sources and s sinks in $G - T$.

We will say that a partite set is covered by a subset T' of T if all of its neighbours in T belong to T'; in particular, if all of the neighbours of a partite set, say X, are the same vertex of T, say x, then X is covered by x. We call a vertex in T *bad* if it has neighbours in both partite sets of $H - T$.

Lemma 10.24. *Any bad vertex of T has degree four in H. If $n \geq 11$ then there is at most one bad vertex.*

Proof. It is easily seen that if a bad vertex has degree ≥ 5 in H, and hence ≥ 3

neighbours in $K_{r-1,r-1}$, then H contains a copy of K_4^-, which is impossible by Lemma 10.9. As any bad vertex of T is adjacent to one vertex of X and one vertex of Y for $r \geq 5$ not all three vertices of T can be bad. Furthermore if two vertices of T are bad then the third vertex of T would have also have to be bad. □

Lemma 10.25. *If there is no bad vertex in T, then either X or Y is covered by a single vertex of T and $s \leq 1$.*

Proof. If there is no bad vertex, then the neighbours of any vertex of T in $K_{r-1,r-1}$ must be entirely contained in one partite set, so one partite set is covered by one vertex of T and the other partite set is covered by the other two vertices of T.

Concerning the value of s, suppose that $s \geq 2$ and that X is covered by x (the argument for Y is similar). There must be an arc from every sink in X to x. But any source in Y has arcs to all the sinks in X and hence will have multiple 2-paths to x, contradicting 2-geodecity. □

Lemma 10.26. *Any vertex of T with neighbours in X has at most one in-neighbour in X. Any vertex of T that is joined to ≥ 2 non-sink vertices of X has no in-neighbour among the non-sink vertices of X. Substituting 'source' for 'sink' and 'out-neighbour' for 'in-neighbour', the analogous results hold for Y.*

Proof. Suppose that a vertex of T, say x, has ≥ 2 in-neighbours x_i and x_j in X. For any $l \in \{1, 2, \ldots, r-1\} - \{i, j\}$ we have $y_l \to x_i \to x$ and $y_l \to x_j \to x$, a contradiction.

Now let x be adjacent to vertices x_i and x_j in X, where we now assume that x_i and x_j are not sinks in $G - T$. If $x_i \to x$, then as x has at most one in-neighbour in X we must have $x \to x_j$. Hence there are paths $x_i \to x \to x_j$ and $x_i \to y_i \to x_j$, a contradiction. The results for Y follow in a similar manner. □

First we shall deal with the case that T has no bad vertices. Assume firstly that X is covered by x. Suppose that $s = 1$ (Figure 10.8). Then x_{r-1} and y_{r-1} are the sink and the source of $G - T$ respectively. Now x must have an arc from the sink so that it does not remain a sink in G; hence by Lemma 10.26 we have $x \to x_i$ for $1 \leq i \leq r-2$. Y is covered by y and z and either y or z has an arc to the source y_{r-1}.

If z has an arc to Y then there would be multiple 2-paths from z to a non-sink vertex in X and similarly if z has an in-neighbour y_i in Y, then there would be 2-paths

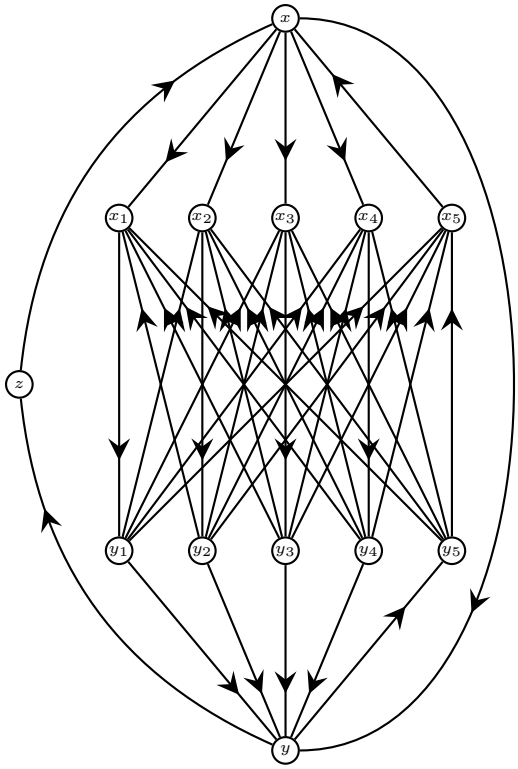

Figure 10.8: A_6

$y_i \to z \to x$ and $y_i \to x_{r-1} \to x$. Therefore z has no neighbours in Y, so y must have an arc to y_{r-1} and by Lemma 10.26 $y_i \to y$ for $1 \leq i \leq r-2$. This yields the 2-geodetic digraph A_r, an example of which is shown in Figure 10.8. This digraph is isomorphic to its converse.

Now let X be covered by x and $s = 0$. By Lemma 10.26 $x \to x_i$ for $1 \leq i \leq r-1$. By reasoning similar to the previous case, y and z can have no out-neighbours in Y. Let the resulting digraph in which y has t in-neighbours in Y be denoted by $B_{r,t}$ for $0 \leq t \leq r-1$ (see Figure 10.9). Each $B_{r,t}$ is a 2-geodetic extremal digraph.

The case of Y being covered by one vertex of T is symmetric. In particular we shall denote the converse of $B_{r,t}$ by $B'_{r,t}$. We have $B'_{r,0} \cong B_{r,0}$ and $B'_{r,r-1} \cong B_{r,r-1}$, but otherwise these digraphs are pairwise non-isomorphic.

We now turn to the case that there is a bad vertex; say z is bad. Hence $d(z) = 4$ in H. It follows by Lemma 10.24 that x and y each have $r-2$ neighbours in $K_{r-1,r-1}$ and each is connected to just one partite set.

Lemma 10.27. *If z is bad, then $s \leq 2$. If z is joined to a source in Y, then X is covered by $\{y, z\}$ and Y is covered by $\{x, z\}$. Likewise, if z is joined to a sink in X, then X is covered by $\{x, z\}$ and Y is covered by $\{y, z\}$. If $s = 2$, then z is connected to a source in Y and a sink in X.*

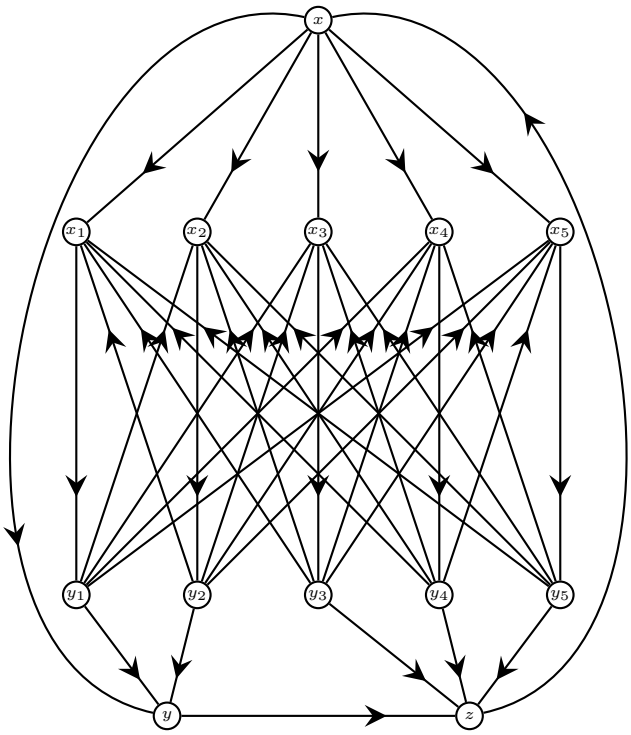

Figure 10.9: $B_{6,2}$

Proof. Suppose that $s \geq 3$. The bad vertex z is adjacent to one vertex of Y in $H - T$, so the vertex of T that also has edges to Y must have arcs to two or more sources in Y, violating Lemma 10.26. This reasoning also demonstrates that if $s = 2$, then z is connected to a source in Y and a sink in X.

For any $s \leq 2$, suppose that z is joined to a source in Y. Suppose that X is covered by $\{x, z\}$. Then z has a 2-path to every vertex of X via the source, but by Lemma 10.26 x has an out-neighbour $x_i \in X$, so there will also be a 2-path from z to x_i via x, violating 2-geodecity. Hence X must be covered by $\{y, z\}$ and hence Y is covered by $\{x, z\}$. The other statement is symmetric to this one. □

Let $s = 2$. The sources in $G - T$ are y_{r-2} and y_{r-1} and the sinks are x_{r-2} and x_{r-1}. By Lemma 10.27 we can assume that $z \to y_{r-2}$ and $x_{r-2} \to z$. Also by Lemma 10.27 X is covered by $\{y, z\}$. There must be an arc from x_{r-1} to y so that x_{r-1} is not a sink in G and $y \to x_i$ for $1 \leq i \leq r - 3$ by Lemma 10.26. Likewise there is an arc from x to y_{r-1}. However, we now have two 2-paths from x to the vertices in $\{x_1, \ldots, x_{r-3}\}$, one via y and the other via y_{r-1}, a contradiction. It follows that $s \leq 1$.

Let $s = 1$. The sink and source of $G - T$ are x_{r-1} and y_{r-1} respectively (Figure 10.10). Suppose that z is joined to x_{r-1} and y_{r-1}. By Lemma 10.27 X is covered by $\{y, z\}$

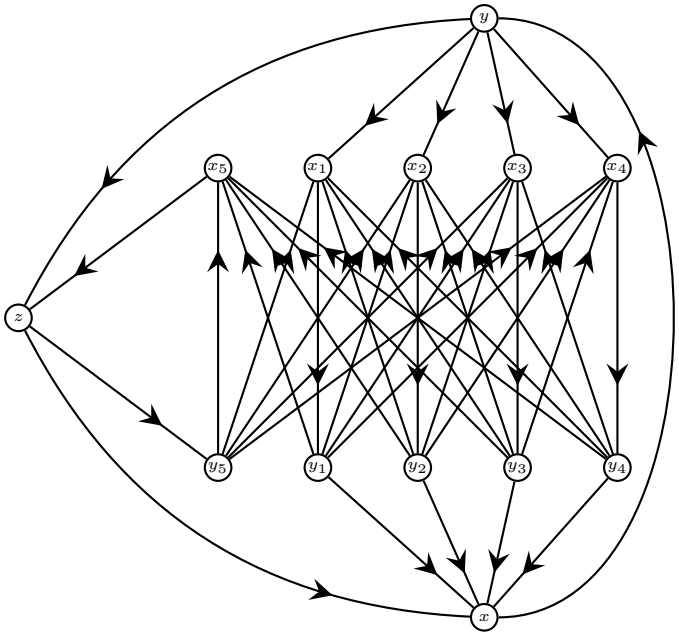

Figure 10.10: C_6

and Y is covered by $\{x, z\}$. By Lemma 10.26 $y \to x_i$ for $1 \leq i \leq r-2$ and $y_i \to x$ for $1 \leq i \leq r-2$. This gives the single solution C_r, an example of which is shown in Figure 10.10. Note that the digraph C_r is isomorphic to its converse.

Suppose that z is joined to the source y_{r-1} but is not joined to the sink x_{r-1} of $G - T$; say z has an edge to x_{r-2} in $H - T$. By Lemma 10.27 X is covered by $\{y, z\}$ and Y is covered by $\{x, z\}$. Hence there is an arc $x_{r-1} \to y$ and by Lemma 10.26 x has at most one out-neighbour in $Y - y_{r-1}$, so that there is a vertex y_i with $y_i \to x$. Hence there would be paths $y_i \to x \to y$ and $y_i \to x_{r-1} \to y$ in G, a contradiction. We will get a similar contradiction if z is joined to the sink x_{r-1} in X, but not to the source y_{r-1} in Y.

Finally, let z be joined to x_i and y_j where $1 \leq i, j \leq r-2$. Suppose that X is covered by $\{x, z\}$ and Y by $\{y, z\}$. If $i = j$, then the triangle is oriented as $x_i \to y_i \to z \to x_i$; however this yields paths $y_i \to z \to x$ and $y_i \to x_{r-1}x$, so we must have $i \neq j$. Without loss of generality we can set $i = r-2$ and $j = r-3$. The triangle is now oriented as $y_{r-3} \to x_{r-2} \to z \to y_{r-3}$. There is an arc $x_{r-1} \to x$, so by Lemma 10.26 there are arcs $x \to x_l$ for $1 \leq l \leq r-3$. In this case we would have paths $z \to y_{r-3} \to x_1$ and $z \to x \to x_1$.

Hence we can assume that X is covered by $\{y, z\}$ and Y by $\{x, z\}$. By Lemma 10.26 y has at least two out-neighbours in X, so if x has any out-neighbour in Y then there would be more than one 2-path from x to an out-neighbour of y in Y. In particular we must have $z \to y_{r-1}$, a case that we have already considered.

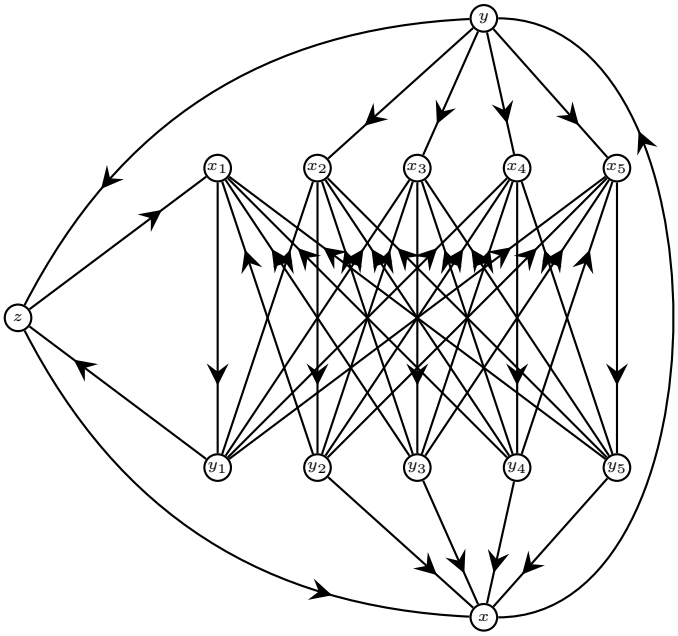

Figure 10.11: D_6

Now we can set $s = 0$. Suppose that z is joined to x_1 and y_2. As $y_2 \to x_1$, we must orient the triangle z, x_1, y_2 as $z \to y_2 \to x_1 \to z$. If X is covered by $\{x, z\}$ and Y is covered by $\{y, z\}$, then by Lemma 10.26 $x \to x_i$ for $2 \leq i \leq r-1$ and so there would be paths $z \to y_2 \to x_3$ and $z \to x \to x_3$. Hence X must be covered by $\{y, z\}$ and Y must be covered by $\{x, z\}$. By Lemma 10.26 we have $y_1 \to x$. Hence there are paths $x_1 \to y_1 \to x$ and $x_1 \to z \to x$.

Therefore we can assume that z is joined to x_1 and y_1. We must have $z \to x_1$ and $y_1 \to z$. If X is covered by $\{y, z\}$ and Y by $\{x, z\}$ then by Lemma 10.26 $y \to x_i$ and $y_i \to x$ for $2 \leq i \leq r-1$. This yields the solution D_r shown in Figure 10.11. D_r is isomorphic to its converse. If X is covered by $\{x, z\}$ and Y by $\{y, z\}$ then by a suitable redrawing of the digraph it can be seen that we obtain a solution isomorphic to C_r in Figure 10.10.

This completes our classification of the strongly connected 2-geodetic digraphs with order $n = 2r + 1$ and size $r^2 + 2$. We therefore have the following theorem.

Theorem 10.28. *Let $K(r)$ be the bipartite digraph with partite sets $X = \{x_1, x_2, \ldots, x_{r-1}\}$ and $Y = \{y_1, y_2, \ldots, y_{r-1}\}$ with $x_i \to y_i$ for $1 \leq i \leq r-1$ and $y_i \to x_j$ for $1 \leq i, j \leq r-1$ and $i \neq j$. Let $K'(r)$ be the digraph obtained from $K(r)$ by reversing the direction of the arc $x_{r-1} \to y_{r-1}$, i.e. in $K'(r)$ we have $y_i \to x_j$ for $1 \leq i, j \leq r-1$ unless $i = j$ and $1 \leq i \leq r-2$, in which case $x_i \to y_i$. Furthermore let T be a directed triangle with vertex set $\{x, y, z\}$ disjoint from $K(r)$ and $K'(r)$ such that $x \to y \to z$.*

We define the following families of digraphs formed from either the disjoint union $K(r) \cup T$ or $K'(r) \cup T$:

- A_r*: $K'(r) \cup T$ with added arcs $x_{r-1} \to x$, $x \to x_i$ for $1 \leq i \leq r-2$, $y \to y_{r-1}$ and $y_i \to y$ for $1 \leq i \leq r-2$,*
- $B_{r,t}$*: $K(r) \cup T$ with added arcs $x \to x_i$ for $1 \leq i \leq r-1$, $y_i \to y$ for $1 \leq i \leq t$ and $y_i \to z$ for $t+1 \leq i \leq r-1$,*
- C_r*: $K'(r) \cup T$ with added arcs $x_{r-1} \to z$, $z \to y_{r-1}$, $y \to x_i$ for $1 \leq i \leq r-2$ and $y_i \to x$ for $1 \leq i \leq r-2$,*
- D_r*: $K(r) \cup T$ with added arcs $z \to x_1$, $y_1 \to z$, $y \to x_i$ for $2 \leq i \leq r-1$ and $y_i \to x$ for $2 \leq i \leq r-1$, and*
- $B'_{r,t}$ *is the converse of $B_{r,t}$ for $0 \leq t \leq r-1$.*

If G is a 2-geodetic digraph with order $n = 2r+1 \geq 11$, size $m = r^2+2$ and no sources or sinks, then G is either isomorphic to one of $A_r, B_{r,0}, B_{r,r-1}, C_r$ or D_r or is isomorphic to a member of the family $B_{r,t}, B'_{r,t}$ for some $1 \leq t \leq r-2$. The digraphs in this list are pairwise non-isomorphic and so there are $2r+1$ extremal digraphs up to isomorphism.

10.4 Extremal strongly connected k-geodetic digraphs for $k \geq 3$

The analysis of Section 10.2 naturally raises the question: what is the largest possible size of a strongly connected k-geodetic digraph with order n for $k \geq 3$? In this section we provide upper and lower bounds for $\mathrm{ex}^*(n;k)$ for $k \geq 3$ and constructions that we conjecture to be extremal for sufficiently large n.

As any k-geodetic digraph with $k \geq 3$ will also be 2-geodetic, it is trivial that for $k \geq 3$ we have $\mathrm{ex}^*(n;k) < \mathrm{ex}^*(n;2)$, where strict inequality follows from the fact that the extremal digraphs for $k = 2$ are not 3-geodetic. However, it is easy to provide a better upper bound for $k \geq 5$.

Lemma 10.29. *For $k \geq 2$ any k-geodetic digraph without sources or sinks has strictly fewer than $\frac{n^2}{k}$ arcs.*

Proof. Let G be a k-geodetic digraph without sinks. Suppose that G contains a vertex u with out-degree $d^+(u) \geq \frac{n}{k}$. As every vertex has out-degree at least one, it follows that $|N^{+t}(u)| \geq d^+(u) = \frac{n}{k}$ for $1 \leq t \leq k$, where $N^{+t}(u)$ denotes the set of vertices at distance t from u. As G is k-geodetic, all of the vertices in these sets are distinct, so it follows that $n \geq 1 + k\frac{n}{k}$, a contradiction. Hence the maximum out-degree of G is

$\Delta^+ < \frac{n}{k}$ and, summing over all vertices of G, the size of G is $m < n\frac{n}{k} = \frac{n^2}{k}$. □

It follows that $\limsup_{n\to\infty} \frac{\mathrm{ex}^*(n;k)}{n^2} \leq \frac{1}{k}$. We now provide constructions that show that $\frac{1}{k^2} \leq \liminf_{n\to\infty} \frac{\mathrm{ex}^*(n;k)}{n^2}$.

Let the quotient and remainder when n is divided by k be r and s respectively, i.e. $n = kr + s$. We assume that $s \leq r$. Form the digraph $G(n,k)$ as follows (see Figure 10.12). The vertex set of $G(n,k)$ consists of vertices $u_{i,j}$ for $1 \leq i \leq r$ and $1 \leq j \leq k$, as well as s further vertices $v_1, v_2, \ldots, v_s$.

We define the adjacencies of $G(n,k)$ as follows:

- i) $u_{i,j} \to u_{i,j+1}$ for $1 \leq i \leq r$ and $1 \leq j \leq k-1$,
- ii) $u_{i,k} \to v_i$ for $1 \leq i \leq s$,
- iii) $u_{i,k} \to u_{j,2}$ for $s+1 \leq i \leq r$ and $1 \leq j \leq s$,
- iv) $u_{i,k} \to u_{i',1}$ for $s+1 \leq i, i' \leq r$ and $i \neq i'$,
- v) $v_t \to u_{i,1}$ for $1 \leq t \leq s$ and all i in the range $1 \leq i \leq r$.

This digraph is k-geodetic and has size

$$m = rs + (k-1)r + s + (r-s)(r-1) = r^2 + (k-2)r + 2s.$$

If $r+1 \leq s \leq k-1$, then we have $\lfloor \frac{n}{k} \rfloor \leq k-2$, which is equivalent to $n \leq k^2 - k - 1$. Therefore these digraphs will certainly exist for $n \geq k^2 - k$. The arcs in part iii) can also be directed to $u_{j,1}$; combined with taking the converse of the resulting digraphs, this generates several different isomorphism classes.

These digraphs admit a particularly simple description when $k|n$. Let $n = kr$ for some $r \geq 2$. Then $G(kr,k)$ is k-geodetic and has order kr and size $r(r-1) + r(k-1) = r^2 + (k-2)r = \frac{n^2}{k^2} + \frac{(k-2)n}{k}$. It has vertices $u_{i,j}$, where $1 \leq i \leq r$ and $1 \leq j \leq k$. We define the adjacencies as follows:

- i) $u_{i,j} \to u_{i,j+1}$ for $1 \leq i \leq r$ and $2 \leq j \leq k-1$,
- ii) $u_{i,1} \to u_{i',2}$ for $1 \leq i, i' \leq r$ and $i \neq i'$,
- iii) $u_{i,k} \to u_{i,1}$ for $1 \leq i \leq r$.

It can also be observed that $G(kr,k)$ can be derived from the extremal strongly connected 2-geodetic digraphs of order $2r$ (i.e. the orientation of $K_{r,r}$ with a perfect matching pointing in one direction and all other arcs directed in the opposite

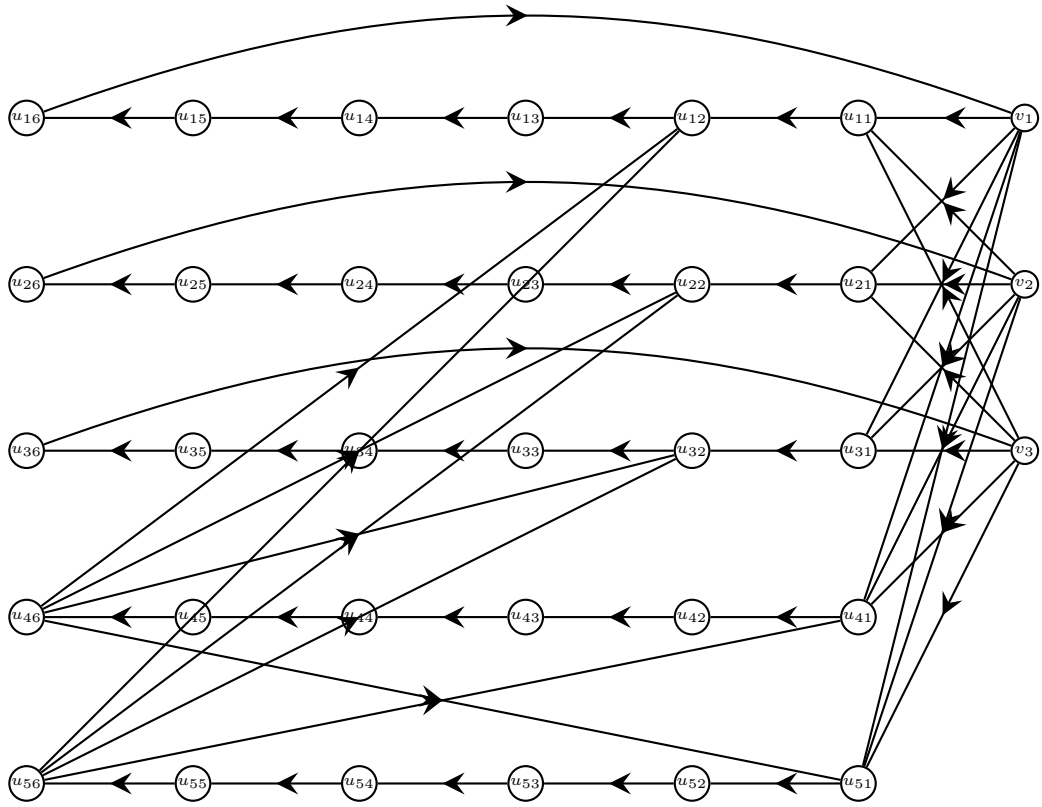

Figure 10.12: $G(33, 6)$

direction) by extending the perfect matching into paths of length $k-1$. The digraph $G(24; 6)$ is shown in Figure 10.13.

Table 10.1 displays the results of computational work by Erskine on the values of $\mathrm{ex}^*(n; k)$ for some small values of n and $k \geq 3$. It can be seen that the digraph $G(n, k)$ has largest possible size whenever $n = kr + s$, where $s \leq \min\{r, k-1\}$. In fact for n and k in the above range such that $k|n$ we can say further that the underlying undirected graph of $G(n, k)$ is the unique graph with size $\frac{n^2}{k^2} + \frac{(k-2)n}{k}$ that has a strongly connected k-geodetic orientation. This leads us to make the following conjecture.

Conjecture 10.30. *If $n \geq k+1$ and $n \leq (k+1)\lfloor \frac{n}{k} \rfloor$ (in particular for $n \geq k^2 - k$),*

$$\mathrm{ex}^*(n; k) = \left\lfloor \frac{n}{k} \right\rfloor^2 - (k+2)\left\lfloor \frac{n}{k} \right\rfloor + 2n.$$

Also if $k|n$, then $G(n, k)$ is the unique extremal strongly-connected k-geodetic digraph with that order.

Theorems 10.23 and 10.13 prove this conjecture for the case $k = 2$.

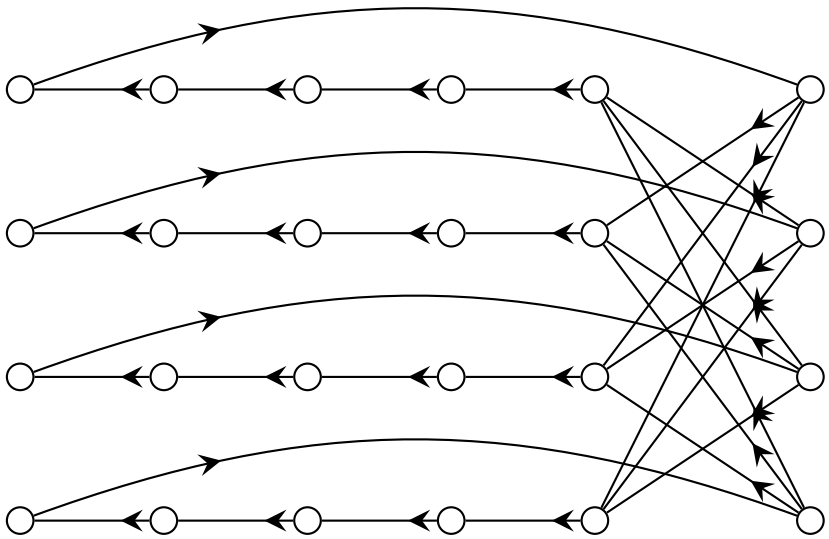

Figure 10.13: $G(24, 6)$

n/k	3	4	5	6
7	8			
8	10			
9	12	10		
10	14	12		
11	16	14	12	
12	20	15	14	
13	22	17	15	14
14	24	19	17	16
15		21	18	17
16			20	19
17			22	20
18				21
19				23

Table 10.1: $\mathrm{ex}^*(n; k)$ for some small values of n and k

10.5 Generalised Turán problems for k-geodetic digraphs

Recently the following extension of Turán's problem has received a great deal of attention: given graphs T and H, what is the largest possible number of copies of T in an H-free graph with order n? Erdős considered this problem in 1962 [58] when T and H are complete graphs. The largest number of 5-cycles in a triangle-free graph was treated in [82, 87] and the converse problem of the largest number of triangles in a graph without a given odd cycle C_{2k+1} is discussed in [27, 83]. The problem was considered in greater generality in [3]. To investigate this problem in digraphs we define the following notation.

Definition 10.31. For any digraph Z and $k \geq 2$ we denote the largest number of copies of Z in a k-geodetic digraph by $\mathrm{ex}(n; Z; k)$.

Observe that if Z is a directed arc then $\mathrm{ex}(n; Z; k) = \mathrm{ex}(n; k)$. We will study the asymptotics of the function $\mathrm{ex}(n; Z; k)$ in the cases that Z is a directed $(k+1)$-cycle or a directed path. We begin with the function $\mathrm{ex}(n; C_{k+1}; k)$, where $k \geq 2$ and C_{k+1} is a directed $(k+1)$-cycle. Earlier we made use of the fact that any arc in a 2-geodetic digraph is contained in at most one triangle; a similar principle applies for larger k.

Lemma 10.32. *Every arc in a k-geodetic digraph is contained in at most one directed $(k+1)$-cycle.*

Proof. Suppose that an arc xy is contained in two distinct $(k+1)$-cycles. Then y has distinct paths of length k to x, violating k-geodecity. □

Using this lemma, Salia proved by induction that the largest number $\mathrm{ex}(n; C_{k+1}; k)$ of directed $(k+1)$-cycles in a k-geodetic digraph with given order n satisfies

$$\mathrm{ex}(n; C_{k+1}; k) \leq \Sigma_{i=1}^{n} i^{1/k} = \frac{k}{k+1} n^{\frac{k+1}{k}} + O(n^{\frac{1}{k}}).$$

For the full proof we refer to [146]. In fact, this upper bound is tight up to a multiplicative constant. We can show this using the permutation digraphs $P(d, k)$. The permutation digraph $P(d, k)$ has order $n = (d+k)(d+k-1)\dots(d+1)$ and size dn. It is easily seen that each arc of $P(d, k)$ is contained in a unique $(k+1)$-cycle; for example $0123\dots(k-1) \to 123\dots(k-1)k$ is contained in the unique $(k+1)$-cycle

$$0123\dots(k-1) \to 123\dots(k-1)k \to 23\dots(k-1)k0 \to \cdots \to k0123\dots(k-2) \to 0123\dots(k-1).$$

Hence $P(d,k)$ contains $\frac{nd}{k+1}$ copies of C_{k+1}. Therefore asymptotically $\mathrm{ex}(n;C_{k+1};k)$ is at least $\frac{1}{k+1}n^{\frac{k+1}{k}}$. In particular, $\mathrm{ex}(n;C_3;2)$ must lie somewhere between $\frac{1}{3}n^{3/2}$ and $\frac{2}{3}n^{3/2}$. It turns out that the lower bound is correct; this was proven by Salia using an application of Hölder's inequality.

Theorem 10.33.

$$\mathrm{ex}(n;C_3;2) = \frac{1}{3}n^{3/2} + O(n^{\frac{1}{2}}).$$

Based on this example, we make the following conjecture.

Conjecture 10.34. *For all $k \geq 2$ we have*

$$\mathrm{ex}(n;C_{k+1};k) = \frac{1}{k+1}n^{\frac{k+1}{k}} + O(n^{\frac{1}{k}}).$$

We turn now to the problem of the largest number of directed paths of given length in a 2-geodetic digraph. Let P_ℓ be the path of length ℓ (i.e. order $\ell+1$). Surprisingly there are some differences between odd and even length paths; in the following theorem we show different lower bounds. The construction for even ℓ is due to the author and for odd ℓ to Erskine.

Theorem 10.35. *If $k \geq 2$ and k divides ℓ, then we have*

$$\mathrm{ex}(n;P_\ell;k) \geq n^{(\ell/k)+1} + O(n^{1+\frac{\ell-1}{k}}).$$

In particular, if ℓ is even then

$$\mathrm{ex}(n;P_\ell;2) \geq n^{(\ell/2)+1} + O(n^{(\ell+1)/2}).$$

If ℓ is odd, we have

$$\mathrm{ex}(n;P_\ell;2) \geq (n/2)^{(\ell+3)/2}.$$

Proof. Let $P(d,k)$ be a permutation digraph with degree d. $P(d,k)$ has order $(d+k)(d+k-1)\dots(d+1)$. From each vertex x there are at least $d^k(d-1)(d-2)\dots(d-\ell+k) = d^\ell + O(d^{\ell-1})$ distinct ℓ-paths with initial vertex x, so there are $d^{\ell+k} + O(d^{\ell+k-1})$ distinct ℓ-paths in $P(d,k)$. Thus there are $n^{(\ell/k)+1} + O(n^{1+\frac{\ell-1}{k}})$ distinct ℓ-paths in $P(d,k)$.

Now let ℓ be odd and consider an orientation of the complete bipartite graph $K_{r,r}$ where $n = 2r$, in which a perfect matching is oriented in one direction and all other

arcs are oriented in the opposite direction. We have already seen that this digraph is 2-geodetic. $\frac{n}{2}$ of the vertices are the initial vertices of $(\frac{n}{2})^{(\ell+1)/2} + O(n^{(l-1)/2})$ distinct ℓ-paths, whereas the vertices in the other partite set are the initial vertices of only $O(n^{(\ell-1)/2})$ ℓ-paths each. Multiplying by $\frac{n}{2}$ yields the result. □

Theorem 10.36. *If $k \geq 2$ and k divides ℓ, then*

$$\mathrm{ex}(n; P_\ell; k) \leq n^{(\ell/k)+1} + O(n^{1+\frac{\ell-1}{k}}).$$

In particular, for every even ℓ

$$\mathrm{ex}(n; P_\ell; 2) = n^{(\ell/2)+1} + O(n^{\ell/2}).$$

Proof. Let $k \geq 2$ divide ℓ. We have a lower bound from Theorem 10.35. For an upper bound, consider a path of length ℓ with vertices $0, 1, \ldots, \ell$. By k-geodecity, given the two endpoints of a path of length k all of the intermediate vertices are determined. Hence we can only choose vertices $0, k, 2k, \ldots, \ell$ independently. Hence $\mathrm{ex}(n; P_\ell; k)$ is at most $n^{(\ell/k)+1}$. □

For paths of odd length we have an asymptotically sharp result only for P_3. The approach of the proof is due to Salia and can be found in [146].

Theorem 10.37. *The largest number of 3-paths in a 2-geodetic digraph with order n satisfies*

$$\mathrm{ex}(n; P_3; 2) = (n/2)^3 + O(n^2).$$

Chapter 11

Conclusion

In this thesis we have discussed several extremal problems for directed and mixed graphs, principally concerning networks with order close to the Moore bound. We will now summarise the main contributions of this thesis, dividing our discussion into two broad sections, i) directed graphs and ii) mixed graphs. We also indicate important problems for future research.

11.1 Bounds for directed graphs

The degree/geodecity problem was first discussed in [132]. We formally defined the problem in Chapter 3 and proved the existence of extremal digraphs (which we named *geodetic cages*) in Corollary 3.20 using the properties of permutation digraphs.

11.1.1 Properties of geodetic cages

In Chapter 3 we discussed some simple properties of geodetic cages. In Theorems 3.26 and 3.27 we proved that the order $N(d,k)$ of a (d,k)-geodetic cage is strictly monotonic in both the degree d and the geodetic girth k. In Theorems 3.31 and 3.33 we proved that directed geodetic cages are strongly connected and 2-weakly-connected; by analogy with Corollary 2.10 for undirected cages, we conjectured that geodetic cages have the following much stronger property.

Conjecture 3.29. *All geodetic cages are maximally connected and super-arc-connected.*

In Chapter 5 we made a further conjecture on the structure of geodetic cages.

Conjecture 5.1. *All (d,k)-geodetic cages are diregular.*

In Section 6.3 we showed that $N(2,2) = 9$ and classified the $(2,2)$-geodetic cages, thereby giving the first known non-trivial examples of geodetic cages. We determined further cages in Section 9.5 for the pairs $(d,k) = (2,3)$ and $(3,2)$; these cages satisfy both Conjecture 3.29 and Conjecture 5.1. As evidence towards Conjecture 3.29 we

noted in Theorem 3.34 that the corresponding result is true for balanced cages with sufficiently large d by the result of [9]; thus if Conjecture 5.1 is true, then Conjecture 3.29 is true for sufficiently large d. However, Conjecture 5.1 appears to be a deep problem.

11.1.2 Digraphs with excess one

As there are no non-trivial Moore digraphs [33], the natural next step is to look for digraphs with excess one. There are no known $(d, k; +1)$-digraphs for $d, k \geq 2$. This motivated us to make the following conjecture.

Conjecture 4.2. *There are no $(d, k; +1)$-digraphs with $d, k \geq 2$.*

The best known results prior to the research contained in this thesis are summarised in Lemma 4.1.

Lemma 4.1. *[116, 132] If G is a $(d, k; +1)$-digraph, then*

- *G is diregular.*
- *Either G is a $(d, 2; +1)$-digraph, where d lies in the range $3 \leq d \leq 7$, or a $(d, k; +1)$-digraph with $d \geq 3$ and $k \geq 5$, or a directed $(k + 2)$-cycle.*
- *The outlier function o of G is an automorphism.*

In Chapter 4 we made a significant step towards proving Conjecture 4.2. Firstly, in Section 4.1, we used counting arguments to deduce strong divisibility conditions on the pairs (d, k) for which there can exist a vertex-transitive $(d, k; +1)$-digraph; this case is of particular interest, as all known undirected Moore graphs are vertex-transitive. In particular, the divisibility conditions demonstrated that any vertex-transitive $(d, k; +1)$-digraph must either have $d > 12$ or $k > 10000$. It appears that the pairs (d, k) that satisfy the conditions in Corollary 4.12 and Theorem 4.14 are very sparse.

Conjecture 11.1. *The set of pairs (d, k) that satisfy Corollary 4.12 and Theorem 4.14 has asymptotic density zero.*

In Section 4.2 we derived the following strong restriction on the structure of any $(3, k; +1)$-digraph and used this to show that there is no $(3, 2; +1)$-digraph.

Theorem 4.21. *Any two distinct vertices of a $(3, k; +1)$-digraph have at most one common out-neighbour and at most one common in-neighbour.*

We then approached the problem of the existence of digraphs with excess one by using results on the fixed point sets of automorphisms of a $(d, k; +1)$-digraph, showing that the digraph induced by a fixed point set must itself have excess one if it contains more than two vertices. Applying this result to the outlier automorphism severely restricts the possible permutation structure of the outlier function of a minimal counterexample to Conjecture 4.2. By combining this analysis with spectral results from [116], we proved that any $(d, k; +1)$-digraph with $d, k \geq 2$ must contain a vertex with order at least three, i.e. there exists a vertex u such that $o(u) \neq o^-(u)$.

Theorem 4.45. *There are no 2-outlier-regular $(d, k; +1)$-digraphs.*

We then employed the same method to deal with the unresolved cases $3 \leq d \leq 7$ for $k = 2$ in Lemma 4.1 using an iterative approach; this completely classifies the $(d, k; +1)$-digraphs with $k \leq 4$.

Theorem 4.56. *If $d, k \geq 2$ and $\epsilon(d, k) = 1$, then $d \geq 3$ and $k \geq 5$.*

11.1.3 Digraphs with excess at least two

For larger values of the excess ϵ our main tool in the diregular case was the Neighbourhood Lemma, which extends the result of [116] that the outlier function of a digraph with excess one is a digraph automorphism.

Lemma 6.1. *For any $d, k \geq 2$ and excess $\epsilon \geq 1$, let G be a diregular $(d, k; +\epsilon)$-digraph. Then for any vertex u of G we have $O(N^+(u)) = N^+(O(u))$ as multisets.*

The following two lemmas gave the analogous relations for a non-diregular $(d, k; +\epsilon)$-digraph, where $S = \{u \in V(G) : d^-(u) < d\}$ and $S' = \{v \in V(G) : d^+(v) > d\}$.

Lemma 5.5. *For every vertex u of an out-regular, but non-diregular $(d, k; +\epsilon)$-digraph G we have*

$$S \subseteq \bigcap_{u \in V(G)} O(N^+(u)).$$

Lemma 5.6. *For every vertex u of an out-regular, but non-diregular $(d, k; +\epsilon)$-digraph G the set S' satisfies*

$$S' \subseteq \bigcap_{u \in V(G)} N^+(O(u)).$$

Using the latter two lemmas and a structural result called the *Amalgamation Lemma* (Lemma 5.12), we showed in Chapter 5 that any $(2, k; +2)$-digraph must be diregular. In Chapter 6 we dealt with the diregular case using the Neighbourhood Lemma, proving that there are no diregular $(2, k; +2)$-digraphs for $k \geq 3$ and classifying the $(2, 2; +2)$-digraphs. In fact, we were able to push this analysis further to show the non-existence of diregular $(2, k; +3)$-digraphs for $k \geq 3$; this represents the first classification of a family of directed graphs with order three away from the Moore bound. As a result, we obtained the following classification of $(2, k; +2)$-digraphs and diregular $(2, k; +3)$-digraphs.

Theorem 11.2. *There are two $(2, 2; +2)$-digraphs (see Figure 9.11) and no $(2, k; +2)$-digraphs for $k \geq 3$. There are also no diregular $(2, k; +3)$-digraphs for $k \geq 3$.*

The obvious question raised by Theorem 11.2 is whether there exists a non-diregular $(2, k; +3)$-digraph. We presented results on the structure of any such digraph in Section 5.4, but the number of in-degree sequences to analyse is prohibitive.

Conjecture 11.3. *There are no non-diregular $(2, k; +3)$-digraphs or $(3, k; +2)$-digraphs.*

Combined with a computer search, the lower bounds derived in Chapters 4, 5 and 6 allowed us to determine geodetic cages for some small values of d and k; the results are contained in Table 9.3.

d	k	M	n	ϵ	Comment
2	2	7	9	2	Figure 9.11
2	3	15	20	5	Figures 9.12 and 9.13
2	4	31	54*	23*	No graphs of order less than 34
3	2	13	16	3	Figure 9.14

Table 9.3: Smallest digraphs of given degree d and geodecity k (* = smallest known)

In Section 3.2 we also touched on the problem of finding a smallest arc-transitive k-geodetic digraph with degree d for $d, k \geq 2$. We showed that the permutation digraphs are arc-transitive and, for fixed k and increasing d, have order asymptotically approaching the Moore bound. In general the permutation digraphs are not smallest possible arc-transitive digraphs for given d and k, but we made the following conjecture for large values of the degree.

Conjecture 3.24. *For fixed k and sufficiently large d, the permutation digraph $P(d, k)$ is the smallest arc-transitive k-geodetic digraph with degree d.*

Given these nice properties of permutation digraphs, it would be interesting to investigate other properties of these digraphs, in particular their diameter behaviour in the cases not covered by Theorems 3.22 and 3.23.

Question 11.4. *What is the diameter of $P(d,k)$ for $3 \leq d \leq k-1$?*

11.1.4 Turán problems

In Chapter 10 we looked at the subject of geodetic girth from a different perspective by asking for the largest possible size of a k-geodetic digraph with given order n. In fact, this problem turned out to be quite simple; we obtain a much more difficult problem if we add the requirement of strong connectivity. We solved this problem for $k = 2$ and classified all of the extremal digraphs.

Theorem 11.5. *The largest size of a strongly connected 2-geodetic digraph with order n is given by $ex^*(2r;2) = r^2$ for $r \geq 2$ and $ex^*(2r+1;2) = r^2+2$ for $r \geq 1$.*

For larger $k \geq 3$, our best upper bound is of asymptotic order only $\frac{n^2}{k}$, whereas we conjecture the true value of $ex^*(n;k)$ to be of order $\frac{n^2}{k^2}$. It would be extremely desirable to close this large gap. In addition to a conjectured asymptotic bound, we presented constructions in Chapter 10 that we believe to be extremal; this leads to the following very precise conjecture.

Conjecture 10.30. *If $n \geq k+1$ and $n \leq (k+1)\left\lfloor \frac{n}{k} \right\rfloor$ (in particular for $n \geq k^2-k$),*

$$ex^*(n;k) = \left\lfloor \frac{n}{k} \right\rfloor^2 - (k+2)\left\lfloor \frac{n}{k} \right\rfloor + 2n.$$

Also if $k|n$, then $G(n,k)$ is the unique extremal strongly-connected k-geodetic digraph with that order.

We closed by considering some generalised Turán problems for k-geodetic digraphs, especially for the largest number of directed $(k+1)$-cycles and paths. We solved these problems for the number of directed triangles and directed paths of even length in 2-geodetic digraphs of given order. These bounds are met asymptotically by the permutation digraphs.

Theorem 10.33.

$$ex(n;C_3;2) = \frac{1}{3}n^{3/2} + O(n^{\frac{1}{2}}).$$

Theorem 10.36. *If $k \geq 2$ and k divides ℓ, then*

$$ex(n; P_\ell; k) = n^{(\ell/k)+1} + O(n^{1+\frac{\ell-1}{k}}).$$

In particular, for every even ℓ we have

$$ex(n; P_\ell; 2) = n^{(\ell/2)+1} + O(n^{\ell/2}).$$

We conjecture that the permutation digraphs $P(d, k)$ are extremal for the number of $(k+1)$-cycles for larger k as well.

Conjecture 10.34. *For all $k \geq 2$ we have*

$$ex(n; C_{k+1}; k) = \frac{1}{k+1} n^{\frac{k+1}{k}} + O(n^{\frac{1}{k}}).$$

For $k = 2$ and paths with odd length we were able to decide the asymptotic order only for paths of length three, which shows that orientations of complete bipartite graphs $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ are extremal for 3-paths.

Theorem 10.37.

$$ex(n; P_3; 2) = (n/2)^3 + O(n^2).$$

The discrepancy between odd and even path lengths is extremely interesting. We have not yet been able to show that this behaviour continues for $k = 2$ and larger odd ℓ; more generally, for larger k, we presume that the asymptotic order of the largest number of paths of length ℓ in a k-geodetic digraph depends upon the conjugacy class of ℓ modulo k.

Conjecture 11.6. *For odd ℓ, we have $ex(n; P_\ell; 2) \sim (n/2)^{(\ell+3)/2}$.*

Directed $(k+1)$-cycles in a k-geodetic digraph represent a 'near-violation' of k-geodecity. Another significant 'near-violation' is a pair of distinct u, v-paths P, Q of length k and $k+1$ or both of length $k+1$; following Ustimenko [149], we could call the corresponding subdigraphs *small hooves*.

Question 11.7. *What is the largest possible number of small hooves in a k-geodetic digraph with order n?*

11.2 Bounds for mixed graphs

In Chapter 7 we shifted our focus to mixed graphs, networks containing both undirected edges and directed arcs. This thesis has made contributions to the degree/diameter problem for mixed graphs and also generalised the degree/geodecity problem to the mixed setting.

11.2.1 Degree/diameter problem for mixed graphs

As discussed in Chapter 7, the degree/diameter problem for mixed graphs has received a great deal of attention. López and Miret presented very strong conditions on the possible values of the undirected degree r and directed out-degree z of an $(r, z, 2; -1)$-graph in [104]; however, this result applies only to totally regular graphs, prompting the authors to ask whether all almost mixed Moore graphs with diameter two are totally regular. Using a combination of counting arguments and spectral methods, we answered this question in the affirmative in Chapter 8.

Theorem 8.10. *Almost mixed Moore graphs with diameter two are totally regular.*

We also extended this result to almost mixed Moore graphs with $k \geq 3$ for $r = z = 1$.

Theorem 8.15. *For $k \geq 3$, $(1, 1, k; -1)$-graphs are totally regular.*

For the degree parameters $r = z = 1$ we also succeeded in improving on a lower bound for the defect of a totally regular mixed graph with diameter $k \geq 3$ due to Dalfó et al. [51].

Theorem 9.25. *Any totally regular $(1, 1, k; -\delta)$-graph has defect*

$$\delta \geq \sum_{t=1}^{k-2} Z'_t \left\lceil \frac{1}{3} + \frac{1}{3} \left\lfloor \frac{k-t}{2} \right\rfloor \right\rceil$$

for $k \geq 3$, where $Z'_1 = 1$ and $Z'_t = \frac{1}{2^{t-1}\sqrt{5}}((1+\sqrt{5})^{t-1} - (1-\sqrt{5})^{t-1})$ for $2 \leq t \leq k-2$.

The noteworthy feature of Theorem 9.25 is that, unlike the bound in [51], it grows with increasing values of the diameter k. It would be of great interest to derive such a bound for other values of r and z.

Question 11.8. *Can the bound in Theorem 9.25 be extended to other values of the degree parameters r and z?*

11.2.2 Degree/geodecity problem for mixed graphs

In Chapter 7 we generalised the degree/geodecity problem to the setting of mixed graphs. We defined a mixed graph G to be k-geodetic if for any pair of (not necessarily distinct) vertices u, v there is at most one non-backtracking mixed walk from u to v with length $\leq k$. The order of a k-geodetic mixed graph with minimum undirected degree r and minimum directed out-degree z is bounded below by the mixed Moore bound $M(r, z, k)$; if such a graph has order $M(r, z, k) + \epsilon$, then we called it an $(r, z, k; +\epsilon)$-graph.

In Chapter 7 we proved the existence of mixed geodetic cages using a truncation argument and proved monotonicity of the order of (r, z, k)-cages in the directed out-degree z and geodetic girth k. We also made the following conjecture on the structure of mixed geodetic cages, which includes Conjecture 5.1 as a special case.

Conjecture 7.19. *All mixed geodetic cages are totally regular.*

In Chapter 8 we proved the analogue of Theorem 8.10 for 2-geodetic mixed graphs with excess one.

Theorem 8.18. *All $(r, z, 2; +1)$-graphs are totally regular.*

A counting argument in Chapter 9 allowed us to derive a strong lower bound on the excess of a totally regular k-geodetic mixed graph.

Theorem 9.5. *For $k \geq 3$, the excess ϵ of a totally regular $(r, z, k; +\epsilon)$-graph satisfies*

$$\epsilon \geq \frac{r}{\phi}\Big[\frac{\lambda_1^{k-1} - 1}{\lambda_1 - 1} - \frac{\lambda_2^{k-1} - 1}{\lambda_2 - 1}\Big],$$

where

$$\phi = \sqrt{(r + z - 1)^2 + 4z},$$

$$\lambda_1 = \frac{1}{2}(r + z - 1 + \phi)$$

and

$$\lambda_2 = \frac{1}{2}(r + z - 1 - \phi).$$

However, the author is not aware of any non-trivial case in which this bound is met.

Question 11.9. *Can the bound in Theorem 9.5 be improved or is it tight?*

Using a more involved argument we generalised Theorem 9.5 to mixed graphs that are not totally regular at the expense of weakening the bound by a factor of $\frac{z}{2r+3z}$.

Theorem 9.9. *The excess of any (r, z, k)-cage satisfies*

$$\epsilon \geq \frac{rz}{(2r+3z)\phi}\left[\frac{\lambda_1^{k-1}-1}{\lambda_1-1} - \frac{\lambda_2^{k-1}-1}{\lambda_2-1}\right],$$

where λ_1, λ_2 and ϕ are as defined in Theorem 9.5.

We applied Theorems 9.5 and 9.9 to the special case of mixed graphs with excess one to show that any such graph must have $k = 2$. This extends the result of [12] for undirected graphs with excess one to the case of mixed graphs.

Theorem 9.15. *If G is an $(r, z, k; +1)$-graph with $r, z \geq 1$, then $k = 2$ and G is totally regular.*

Combined with the spectral analysis from [104], which gives strong conditions on the degree parameters in a totally regular $(r, z, k; +1)$-graph, this means that mixed graphs with excess one are very rare.

Theorem 7.18. *Let G be a totally regular $(r, z, 2; +1)$-graph. Then either*

- $r = 2$,
- $4r + 1 = c^2$ *for some* $c \in \mathbb{N}$ *and* $c|(16z^2 - 24z + 25)$, *or*
- $4r - 7 = c^2$ *for some* $c \in \mathbb{N}$ *and* $c|(16z^2 + 40z + 9)$.

However, we did identify a $(2, 1, 2; +1)$-graph (see Figure 9.4) and proved that this is the unique 2-geodetic mixed graph with excess one and $r = z = 1$.

Chapter 9 also presented the results of a computer search that found new mixed cages for some small r, z and k and established upper bounds for other combinations of r, z and k by finding smallest Cayley $(r, z, k; +\epsilon)$-graphs. Some results are shown in Table 9.2. In some cases the lower bounds from Theorem 9.5 combined with computer search are close to the upper bound provided by our new record graphs. This suggests that further geodetic cages will be identified by extending the search and improving the lower bounds for particular combinations of r, z and k.

Problem 11.10. *Identify further mixed and directed geodetic cages.*

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