

EGERVÁRY RESEARCH GROUP
ON COMBINATORIAL OPTIMIZATION



TECHNICAL REPORTS

TR-TR-2023-01. Published by the Egerváry Research Group, Pázmány P. sétány 1/C,
H-1117, Budapest, Hungary. Web site: www.cs.elte.hu/egres. ISSN 1587-4451.

**A network flow approach to
a common generalization of
Clar and Fries numbers**

Erika Bérczi-Kovács and András Frank

July 6, 2023

A network flow approach to a common generalization of Clar and Fries numbers

Erika Bérczi-Kovács ^{*} and András Frank ^{**}

Abstract

Clar number and Fries number are two thoroughly investigated parameters of plane graphs emerging from mathematical chemistry to measure stability of organic molecules. We consider first a common generalization of these two concepts for bipartite plane graphs, and then extend it to a framework on general (not necessarily planar) directed graphs. The corresponding optimization problem can be transformed into a maximum weight feasible tension problem which is the linear programming dual of a minimum cost network flow (or circulation) problem. Therefore the approach gives rise to a min-max theorem and to a strongly polynomial algorithm that relies exclusively on standard network flow subroutines. In particular, we give the first network flow based algorithm for an optimal Fries structure and its variants.

1 Introduction

This paper considers some optimization problems arising in mathematical chemistry. A natural graph model to capture the basic structure of an organic molecule uses a planar graph G where the atoms are represented by nodes of G while the bonds between atoms correspond to the edges of G . An important tool in mathematical chemistry is the notion of a Kekulé structure, which corresponds to a perfect matching of the representing graph G .

Several important parameters can be described with this approach, which gives rise to challenging problems in combinatorial optimization. One of the most well-known of these problems concerns the Clar number [6]. Clar's empirical observation states a connection between the stability of a so-called aromatic hydrocarbon molecule and the maximum number of disjoint benzenoid rings, called the Clar number. In the graph model, the Clar number of a molecule is the cardinality of the largest Clar-set, where

^{*}Alfréd Rényi Institute of Mathematics, Department of Operations Research, Eötvös Loránd University, Budapest, Hungary, and ELKH-ELTE Egerváry Research Group on Combinatorial Optimization. erika.berczi-kovacs@ttk.elte.hu

^{**}Department of Operations Research, Eötvös Loránd University, Budapest, Hungary, and ELKH-ELTE Egerváry Research Group on Combinatorial Optimization. andras.frank@ttk.elte.hu

a Clar-set of a perfectly matchable planar graph G embedded in the plane consists of some disjoint bounded (= inner) faces of G that can simultaneously alternate with respect to an appropriate perfect matching of G .

Another important parameter of a molecule is its Fries number [10, 15]. In the graph model, the Fries number of a perfectly matchable planar graph G embedded in the plane is the maximum cardinality of a Fries-set, where a Fries-set consists of some distinct but not necessarily disjoint inner faces that can simultaneously alternate with respect to an appropriate perfect matching of G .

We note that the Clar and Fries numbers are closely related to other parameters investigated in mathematical chemistry, called the forcing and anti-forcing numbers. In bipartite planar graphs with a given embedding the Clar and Fries numbers are lower bounds for the forcing and anti-forcing numbers, respectively, and in some cases these bounds are sharp, e.g. for hexagonal systems and (4,6)-fullerenes [27], [18], [21].

A major issue of the investigations is the algorithmic and structural aspects of Clar and Fries numbers and sets, in which the polyhedral approach (that is, linear programming) plays a central role. We concentrate on 2-connected perfectly matchable bipartite plane graphs $G = (S, T; E)$, where a plane graph means a planar graph with a given embedding in the plane. (Recall that a polyhedron is the solution set of a linear inequality system, while a polytope is the convex hull of a finite number of points. A fundamental theorem of linear programming states that every polytope is a bounded polyhedron. In discrete optimization, it is often a basic, non-trivial approach to provide explicitly such a linear description of the polytope of combinatorial objects to be investigated.)

Consider first the situation with Clar numbers and sets. Hansen and Zheng [14] (using different notation) introduced a polyhedron $P = \{(x', x'') : Fx' + Qx'' = 1, (x', x'') \geq 0\}$, where F is the node vs bounded-face incidence matrix of G while Q is the standard node-edge incidence matrix of G (and hence $[F, Q]$ is a small size $(0, 1)$ -matrix). They considered the projection $P_{\text{Cl}} := \{x' : \exists x'' \text{ with } (x', x'') \in P\}$ of P to the variables x' and observed that the integral (that is, $(0, 1)$ -valued) elements of P_{Cl} correspond to the Clar-sets of G . Hansen and Zheng conjectured that P (and hence P_{Cl}) is an integral polyhedron, which property, if true, implies that the vertices of P_{Cl} correspond to the Clar-sets of G .

Abeledo and Atkinson [2] (Theorem 3.5) proved that $[F, Q]$ is a unimodular matrix (though not always totally unimodular). This implied the truth of the conjecture of Hansen and Zheng since a theorem of Hoffman and Kruskal [17] (see Theorem 21.5 in the book [23] of Schrijver) implies that, for a unimodular matrix $[A, A']$ and integral vector b , the polyhedron $\{(x, x') : Ax + Ax' = b, x \geq 0\}$ is integral (and so is the dual polyhedron $\{y : yA \geq c, yA' = c'\}$ whenever (c, c') is an integral vector.)

A tiny remark is in order. It follows from the previous approach that P_{Cl} is the polytope of Clar-sets, and P_{Cl} was obtained as a projection of the polyhedron P . At first sight, it may seem more natural to figure out an explicit polyhedral description of P_{Cl} itself. However, the linear inequality system describing P_{Cl} may consist of an exponential number of inequalities. This is why it is more efficient to produce P_{Cl} as the projection of the (integral) polyhedron P that is described by only $O(|E|)$ constraints. Of course, a maximum weight vertex of P_{Cl} (that is, a maximum weight

Clar-set) can be computed once a maximum weight vertex of P can be.

Abeledo and Atkinson [2] noted that an analogous approach works for Fries-sets, as well. Namely, in Theorem 3.6 of [2] they claimed (without a proof) that a certain matrix A is unimodular, and indicated that the Fries-sets correspond to the vertices of the a projection P_{Fr} of the polyhedron defined by A . It should be noted that A is a small size $(0, \pm 1)$ -matrix.

Since the sizes of the describing unimodular matrices are small (a linear function of the size of the graph G), a general purpose linear programming algorithm can be used to compute an optimal (maximum weight) basic solution which corresponds to an optimal Clar-set (Fries-set). Moreover, as the matrices are $(0, \pm 1)$ -valued, the strongly polynomial time algorithm of Tardos [24] for solving such linear programs can be applied. Therefore, there exists a strongly polynomial algorithm for computing both a maximum weight Clar-set and a maximum weight Fries-set.

In addition, Abeledo and Atkinson [3] provided a network flow formulation for the dual of the Clar problem, and hence, as they write: *"the Clar number and the cut cover can be found in polynomial time by solving a minimum cost network flow problem"*. Yet another fundamental result of Abeledo and Atkinson [3] is an elegant min-max formula for the Clar number of a plane bipartite graph, which was conjectured by Hansen and Zheng [13, 14].

As for a min-max formula concerning the Fries number, the above-mentioned linear programming approach of Fries-sets [2] does provide one through the l.p. duality theorem, though this was not explicitly formulated (in a form similar to the one mentioned before concerning Clar numbers). Moreover, to our best knowledge, no purely combinatorial or network flow based algorithm appears in the literature for computing the Fries number of G .

The major goal of the present work is to develop a common generalization of the Clar number and Fries number problems, and based on this, to develop a strongly polynomial algorithm relying exclusively on standard network flow subroutines. Our approach is self-contained, in particular, it does not rely on any earlier polyhedral results on Clar-sets and Fries-sets.

We note that the presented common framework for Clar-sets and Fries-sets has nothing to do with a popular conjecture stating that a plane graph has a largest Clar-set that can be extended to a largest Fries-set. This conjecture was disproved by Hartung [16] for general plane graphs (for fullerenes), proved for a special class of benzenoids by Graver et al. [12], but it is still open for general perfectly matchable bipartite plane graphs.

A basic tool of our approach is that we reformulate the original problem on G for the planar dual graph of G , and then we can drop the planarity assumption. This idea appeared in the work of Erdős, Frank, and Kun [7], where the major problem was to find a largest (weight) sink-stable set of a (not necessarily planar) digraph $D = (V, A)$. Here the term sink-stable refers to a stable set of D whose elements are sink-nodes in an appropriate dicut equivalent reorientation of D . We call two orientations of a graph **dicut equivalent** if one of them can be obtained from the other by reorienting some disjoint one-way cuts (= dicuts). (Incidentally we remark that this digraph model not only covered the (weighted) Clar number problem but implied an elegant theorem of

Bessy and Thomassé [5] as well as its extension by Sebó [20].)

The Fries number problem can also be embedded into this general digraph framework, where it transforms into finding a dicut equivalent reorientation of a digraph in which the set of sink and source nodes is as large as possible. However, this requires a technique more involved than the one needed for Clar numbers (see Remark 5.4).

Our goal, in fact, is to introduce a common framework for these extensions of the Clar and Fries problems. For two given weight-functions w_o and w_i on the node-set of D , our objective is to find a dicut equivalent reorientation of D in which the w_o -weight of the set of source nodes plus the w_i -weight of the set of sink nodes is as large as possible. We shall show that the corresponding optimization problem can be transformed into a maximum weight feasible tension problem which is the linear programming dual of a minimum cost network flow (or circulation) problem. Therefore the approach gives rise to a (combinatorial) min-max theorem and to a strongly polynomial algorithm that relies exclusively on standard network flow subroutines.

1.1 Notation, terminology

Given a ground-set S , we do not distinguish between a vector $c \in \mathbf{R}^S$ and a function $c : S \rightarrow \mathbf{R}$. For a vector or function c on S , let $\tilde{c}(X) := \sum [c(s) : s \in X]$.

We call a digraph **weakly connected** or just **connected** if its underlying undirected graph is connected. Often we refer to the edges of a digraph as **arcs**. Let $D = (V, A)$ be a loopless connected digraph with $n \geq 2$ nodes. For a subset U of nodes, the **in-degree** $\varrho(U) = \varrho_D(U) = \varrho_A(U)$ is the number of arcs entering U , while the **out-degree** $\delta(U) = \delta_D(U) = \delta_A(U)$ is the number of arcs leaving U . Typically, we do not distinguish between a one-element set $U = \{u\}$ and its only element u , for example, $\varrho(u) = \varrho(\{u\})$. For a vector (or function) z on the arc-set A of D , let $\varrho_z(U) := \sum [z(e) : e \text{ enters } U]$ and $\delta_z(U) := \sum [z(e) : e \text{ leaves } U]$.

A function z defined on the arc-set of D is called a **circulation** if $\varrho_z(v) = \delta_z(v)$ holds for every node v . This is equivalent to requiring that $\varrho_z(v) \leq \delta_z(v)$ holds for every node v . Furthermore, for a circulation z , $\varrho_z(U) = \delta_z(U)$ holds for any subset $U \subseteq V$. For lower and upper bound functions f, g , we say that a circulation z is **feasible** if $f \leq z \leq g$. (Here $-\infty$ is allowed for the components of f and $+\infty$ for the components of g .)

A function π defined on the node-set of D is often referred to a **potential**, which **induces** the **tension** Δ_π (sometimes called potential-drop) on the arc-set of D , where $\Delta_\pi(uv) := \pi(v) - \pi(u)$ for $uv \in A$. An integer-valued tension can be obtained as the potential-drop of an integer-valued potential. It is a well-known property that the set of circulations and the set of tensions are complementary orthogonal subspaces (over the rationals or the reals), that is, $z\Delta_\pi = 0$ holds for any circulation z and potential π . We call an integer-valued potential π **small-dropping** if its potential-drop Δ_π is $(0, 1)$ -valued. When Δ_π is $(0, 1)$ -valued only on a subset $A_0 \subseteq A$ of arcs, we say that π is **small-dropping on A_0** .

For given lower bound $c_\ell : A \rightarrow \mathbf{R} \cup \{-\infty\}$ and upper bound $c_u : A \rightarrow \mathbf{R} \cup \{+\infty\}$, we say that a potential π or the potential drop Δ_π is (c_ℓ, c_u) -**feasible** if $c_\ell \leq \Delta_\pi \leq c_u$. When $c_\ell \equiv -\infty$ (that is, when no lower bound is given), we speak of c_u -**feasibility**.

A **circuit** is a connected undirected graph in which the degree of every node is 2. For a circuit C , we use the convention that C also denotes the edge-set of the circuit while $V(C)$ denotes its node-set. A directed graph is also called a **circuit** if it arises from an undirected circuit by arbitrarily orienting its edges. A directed graph obtained from an undirected circuit by orienting each edge in the same direction is called a **one-way circuit** or just a **di-circuit**.

We call two orientations of an undirected graph **di-circuit equivalent** if one of them can be obtained from the other one by reorienting a set of arc-disjoint di-circuits. This is clearly equivalent to requiring that the in-degree of a node on one orientation is equal to the in-degree in the other orientation.

By **reorienting** (or **reversing**) an arc uv , we mean the operation of replacing uv by vu . The reorientation of a subset B of arcs (that is, reversing B) means that we reorient all the elements of B .

By a **cut** of a connected graph $G = (V, E)$, we mean the set of edges connecting Z and $V - Z$ for some subset Z of nodes. An inclusionwise minimal cut is called **elementary**. A useful observation is that a cut is elementary if and only if both Z and $V - Z$ induce a connected subgraph of G . Furthermore, every cut can be partitioned into elementary cuts. An elementary cut is sometimes called a **bond**, but this term should not be confused with a bond used in chemistry (which corresponds to an edge of the modelling graph).

By a **cut** of a digraph $D = (V, A)$ defined by a subset Z of nodes, we mean the set of arcs connecting Z and $V - Z$ (in either direction). In the special case when no arc enters Z , the cut is called a **directed cut** or a **dicut** of D . Sometimes the term **one-way cut** is used for a dicut. A node of D will be called a **sink node** (or just a sink) if it admits no leaving arcs. A node is a **source node** if it admits no entering arcs. A subset of nodes is a **sink set** (respectively, a **source set**) if each of its elements is a sink (resp., a source). Clearly, a sink set is always stable.

We call a subset Y of nodes of D **sink-stable** (**source-stable**) if there is a dicut equivalent reorientation of D in which every node in Y is a sink node (source node). Obviously, a set is sink-stable precisely if it is source-stable. These are special stable sets of D , and an element of a one-way circuit never belongs to a sink-stable set.

For two disjoint sets $Y_o, Y_i \subseteq V$, we call the ordered pair (Y_o, Y_i) a **source-sink** (= **so-si**) **pair** if there is a dicut equivalent reorientation of D in which Y_o is a source set while Y_i is a sink set. It may be the case that (Y_o, Y_i) is a so-si pair, but (Y_i, Y_o) is not (as exemplified by an acyclic orientation of a triangle). For a subset Y of nodes the following are obviously equivalent: Y is sink-stable (source-stable) set, (Y, \emptyset) is a so-si pair, (\emptyset, Y) is a so-si pair.

We call a subset Y of nodes of D **resonant** if it can be partitioned into subsets Y_o and Y_i where (Y_o, Y_i) is a so-si pair. (The name is motivated by the term resonant set of faces of a plane graph, see, for example, [28]). A sink-stable (or source-stable) set is clearly resonant.

2 Undirected plane graphs and directed general graphs

Recall a basic result of Fáry [8] stating that every simple planar graph admits an embedding in the plane where each edge is represented by a straight-line segment. A deeper result of Tutte [25] states that a 3-connected simple planar graph admits an embedding into the plane in which every edge is represented by a straight-line segment and the faces are convex sets.

Let $G = (V, E)$ be a loopless 2-connected planar graph. Throughout we consider a specified embedding of G into the plane, and say that G is a **plane** graph. Such an embedded graph divides the plane into disjoint (connected) regions, exactly one of them is infinite. We refer to these regions as the **faces** of the plane graph. Since G is 2-connected, its faces are surrounded by a circuit of G , and we refer to these as **face-bounding circuits** or just **face-circuits**. (In the literature, often the longer term boundary circuit is used.) With a slight abuse of terminology, sometimes we do not distinguish between a face and its face-circuit. The single infinite face is called the **outer face** of G while all the other faces are the **inner** faces of G . For their surrounding circuits, we use the term **outer (inner)** face-circuit.

Note that the set of face-circuits may be different for another embedding of a planar graph into the plane, but for 3-connected planar graphs, by a theorem of Tutte, the set of face-circuits is independent from the embedding.

Let F be a face of G and C_F its face-circuit. Let \vec{G} be an orientation of G in which the orientation \vec{C}_F of C_F is a one-way circuit. When we say that the face F and the di-circuit \vec{C}_F is clockwise (anti-clockwise) oriented, we mean that it is clockwise (anti-clockwise) when looked at from the inside of F . (Or putting it in another way, we may imagine that \vec{G} is embedded on the surface of a sphere, with no distinction between the outer face and the inner faces, and a one-way face-circuit is clockwise in the usual sense.)

As a simple example, let the graph be a single circuit C embedded in the plane and let \vec{C} be an orientation of C which is a one-way circuit. Now the graph has one inner face and one outer face, C is a one-way face-circuit belonging to both faces, and \vec{C} is clockwise with respect to the inner face precisely if it is anti-clockwise with respect to the outer face.

It follows from this definition that if F_1 and F_2 are neighbouring (incident) faces of G (that is, they have an edge in common) and their face-circuits are one-way circuits in \vec{G} , then one of F_1 and F_2 is clockwise in \vec{G} while the other is anti-clockwise.

Throughout the paper, we assume that $G = (S, T; E)$ is a perfectly matchable, 2-connected, loopless, bipartite plane graph. Let M be a perfect matching of G . A circuit C of G is called **M -alternating** if every second edge of C belongs to M . If M' is another perfect matching of G , then the symmetric difference $M \ominus M'$ of M and M' consists of disjoint circuits which are both M -alternating and M' -alternating.

A set \mathcal{C}' of node-disjoint face-circuits of G forms a **Clar-set** if G has a perfect matching M such that each member of \mathcal{C}' is M -alternating. A set \mathcal{C}' of (distinct)

face-circuits of G forms a **Fries-set** if G has perfect matching M such that each member of \mathcal{C}' is M -alternating. Sometimes a Fries-set is called a resonant set of faces or face-circuits [28].

Let \mathcal{C}_G denote the set of face-circuits of G (including the outer face). For a non-empty subset \mathcal{C}' of \mathcal{C}_G , the **Clar number** $\text{Cl}(\mathcal{C}') = \text{Cl}_G(\mathcal{C}')$ of G **within** \mathcal{C}' is the maximum cardinality of a Clar-set consisting of some members of \mathcal{C}' . When \mathcal{C}' is the set of inner faces, we simply speak of the **Clar number** of G . It should be noted that the Clar number of two different embeddings of a planar graph into the plane with the same outer face may be different (unless the graph is 3-connected).

For a non-empty subset \mathcal{C}' of face-circuits, the **Fries number** $\text{Fr}(\mathcal{C}') = \text{Fr}_G(\mathcal{C}')$ of G **within** \mathcal{C}' is the maximum cardinality of a Fries-set consisting of some members of \mathcal{C}' . When \mathcal{C} is the set of all inner faces, we simply speak of the **Fries number** of G .

The basic optimization problem for Clar (respectively, Fries) numbers is (A) to compute the Clar (Fries) number of G as well as a maximizing Clar-set (Fries-set) consisting of inner face-circuits. In a slightly more general version, we are interested in (B) finding a maximum cardinality Clar-set (Fries-set) within a specified subset of face-circuits. An even more general form is (C) the weighted Clar-set (Fries-set) problem where we are given a non-negative weight-function w on the set of faces (face-circuits), and want to construct a Clar-set (Fries-set) of largest weight. (When w is $(0, 1)$ -valued we are back at Problem (B), while Problem (A) is obtained for the special weight-function w defined to be 1 on all inner faces and 0 on the outer face.) In what follows, we consider a weighted version of a common generalization of Clar-sets and Fries-sets.

2.1 Common framework for Clar and Fries

For any perfect matching M of G , we define an orientation \vec{G}_M of G , as follows. Orient each element of M toward S while all the other edges of G toward T . Then a face (and its face-circuit) of G is M -alternating precisely if it is a one-way circuit in the orientation \vec{G}_M . Note that every one-way circuit of \vec{G}_M is clockwise or anti-clockwise.

We will say that an M -alternating face-circuit of G is **clockwise** (**anti-clockwise**) if the corresponding one-way circuit in \vec{G}_M is clockwise (anti-clockwise). It follows for two adjacent M -alternating faces that one of them is clockwise, while the other one is anti-clockwise. Furthermore, both the sets of clockwise M -alternating face-circuits and the sets of anti-clockwise M -alternating face-circuits are Clar-sets, and their union is a Fries-set. And conversely, every Fries-set \mathcal{F}' can be obtained in this way. Indeed, if M is a perfect matching for which the members of \mathcal{F}' are M -alternating, then both the set of clock-wise M -alternating members and the set of anti-clockwise M -alternating members of \mathcal{F}' are Clar-sets.

Observe that for any Clar-set \mathcal{C}' there is a perfect matching M' for which each member of \mathcal{C}' is alternating and clockwise. Indeed, by definition, there is a perfect matching M for which each member of \mathcal{C}' is M -alternating. Then the perfect matching M' obtained by taking the symmetric difference of M and the union of anti-clockwise members of \mathcal{C}' will do.

Let w_1 and w_2 be two non-negative weight-functions on the set of faces of G . In the common generalization of the weighted Fries and Clar problems, we look for a perfect matching M of G for which the sum of the total w_1 -weight of the clockwise M -alternating face-circuits plus the total w_2 -weight of the anti-clockwise M -alternating face-circuits is as large as possible. We refer to this common framework as the **double-weighted Clar-Fries** problem. In the special case when $w_1 := w$ and $w_2 := 0$, we are back at the maximum w -weighted Clar-set problem. In the special case when $w_1 := w$ and $w_2 := w$, we are back at the maximum w -weighted Fries-set problem.

Observe that for two perfect matchings M and M' of G , the orientations \vec{G}_M and $\vec{G}_{M'}$ are di-circuit equivalent. In the solution of the double-weighted Clar-Fries problem, we start with an arbitrary perfect matching M of G , consider the digraph \vec{G}_M , and try to find a di-circuit equivalent reorientation of \vec{G}_M maximizing the double weight-function.

The problem can be reformulated in terms of the directed planar dual graph $D = (V, A)$ of \vec{G}_M , as follows. Instead of w_1 and w_2 , we use the non-negative weight-functions w_o and w_i defined on V . Recall the definition of source-sink pair (Y_o, Y_i) in a general digraph. The double-weighted Clar-Fries problem is equivalent to finding a dicut equivalent reorientation of D for which the w_o -weight of the set of source nodes plus the w_i -weight of the set of sink nodes is as large as possible. We solve this problem for an arbitrary (non-necessarily planar) weakly connected digraph D .

Note that the problem of finding a dicut equivalent reorientation of a digraph D for which the total weight of the set of sink nodes is as large as possible is a special case of this problem and was solved by Erdős, Frank, and Kun [7]. Theorem 4.1 of [7] states that a stable set of D is sink-stable if and only if $|S \cap V(C)| \leq \eta(C)$ holds for every circuit C of D , where $\eta(C)$ denotes the minimum of the number of forward arcs of C and the number of backward arcs of C . By extending this result, we shall derive an analogous characterization of source-sink pairs in Section 3. Resonant sets will be characterized in Corollary 5.3 in terms of integer-valued circulations (and not only circuits). Perhaps a bit surprisingly, no characterization of resonant sets may exist that requires an inequality only for circuits, see Remark 5.4.

In another approach, clockwise and anti-clockwise M -alternating edge sets appear in the formulation of Abeledo and Ni [1], who gave an LP description for the Fries number of plane bipartite graphs using a TU matrix.

Shi and Zhang [22] considered (4,6)-fullerenes, and gave a formula for a variation of the Fries number problem when only the number of alternating hexagonal faces is to be maximized. Note that this problem is a special case of the Fries number within a subset \mathcal{C}' of face-circuits defined above, by choosing \mathcal{C}' to be the set of hexagonal faces.

We conclude this section by remarking that the problems above concerning Clar and Fries numbers can be considered for non-bipartite plane graphs, as well. It was shown by Bérczi-Kovács and Bernáth [4] that computing the Clar number is **NP**-hard for general plane graphs, but the problem is open if the number of odd faces is constant. This is the case, for example, for fullerene graphs (a 3-connected 3-regular planar graph with hexagonal faces and exactly six pentagonal faces). The status of the Fries number problem for general plane graphs is open. Salami and Ahmadi in [19] gave both integer

and quadratic programming formulations for the Fries number of fullerenes.

3 Characterizing source-sink pairs

In this section we describe a characterization of source-sink pairs. Recall the notion of dicut equivalence of two orientations of an undirected graph. It was observed in [7] (Lemma 3.1) that a subset $F \subseteq A$ of arcs is the union of disjoint one-way cuts if and only if there is an integer-valued potential π for which $\chi_F = \Delta_\pi$. This immediately implies the following observation.

Claim 3.1. *Two orientations D and D' of an undirected graph are dicut equivalent precisely if there is a small-dropping potential $\pi : V \rightarrow \mathbf{Z}_+$, and D' arises from D by reorienting those arcs $a \in A$ of D for which $\Delta_\pi(a) = 1$. \blacksquare*

Let $f : A \rightarrow \mathbf{R} \cup \{-\infty\}$ be a lower bound function on the arc-set of $D = (V, A)$ while $g : A \rightarrow \mathbf{R} \cup \{+\infty\}$ an upper bound function, for which $f \leq g$. By the extended (but equivalent) form of Gallai-lemma [11], there is an (f, g) -feasible tension if and only if, for every circuit C of D , the total f -value on the arcs of C in one direction is at most the total g -value on the arcs in the other direction. (In the original Gallai-lemma $f \equiv -\infty$ in which case the condition reduces to requiring that g is conservative, that is, D admits no one-way circuit with negative g -weight. This immediately implies the extended form by adding the reverse \overleftarrow{e} of each arc $e \in A$ to D and define $g(\overleftarrow{e}) := -f(e)$.)

Let F and R be two disjoint subsets of arcs of digraph $D = (V, A)$. We consider the members of F as fixed arcs while the elements of R must be reversed. The members of complementary set $N := A - (F \cup R)$ are the neutral arcs.

Claim 3.2. *For a partition $\{F, R, N\}$ of the arc-set of digraph $D = (V, A)$, the following are equivalent.*

- (A) *D admits a dicut equivalent reorientation for which every element of R is reversed while the orientation of every element of F is unchanged.*
- (B) *There is a small-dropping potential π for which*

$$\Delta_\pi(e) = \begin{cases} 1 & \text{if } e \in R \\ 0 & \text{if } e \in F. \end{cases} \quad (1)$$

- (C) *For every circuit of D , the number of R -arcs in one direction is at most the number of $(R \cup N)$ -arcs in the other direction.*

Proof. The equivalence of conditions (A) and (B) follows from Claim 3.1. Let

$$(f(e), g(e)) := \begin{cases} (0, 0) & \text{if } e \in F \\ (1, 1) & \text{if } e \in R \\ (0, 1) & \text{if } e \in N. \end{cases}$$

It follows from this definition that a small-dropping potential meets (1) precisely if Δ_π is (f, g) -feasible. For a circuit of D , the sum of the f -values of the the arcs in

one direction is the number of R -arcs in this direction, and the sum of the g -values of the arcs of C in the other direction is the number of $(R \cup N)$ -arcs in that direction. Therefore the extended Gallai-lemma implies the equivalence of Conditions **(B)** and **(C)**. ■

In digraph $D = (V, A)$, let $Y_o \subseteq V$ and $Y_i \subseteq V$ be disjoint stable sets for which we want to decide whether (Y_o, Y_i) is a so-si pair. Of course, if no arc enters Y_o and no arc leaves Y_i , then (Y_o, Y_i) is a so-si pair. We refer to an arc $e \in A$ as incorrect if it enters Y_o or leaves Y_i , while e is considered correct if it leaves Y_o or enters Y_i . The arcs neither leaving nor entering $Y_o \cup Y_i$ are neutral.

Theorem 3.3. *For disjoint node-sets $Y_o \subseteq V$, $Y_i \subseteq V$ of digraph $D = (V, A)$, the following properties are equivalent.*

- (A)** (Y_o, Y_i) is a so-si pair.
- (B)** There is a small-dropping potential π on V for which

$$\Delta_\pi(e) = \begin{cases} 1 & \text{if } e \in A \text{ incorrect} \\ 0 & \text{if } e \in A \text{ correct.} \end{cases} \quad (2)$$

- (C)** For every circuit of D , the number of incorrect arcs in one direction is at most the total number of correct arcs and neutral arcs in the other direction.

Proof. By definition, (Y_o, Y_i) is a so-si pair precisely if D admits a dicut equivalent reorientation D' in which Y_o is a source set and Y_i is a sink set, that is, the incorrect arcs in D' are reversed while the correct arcs are unchanged. Let R denote the set of incorrect arcs and F the set of correct arcs. Then the properties **(A)**, **(B)**, and **(C)** occurring in Claim 3.2 are just equivalent to those in the theorem. ■

In the rest of the paper, we are going to prove a min-max theorem for the maximum w -weight of a resonant set. Actually, we do this in a more general form when $w_o : V \rightarrow \mathbf{R}_+$ and $w_i : V \rightarrow \mathbf{R}_+$, are two given weight-functions and we are interested in finding a so-si pair (Y_o, Y_i) whose (w_o, w_i) -**weight** defined by $\tilde{w}_o(Y_o) + \tilde{w}_i(Y_i)$ is maximum. As the problem will be formulated as a network circulation problem in a larger digraph D^* , a standard algorithm for the latter one will compute the optimal solutions occurring in the min-max theorem (Theorem 4.1).

4 Min-max formula and algorithm for weighted source-sink pairs

In this section, we exhibit first a min-max formula for the maximum (w_o, w_i) -**weight** of a so-si pair of digraph $D = (V, A)$. To prepare its proof in Section 5, we describe here a feasible circulation problem on a larger digraph D^* along with its linear programming dual, a feasible tension problem. The algorithmic aspects of the approach will be discussed in Section 5.2.1.

4.1 The main theorem

Let \overleftarrow{A} denote the set of arcs obtained from A by reversing all the arcs in A . Let $\overleftrightarrow{A} := A \cup \overleftarrow{A}$ and $\overleftrightarrow{D} := (V, \overleftrightarrow{A})$. That is, \overleftrightarrow{D} is the digraph arising from D by adding the reverse of its arcs.

For a non-negative vector z_i defined on the arc-set \overleftrightarrow{A} , we say that z_i is an **in-cover** of w_i if $\varrho_{z_i}(v) \geq w_i(v)$ holds for every node $v \in V$ (where $\varrho_{z_i}(v)$ denotes the sum of z_i -values on the arcs in \overleftrightarrow{A} entering v). Analogously, a non-negative vector z_o is said to be an **out-cover** of w_o if $\delta_{z_o}(v) \geq w_o(v)$ holds for every node $v \in V$. We say that pair (z_o, z_i) is a **cover** which is **circular** if $z := z_o + z_i$ is a circulation. If a circulation z can be obtained in this way, we say that z is a **bi-cover** of (w_o, w_i) .

Let $c := \chi_A$ denote the characteristic function of A defined on the arc-set \overleftrightarrow{A} , that is,

$$c(e) := \begin{cases} 1 & \text{if } e \in A \\ 0 & \text{if } e \in \overleftarrow{A}. \end{cases} \quad (3)$$

In what follows, the cost-function c always refers to the function defined in (3). The **c-cost** of a circular pair (z_o, z_i) or a bi-cover z is $cz = cz_o + cz_i$.

The main result of the paper (beside the algorithmic aspects) is the following min-max formula.

Theorem 4.1. *Let $w_o : V \rightarrow \mathbf{R}_+$ and $w_i : V \rightarrow \mathbf{R}_+$ be weight-functions on the node-set of digraph $D = (V, A)$. Then*

$$\begin{cases} \max\{\tilde{w}_o(Y_o) + \tilde{w}_i(Y_i) : (Y_o, Y_i) \text{ a source-sink pair}\} \\ = \\ \min\{c(z_o + z_i) : (z_o, z_i) \text{ a circular cover of } (w_o, w_i)\}. \end{cases} \quad (4)$$

If (w_o, w_i) is integer-valued, the minimum c -cost circular cover may be chosen integer-valued.

4.2 A primal circulation problem and its dual tension problem

We assign a digraph $D^* = (V^*, A^*)$ to D and investigate a minimum cost feasible circulation problem on D^* along with its linear programming dual which is a maximum weight feasible tension problem. On one hand, an optimal integer-valued tension in D^* shall define a maximum (w_o, w_i) -weight so-si pair. On the other hand, an optimal feasible circulation in D^* shall define a minimum c -cost circular cover (z_o, z_i) of (w_o, w_u) .

Let V_i and V_o be disjoint copies of V and let $V^* := V_o \cup V \cup V_i$. (For an intuition, we think on these three sets to be drawn in three parallel horizontal lines so that V_o is the lower, V is the middle, and V_i is the upper set, and their elements are positioned in such a way that v_o, v, v_i are in a vertical position for every $v \in V$.)

Define a digraph $D^* = (V^*, A^*)$ as follows. For every node $v \in V$, let $v_i v$ and $v v_o$ be ‘vertical’ arcs of D^* (which are directed downward). Furthermore, for every arc $uv \in \overleftrightarrow{A}$,

let uv , uv_i , and $u_o v$ be arcs in D^* . (Therefore D^* has $3|V|$ nodes and $2|V| + 6|A|$ arcs, and the restriction of D^* to V is just \overleftrightarrow{D} . See Figure 1.)

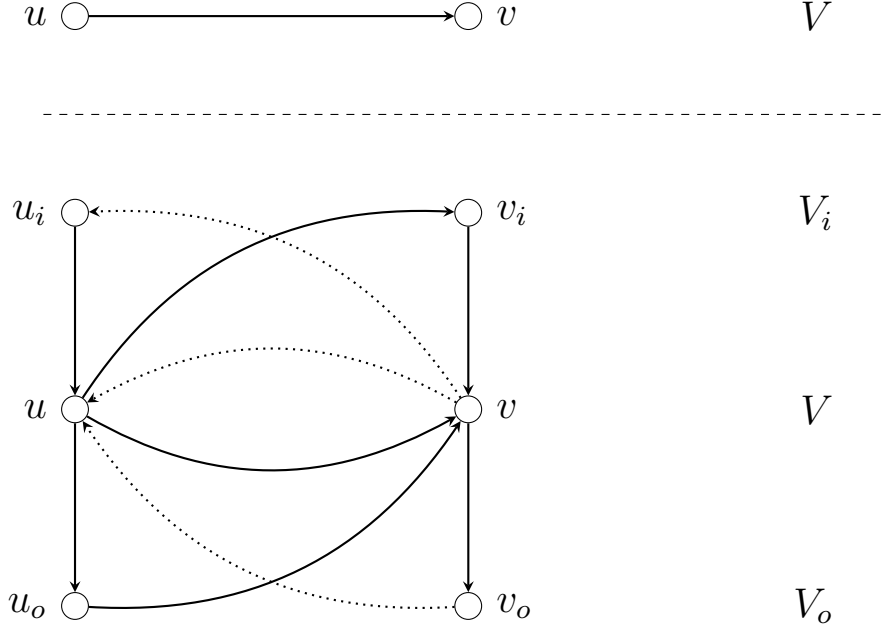


Figure 1: Auxiliary digraph D^* assigned to D

On the arc-set of D^* , we define a lower bound function $f^* : A^* \rightarrow \mathbf{R}^+$ and a cost-function $c^* : A^* \rightarrow \{0, 1\}$, as follows.

$$f^*(e) := \begin{cases} w_i(v) & \text{if } e = v_i v \ (v \in V) \\ w_o(v) & \text{if } e = v v_o \ (v \in V) \\ 0 & \text{otherwise,} \end{cases} \quad (5)$$

$$c^*(e) := \begin{cases} 1 & \text{if } e = uv \ (uv \in A) \\ 1 & \text{if } e = uv_i \ (uv \in A) \\ 1 & \text{if } e = u_o v \ (uv \in A) \\ 0 & \text{otherwise.} \end{cases} \quad (6)$$

Let Q^* denote the $(0, \pm 1)$ -valued incidence matrix of D^* , in which the columns correspond to the nodes and the rows correspond to the arcs of D^* . An entry of the row corresponding to $e = uv$ is $+1$ in the column of v and -1 in the column of u , and 0 otherwise. Consider the following (primal) polyhedron of feasible circulations.

$$R_{\text{pr}} := \{x^* : Q^* x^* = 0, x^* \geq f^*\}. \quad (7)$$

Below we refer to the members of R_{pr} as **feasible** circulations. Consider the primal linear program

$$\text{OPT}_{\text{pr}} := \min\{c^*x^* : Q^*x^* = 0, x^* \geq f^*\}, \quad (8)$$

which is a cheapest feasible circulation problem.

The dual polyhedron belonging to (8) and the dual linear program are the following

$$R_{\text{du}} := \{(\pi^*, y^*) : \pi^*Q^* + y^* = c^*, y^* \geq 0\}, \quad (9)$$

$$\text{OPT}_{\text{du}} := \max\{f^*y^* : \pi^*Q^* + y^* = c^*, y^* \geq 0\}, \quad (10)$$

where $\pi^* = (\pi_o, \pi, \pi_i)$ is a function defined on V^* , while y^* is defined on A^* .

The duality theorem of linear programming states that $\text{OPT}_{\text{pr}} = \text{OPT}_{\text{du}}$. As the describing incidence matrix Q^* is known to be totally unimodular (TU) and c^* is $(0, 1)$ -valued, the dual optimum is attained at an integral vector. If f^* is integer-valued (that is, if (w_o, w_i) is integer-valued), then the primal optimum is also attained at an integral vector.

The constraint equality $\pi^*Q^* + y^* = c^*$ in the dual program requires for every arc $a \in A^*$ that

$$\Delta_{\pi^*}(a) + y^*(a) = c^*(a).$$

Since y^* is non-negative, π^* is a feasible potential with respect to c^* , that is, $\Delta_{\pi^*}(a) \leq c^*(a)$ holds for each arc $a \in A^*$. Therefore, if we assign a vector $y^* := c^* - \Delta_{\pi^*}$ (on A^*) to a c^* -feasible potential π^* , the vector (π^*, y^*) obtained in this way is in the dual polyhedron (9). (This means that the polyhedron of c^* -feasible potentials is the projection of R_{du} .) In this case, we say that y^* **belongs to** π^* . In particular, it follows that

$$y^*(a) = -\Delta_{\pi^*}(a) \text{ holds for each vertical arc } a \in A^* \text{ of } D^*, \quad (11)$$

and hence the weight $M(\pi^*)$ of π^* in the dual linear program is

$$M(\pi^*) := f^*y^* = \sum [-\Delta_{\pi^*}(a)f^*(a) : a \in A^* \text{ a vertical arc}]. \quad (12)$$

4.3 From feasible potentials in D^* to so-si pairs in D

Consider an integer-valued c^* -feasible potential $\pi^* = (\pi_o, \pi, \pi_i)$ along with the vector y^* for which $(\pi^*, y^*) \in R_{\text{du}}$. We show how to assign a so-si pair (Y_o, Y_i) to π^* for which

$$\tilde{w}_o(Y_o) + \tilde{w}_i(Y_i) = M(\pi^*) \quad (= f^*y^*). \quad (13)$$

holds.

Claim 4.2. *The potential π (on V) occurring in $\pi^* = (\pi_o, \pi, \pi_i)$ is small-dropping on the arc-set of D , that is, $\Delta_{\pi}(e) \in \{0, 1\}$ holds for each arc $e \in A$.*

Proof. What we prove is that $0 \leq \Delta_\pi(e) \leq 1$. On one hand, clearly

$$\Delta_\pi(e) = \Delta_{\pi^*}(e) \leq c^*(e) = 1.$$

On the other hand, $\Delta_\pi(e) + \Delta_\pi(\overleftarrow{e}) = 0$ holds for the arc $\overleftarrow{e} \in \overleftarrow{A}$ arising by reversing e , and hence

$$-\Delta_\pi(e) = \Delta_\pi(\overleftarrow{e}) = \Delta_{\pi^*}(\overleftarrow{e}) \leq c^*(\overleftarrow{e}) = 0,$$

that is, $\Delta_\pi(e) \geq 0$. ■

Claim 4.3. *For every node $v \in V$, the sum $y^*(v_i v) + y^*(v v_o)$ is either 0 or 1. In particular, the non-negativity of y^* implies that $y^*(v_i v) \in \{0, 1\}$ and $y^*(v v_o) \in \{0, 1\}$.*

Proof. Assume first that there is an arc $vu \in A$ leaving v . By (11) we have

$$\begin{aligned} y^*(v_i v) + y^*(v v_o) &= [\pi^*(v_i) - \pi^*(v)] + [\pi^*(v) - \pi^*(v_o)] = \pi^*(v_i) - \pi^*(v_o) = \\ &[\pi^*(v_i) - \pi^*(u)] + [\pi^*(u) - \pi^*(v_o)] \leq c^*(uv_i) + c^*(v_o u) = 0 + 1 = 1. \end{aligned}$$

If no arc of D leaves v , then there is an arc $uv \in A$ entering v , for which the proof runs analogously:

$$\begin{aligned} y^*(v_i v) + y^*(v v_o) &= [\pi^*(v_i) - \pi^*(v)] + [\pi^*(v) - \pi^*(v_o)] = \pi^*(v_i) - \pi^*(v_o) = \\ &[\pi^*(v_i) - \pi^*(u)] + [\pi^*(u) - \pi^*(v_o)] \leq c^*(uv_i) + c^*(v_o u) = 1 + 0 = 1. \end{aligned}$$
■

Define subsets Y_o and Y_i of V , as follows.

$$\begin{cases} Y_o := \{v \in V : y^*(v v_o) = 1\}, \\ Y_i := \{v \in V : y^*(v_i v) = 1\}. \end{cases} \quad (14)$$

We say that the pair (Y_o, Y_i) defined in this way **belongs to** the c^* -feasible potential π^* .

Lemma 4.4. *The pair (Y_o, Y_i) of subsets belonging to an integer-valued c^* -feasible potential π^* forms a source-sink pair for which (13) holds.*

Proof. Observe first that $Y_o \cap Y_i = \emptyset$ since if there were a node $v \in Y_o \cap Y_i$, then $y^*(v_i v) = 1 = y^*(v v_o)$, contradicting Claim 4.3. Furthermore, we have

$$\tilde{w}_o(Y_o) = \sum [w_o(v) y^*(v v_o) : v \in V] = \sum [f^*(v v_o) y^*(v v_o) : v \in V],$$

and

$$\tilde{w}_i(Y_i) = \sum [w_i(v) y^*(v_i v) : v \in V] = \sum [f^*(v_i v) y^*(v_i v) : v \in V],$$

from which (13) follows immediately.

Next, we show that Y_o is a source-stable set in D . By Claim 4.2, π is small-dropping on the arc-set of D . Let D' denote a dicut equivalent digraph of D which arises from D by reversing those arcs $e \in A$ for which $(\Delta_{\pi^*}(e) =) \Delta_\pi(e) = 1$.

Claim 4.5. *The elements of Y_o are source nodes in D' .*

Proof. Consider an arbitrary node $v \in Y_o$. By Claim 3.1, what we have to show for every arc $vt \in A$ leaving v is that $\pi^*(t) - \pi^*(v) = 0$, and for every arc $sv \in A$ entering v that $\pi^*(v) - \pi^*(s) = 1$.

By (11) it follows for $v_o \in V_o$ that $\pi^*(v_o) - \pi^*(v) = -y^*(v_o v) = -1$, and hence we have for each arc $vt \in A$ the following.

$$\begin{aligned} \pi^*(t) - \pi^*(v) &= [\pi^*(t) - \pi^*(v_o)] + [\pi^*(v_o) - \pi^*(v)] = \\ &[\pi^*(t) - \pi^*(v_o)] - 1 \leq c^*(v_o t) - 1 = 0, \end{aligned}$$

that is, $\pi^*(t) - \pi^*(v) \leq 0$. On the other hand, as $tv \in \overleftarrow{A}$, we have $\pi^*(v) - \pi^*(t) \leq c^*(tv) = 0$, from which $0 \leq \pi^*(t) - \pi^*(v) \leq 0$, that is, $\pi^*(t) - \pi^*(v) = 0$ follows.

Similarly, for an arc $sv \in A$ we get:

$$\begin{aligned} \pi^*(s) - \pi^*(v) &= [\pi^*(s) - \pi^*(v_o)] + [\pi^*(v_o) - \pi^*(v)] = \\ &[\pi^*(s) - \pi^*(v_o)] - 1 \leq c^*(v_o s) - 1 = -1, \end{aligned}$$

from which $\pi^*(v) - \pi^*(s) \geq 1$. On the other hand $\pi^*(v) - \pi^*(s) \leq c^*(cs) = 1$, and hence $1 \leq \pi^*(v) - \pi^*(s) \leq 1$, that is, $\pi^*(s) - \pi^*(v) = 1$ follows, and the proof of the claim is complete. \blacksquare

An analogous argument shows that Y_i is a sink-stable set of D , completing the proof of the lemma. $\blacksquare \blacksquare$

It follows from Lemma 4.4 that:

$$\begin{aligned} \max\{\tilde{w}_o(Y_o) + \tilde{w}_i(Y_i) : (Y_o, Y_i) \text{ a so-si pair}\} &\geq \\ \max\{M(\pi^*) : \pi^* \text{ a } c^*\text{-feasible potential}\} &= \text{OPT}_{\text{du}}. \end{aligned} \quad (15)$$

4.4 From feasible circulations in D^* to circular covers of (w_o, w_i)

Next, we assign a circular pair (z_o, z_i) covering (w_o, w_i) to an optimal solution z^* of the primal problem (8) in such a way that $c(z_o + z_i) = c^* z^*$ (where $c = \chi_A$ is defined in (3)). Here both z_o and z_i are non-negative vectors on the arc-set \overleftrightarrow{A} , and their sum $z_o + z_i$ is a circulation in \overleftrightarrow{D} .

We may assume that $z^*(uv) = 0$ for every arc $uv \in A$ since if $\alpha = z^*(uv)$ were positive for an arc uv , then, by decreasing $z^*(uv)$ to 0 and increasing both $z^*(uv_i)$ and $z^*(v_i v)$ by α , we obtain a new circulation which is also f^* -feasible and its c^* -cost is unchanged.

Define functions $z_i : \overleftrightarrow{A} \rightarrow \mathbf{R}_+$ and $z_o : \overleftrightarrow{A} \rightarrow \mathbf{R}_+$ as follows.

$$z_o(uv) := z^*(u_o v) \text{ and } z_i(uv) := z^*(u v_i). \quad (16)$$

Now the sum $z := z_o + z_i$ is a circulation in \overleftrightarrow{D} for which $cz = c^*z^*$. Moreover, we have for every node $u \in V$ the following.

$$\begin{cases} \delta_{z_o}(u) = \delta_{z^*}(u_o) = z^*(uu_o) \geq f^*(uu_o) = w_o(u) \\ \varrho_{z_i}(u) = \varrho_{z^*}(u_i) = z^*(u_iu) \geq f^*(u_iu) = w_i(u), \end{cases} \quad (17)$$

from which it follows that (z_o, z_i) is indeed a circular cover of (w_o, w_i) .

This implies that:

$$\min\{cx : x \geq 0 \text{ a bi-covering integer-valued circulation in } \overleftrightarrow{D}\} \leq \begin{matrix} cz = c^*z^* = \text{OPT}_{\text{pr.}} \end{matrix} \quad (18)$$

5 The proof of Theorem 4.1

5.1 Proving $\max \leq \min$

Claim 5.1. *Let $D' = (V, A')$ be a dicut equivalent reorientation of D and let $c' := \chi_{A'}$ denote the characteristic function of A' on \overleftrightarrow{A} . Then $cz = c'z$ holds for every circulation $z \geq 0$ (defined on digraph \overleftrightarrow{D}).*

Proof. Recall the notation \tilde{c} . Since a non-negative circulation can be expressed as the non-negative linear combination of one-way circuits it suffices to show that $\tilde{c}(K) = \tilde{c}'(K)$ holds for every one-way circuit K of \overleftrightarrow{D} . But this will follow once we prove it for the case when D' arises from D by reversing a single dicut.

Let this dicut be the set of arcs of D entering a subset $Z \subset V$ of nodes with no leaving arcs of D . In this case c' arises from c in such a way that the c -cost of A -arcs entering Z is changed from 1 to 0 while c -cost of \overleftarrow{A} -arcs leaving Z is changed from 0 to 1. But this implies, as $\varrho_K(Z) = \delta_K(Z)$, that the cost of one-way circuit K does not change, that is, $\tilde{c}(K) = \tilde{c}'(K)$. ■

Remark 5.1. A more concise proof of Claim 5.1, where the non-negativity of z is not used, is as follows. By Claim 3.1, there is a potential $\pi \in V \rightarrow \mathbf{Z}$ (which is small-dropping on A) for which A' arises from A by reorienting those arcs $e \in A$ for which $\Delta_\pi(e) = 1$. Now $c' = c - \Delta_\pi$ and $z\Delta_\pi = 0$ since the scalar product of a circulation and a tension is always zero. Therefore $c'z = cz$ follows indeed. •

The requested inequality $\max \leq \min$ immediately follows from the following claim.

Claim 5.2. *Let (Y_o, Y_i) be a so-si pair in D , and let (z_o, z_i) be a circular cover of (w_o, w_i) . Then $cz \geq \tilde{w}_o(Y_o) + \tilde{w}_i(Y_i)$ holds for the circulation $z = z_o + z_i$.*

Proof. Consider the dicut equivalent reorientation D' of D for which the elements of Y_o are source nodes and the elements of Y_i are sink nodes. For a vector $x : \overleftrightarrow{A} \rightarrow \mathbf{Z}$, let $\delta'_x(Z) := \sum [x(e) : e \in A', e \text{ leaves } Z]$ and $\varrho'_x(Z) := \sum [x(e) : e \in A', e \text{ enters } Z]$. By Claim 5.1, $cz = c'z (= c'z_o + c'z_i)$. But we have $c'z_o \geq \delta'_{z_o}(Y_o) \geq \tilde{w}_o(Y_o)$ and $c'z_i \geq \varrho'_{z_i}(Y_i) \geq \tilde{w}_i(Y_i)$ from which $cz \geq \tilde{w}_o(Y_o) + \tilde{w}_i(Y_i)$ follows. ■

5.2 Proving $\max \geq \min$

By combining (18) with inequality (15), we get the following.

$$\begin{cases} \max\{\tilde{w}_o(Y_o) + \tilde{w}_i(Y_i) : (Y_o, Y_i) \text{ so-si pair} \} \geq \\ \text{OPT}_{\text{du}} = \text{OPT}_{\text{pr}} \geq \\ \min\{c(z_o + z_i) : (z_o, z_i) \text{ a non-negative circular cover of } (w_o, w_i)\}, \end{cases} \quad (19)$$

and this is exactly the non-trivial inequality $\max \geq \min$ of Theorem 4.1.

Finally, observe that if (w_o, w_i) is integer-valued, then f^* in the primal linear program (8) is also integer-valued, and hence the optimal circulation can be chosen integer-valued. In this case, the pair (z_o, z_i) assigned to z^* in (16) is an integer-valued circular cover of (w_o, w_i) , and hence the proof of Theorem 4.1 is complete. ■ ■

Corollary 5.2. *Let z^* be an optimal solution to the primal linear program (8), and let (z_o, z_i) be the circular cover of (w_o, w_i) assigned to z^* in (16), which is integer-valued when (w_o, w_i) is integer-valued. Let (π^*, y^*) be an optimal integral solution to the dual linear program (10), and let (Y_o, Y_i) be the so-si pair assigned to π^* in (14). Then $c(z_o + z_i) = \tilde{w}_o(Y_o) + \tilde{w}_i(Y_i)$. Moreover, (z_o, z_i) is a minimum c -cost circular cover of (w_o, w_i) , and (Y_o, Y_i) is a maximum (w_o, w_i) -weight so-si pair. ■*

5.2.1 Algorithmic aspects

In the proof of Theorem 4.1, we introduced a network circulation problem on a digraph $D^* = (V^*, A^*)$ along with its dual tension problem. These problems are special in the sense that the (primal) cost-function c^* on A^* is $(0, 1)$ -valued. It is a standard reduction to reformulate such a circulation problem as a minimum cost network flow problem in which the cost-function is $(0, 1)$ -valued. The min-cost flow algorithm of Ford and Fulkerson [9] in this case is strongly polynomial, provided that a strongly polynomial subroutine is used for the intermediate maximum flow computations (for example, the classic shortest augmenting path type algorithms of Edmonds and Karp, and of Dinitz, or the push-relabel algorithm of Goldberg and Tarjan).

Therefore, an optimal solution to the primal and to the dual linear programs (8) and (10) can be computed in strongly polynomial time, where the dual optimal vector is integer-valued and the primal optimal vector is integer-valued when (w_o, w_i) is integer-valued. By Corollary 5.2, a maximum (w_o, w_i) -weight so-si pair occurring in Theorem 4.1 as well as a minimum c -cost circular cover of (w_o, w_i) can be computed in strongly polynomial time.

5.3 Consequences

Theorem 5.1 in [7] provided a min-max formula for the maximum w -weight of a sink-stable set for an integer-valued weight-function w . Here we show how this formula follows immediately from Theorem 4.1.

We say that a set of one-way circuits of digraph $D = (V, A)$ covers w if every node $u \in V$ belongs to at least $w(u)$ circuits. The **A-value** of a one-way circuit K of digraph $\overset{\leftrightarrow}{D}$ is $|K \cap A|$. In particular, $\{e, \overleftarrow{e}\}$ is a two-element one-way circuit of $\overset{\leftrightarrow}{D}$ for every arc $e \in A$, whose A-value is 1. With this terminology, Theorem 5.1 in [7] is equivalent to the following.

Theorem 5.3. *The maximum w -weight of a sink-stable set of a digraph $D = (V, A)$ is equal to the minimum sum of A-values of a family of one-way circuits of digraph $\overset{\leftrightarrow}{D}$ that cover w .*

Proof. Let $w_o := 0$ and $w_i := w$. If (Y_o, Y_i) is a so-si pair for which $\tilde{w}_o(Y_o) + \tilde{w}_i(Y_i) = \tilde{w}(Y_i)$ is maximum, then Y_i is a maximum w -weight sink-stable set since any sink-stable set Y defines a so-si pair (\emptyset, Y) for which $\tilde{w}_i(Y) = \tilde{w}(Y)$. Let (z_o, z_i) be an integer-valued circular cover of $(0, w)$. Then $z = z_o + z_i$ is a circulation for which $(0, z)$ is a cover of $(0, w)$. Conversely, if $z \geq 0$ is a circulation covering w in the sense that $\rho_z(u) \geq w(u)$ for every node $u \in V$, then $(0, z)$ is a circular covering of $(0, w)$.

By Theorem 4.1, the maximum w -weight of a sink-stable set is equal to the minimum of cz over non-negative (integer-valued) circulations z covering w . But z can be obtained as non-negative integral combination of one-way circuits of $\overset{\leftrightarrow}{D}$, and the property that z covers w means that every node u belongs to at least $w(u)$ one-way circuits. ■

Next, we show a min-max formula concerning maximum weight resonant sets. We say that the pair (z_i, z_o) **covers** a vector $w \in \mathbf{R}_+^V$ if $\min\{\delta_{z_i}(v), \rho_{z_o}(v)\} \geq w(v)$ holds for every node $v \in V$. Recall the definition of the cost-function c on arc-set $\overset{\leftrightarrow}{A}$ given in (3). In the special case $w := w_o = w_i$, Theorem 4.1 is as follows.

Theorem 5.4. *Let $w : V \rightarrow \mathbf{R}_+$ be a non-negative weight-function on the node-set of digraph $D = (V, A)$. Then*

$$\left\{ \begin{array}{l} \max\{\tilde{w}(Y) : Y \subseteq V \text{ resonant set}\} \\ = \\ \min\{c(z_o + z_i) : (z_o, z_i) \text{ circular cover of } (w, w)\}. \end{array} \right. \quad (20)$$

When (w_o, w_i) is integer-valued, a circular cover of minimum c -cost can be chosen integer-valued. ■

We say for a non-negative integer vector z_i on arc-set $\overset{\leftrightarrow}{A}$ that it is an **in-cover** of a subset $U \subseteq V$ of nodes if $\rho_{z_i}(v) \geq 1$ holds for each node $v \in U$. A non-negative vector z_o is an **out-cover** of U if $\delta_{z_o}(v) \geq 1$ holds for every node $v \in U$.

Let $U_o \subseteq V$ and $U_i \subseteq V$ be two disjoint subsets. The pair (z_o, z_i) of vectors is a **cover** of the pair (U_o, U_i) of sets if z_o is an out-cover of U_o and z_i is an in-cover of U_i . If a circulation z arises in this way, we say that z is a bi-cover of (U_o, U_i) .

In the special case when $U := U_o = U_i$, a circulation z is a **bi-cover** of U if it is a bi-cover of (U_o, U_i) , that is, if z can be obtained as the sum of an in-cover of U and an out-cover of U . By applying Theorem 4.1 to weight-functions $w_o := \chi_{U_o}$ and $w_i := \chi_{U_i}$, we obtain the following.

Theorem 5.5. *In a digraph $D = (V, A)$, let $U_o \subseteq V$ and $U_i \subseteq V$ be two disjoint subsets of nodes. Then the value*

$$\max\{|Y_o| + |Y_i| : (Y_o, Y_i) \text{ a so-si pair, } Y_o \subseteq U_o, Y_i \subseteq U_i\}$$

is equal to the minimum of $c(z_o + z_i)$ over the integer-valued circular pairs (z_o, z_i) covering (U_o, U_i) . In the special case when $U := U_i = V_i$, this reduces to the formula stating that the maximum cardinality of a resonant subset of U is equal to the minimum c -cost of a non-negative integer-valued circulation that is a bi-cover of U . ■

Theorem 5.5 implies the following.

Corollary 5.3. *A subset $Y \subseteq V$ of nodes is resonant if and only if $cz \geq |Y|$ holds for every non-negative integer-valued circulation (in \vec{D}) which is a bi-cover of Y . ■*

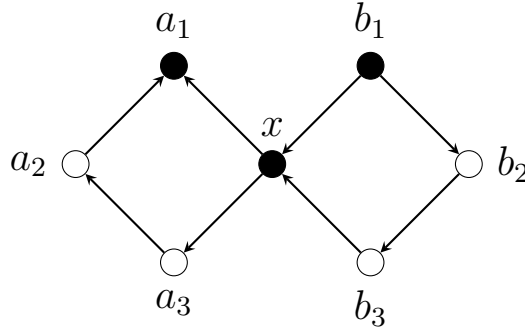


Figure 2: An example

Remark 5.4. Theorem 3.3 implies that a pair (Y_o, Y_i) of disjoint stable sets is a so-si pair if it is a so-si pair when restricted to any circuit of D . Theorem 4.1 in [7] states that a stable set $Y \subseteq V$ is sink-stable if and only if, for every circuit C of D , there are at least $|V(C) \cap Y|$ arcs in both directions. In the present terminology this is equivalent to requiring that $\tilde{c}(K) \geq |V(K) \cap Y|$ holds for every one-way circuit K of \vec{D} . This implies that Y is a sink-stable set if and only if it is sink stable when restricted to any circuit of D .

This fact gives rise to the question whether there is an analogous characterization for a set being resonant, that is, when we require a certain inequality only for circuits but not for every integer-valued circulation (as formulated in Corollary 5.3). Such a simplified characterization of resonant sets would imply that Y is resonant if and only if it is resonant when restricted to any circuit of D . However, this fails to hold, as demonstrated by a digraph $D = (V, A)$ where

$$V := \{a_1, a_2, a_3, x, b_1, b_2, b_3\}, \quad A := \{xa_1, xa_3, a_3a_2, a_2a_1, b_1x, b_3x, b_2b_3, b_1b_2\}.$$

Then D has exactly two circuits, and $Y := \{x, a_1, b_1\}$ is a set which is resonant when restricted to any of these two circuits, but this Y is not a resonant set. (See Figure 2.)

Therefore we cannot expect a characterization of resonant sets that requires an inequality only for single circuits. •

Finally we remark that Theorem 4.1 can be applied to manage further special cases. For example, the one when we are interested in finding a maximum weight resonant set including a specified subset. Or more generally, one may be interested in finding a (maximum weight) so-si pair (Y_i, Y_o) for which $U'_o \subseteq Y_o \subseteq U_o$ and $U'_i \subseteq Y_i \subseteq U_i$. By defining w_o (w_i) to be an appropriately large number on the elements of U'_o (U'_i), and zero on the elements of $V - U_o$ ($V - U_i$), Theorem 4.1 and the algorithmic approach described above can be applied.

Acknowledgement

This research was supported by the ÚNKP-22-5 New National Excellence Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund. This research has been implemented with the support provided by the Ministry of Innovation and Technology of Hungary from the National Research, Development and Innovation Fund, financed under the ELTE TKP 2021-NKTA-62 funding scheme, and supported by the János Bolyai Research Scholarship of the Hungarian Academy of Science. This research is in part supported by the project no. FK 132524, provided by the National Research, Development and Innovation Fund of Hungary.

References

- [1] H. Abeledo, *personal communication*, 2010
- [2] H. Abeledo and G.W. Atkinson, *Unimodularity of the Clar number problem*, Linear Algebra and its Applications, 420(2-3) (2007) 441–448.
- [3] H. Abeledo and G.W. Atkinson, *A min-max theorem for plane bipartite graphs*, Discrete Applied Mathematics, 158(5) (2010) 375–378.
- [4] E.R. Bérczi-Kovács and A. Bernáth, *The complexity of the Clar number problem and an exact algorithm*, J. of Mathematical Chemistry, 56 (2018) 597–605.
- [5] S. Bessy and S. Thomassé, *Spanning a strong digraph by α circuits: A proof of Gallai's conjecture*, Combinatorica, 27(6) (2007) 659–667.
- [6] E. Clar, *The aromatic sextet*, John Wiley and Sons, London, 1972.
- [7] D. Erdős, A. Frank, K. Kun, *Sink-stable sets of digraphs*, SIAM J. on Discrete Mathematics, 28(4) (2014) 1651–1674.

-
- [8] I. Fáry, *On the straight line representation of planar graphs*, Acta Scientiarum Mathematicarum, 11(4) (1948) 229–233.
- [9] L.R. Ford and D.R. Fulkerson, *Flows in Networks*, Princeton Univ. Press, Princeton NJ., 1962.
- [10] K. Fries, *Über bicyclische Verbindungen und ihre Vergleich mit dem Naphtalin*, (3. Mitteilung), Justus Liebigs Annalen der Chemistry, 454(1) (1927) 121–324.
- [11] T. Gallai, *Maximum-Minimum Sätze über Graphen*, Acta Mathematica Academiae Scientiarum Hungariae, 9(3-4) (1958) 395–434.
- [12] J.E. Graver, E.J. Hartung, A.Y. Soud, *Clar and Fries numbers for benzenoids*, J. of Mathematical Chemistry, 51(8) (2013) 1981–1989.
- [13] P. Hansen and M. Zheng, *Upper bounds for the Clar number of a benzenoid hydrocarbon*, J. of the Chemical Society, Faraday Transactions, 88(12) (1992) 1621–1625.
- [14] P. Hansen and M. Zheng, *The Clar number of a benzenoid hydrocarbon and linear programming*, J. of Mathematical Chemistry, 15(1) (1994) 93–107.
- [15] P. Hansen and M. Zheng, *Numerical bounds for the perfect matching vectors of a polyhex*, J. of Chemical Information and Computer Sciences, 34(2) (1994) 305–308.
- [16] E.J. Hartung, *Clar chains and a counter-example*, J. of Mathematical Chemistry, 52(3) (2014) 990–1006.
- [17] A. J. Hoffman and J.B. Kruskal, Jr, *Integral boundary points of convex polyhedra*, Linear Inequalities and Related Systems, Annals of Mathematics Study, 38 (1956) 223–346, Princeton University Press.
- [18] H. Lei, Y-N. Yeh, H. Zhang, *Anti-forcing numbers of perfect matchings in graphs*, Discrete Applied Mathematics, 202 (2016) 95–105.
- [19] M. Salami and M. B. Ahmadi, *A mathematical programming model for computing the Fries number of a fullerene*, Applied Mathematical Modelling, 39(18) (2015) 5473–5479.
- [20] A. Sebő, *Minmax relations for cyclically ordered digraphs*, J. Combinatorial Theory, Ser. B, 97(4) (2007) 518–552.
- [21] L. Shi, H. Wang, H. Zhang, *On the maximum forcing and anti-forcing numbers of (4,6)-fullerenes*, Discrete Applied Mathematics, 233 (2017) 187–194.
- [22] L. Shi and H. Zhang, *The maximum number of alternating hexagonal faces in (4, 6)-fullerenes*, Advances in Mathematics (China), 51(3) (2022) 407–414.

-
- [23] A. Schrijver, *Theory of Linear and Integer Programming*, Wiley, Chichester, 1986.
- [24] É. Tardos, *A strongly polynomial algorithm to solve combinatorial linear programs*, *Operations Research*, 32(2) (1986) 250–256.
- [25] W.T. Tutte, *How to draw a graph*, *Proceedings of the London Mathematical Society*, 13(3) (1963) 743–768.
- [26] Y. Wang, *Extension and Quantification of the Fries Rule and Its Connection to Aromaticity: Large-Scale Validation by Wave-Function-Based Resonance Analysis*, *J. of Chemical Information and Modeling*, 62(21) (2022) 5136–5148.
- [27] L. Xu, B. Hong, F. Zhang, *Maximum forcing number of hexagonal systems*, *MATCH Communications in Mathematical and in Computer Chemistry*, 70(2) (2013) 493–500.
- [28] S. Zhai, D. Alrowaili, D. Ye, *Clar structures vs Fries structure in hexagonal systems*, *Applied Mathematics and Computation*, 329 (2018) 384–394.
- [29] S. Zhou, H. Zhang, I. Gutman, *Relations between Clar structures, Clar covers, and the sextet-rotation tree of a hexagonal system*, *Discrete Applied Mathematics*, 156(10) (2008) 1809–1821.