On Topological Indices, Graph Compression, and Threshold Graphs

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Abstract

A graph transformation known in the graph theory literature as the compression of a graph G from u to v has been shown to uniformly decrease or increase a wide variety of graph parameters. Repeated applications of compression are also known to eventually produce threshold graphs. This implies that when compression does uniformly affect a graph parameter, the parameter has at least one threshold graph as an extremal graph. In this paper we demonstrate that a number of topological indices from the mathematical chemistry literature are uniformly affected by the compression operation. As a consequence, many extremal results on topological indices can be reproduced and generalized in a unified way, and new extremal results obtained as well.

1 Introduction

Let G be a graph, let u, v be two vertices of G, and let $N_G(u)$ and $N_G(v)$ respectively denote the open neighborhoods in G of u and v. The *compression of G from u to v* is a graph transformation that produces the new graph $G_{u\to v}$ by, for each $x \in N_G(u) - N_G(v) - \{v\}$, removing all edges from G of the form ux and replacing them with corresponding edges of the form vx. An illustration of compression appears in Figure 1.

The compression operation appears to have been first employed by Kelmans in [39] who used it to investigate all-terminal reliability, the probability that a network (i.e., graph) remains connected when the network's links fail (i.e., edges are removed) independently and with fixed probability. The operation has been rediscovered many times since, and so it has also acquired a number of distinct names; we have also seen this operation variously called a path property transformation [8], a shift transformation [9, 10, 12], a swing surgery [48], and a Kelmans transformation [16, 17], to mention just a few. Our choice of the "compression" terminology here follows recent use [18, 19, 38] and is motivated by the following important fact, first observed by Satyanarayana, Schoppmann, and Suffel [48], but also rediscovered by many other authors as well [9, 16, 18, 19].

Theorem 1.1 ([48])**.** *Any connected graph G can be transformed into a connected threshold graph by repeated applications of graph compression.*

We will say much more about threshold graphs and their properties later, for now we simply note that threshold graphs are a well-known and widely-studied class of graphs with many nice properties. One of these properties is that all connected threshold graphs have diameter 2 or less, which motivates the "compression" terminology.

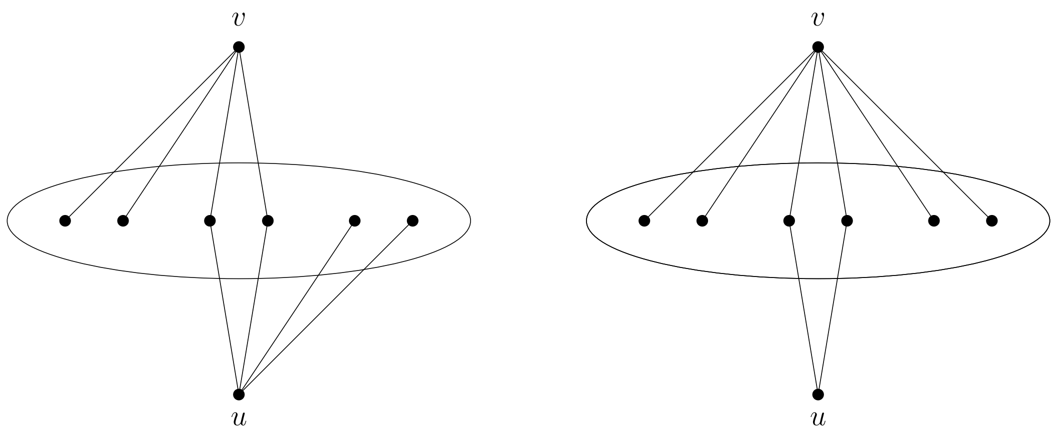

Figure 1: An illustration of graph compression. The compression of G from u to v transforms the graph G on the left to the graph $G_{u\to v}$ on the right. If edge uv had been present in G, it would also be present in $G_{u\to v}$.

One reason compression has been rediscovered so many times is that a remarkable number of graph parameters have turned out to be affected, in a uniform way, by compression. To give the reader some idea of their scope, in what follows we will indicate by "compression decreases parameter p" the relationship $p(G) \geq p(G_{u\to v})$, and in a similar manner use "increases." In [39] Kelmans showed that compression decreases all-terminal reliability, but compression has also been shown to decrease other measures of network strength such as the number of spanning trees [8], graph toughness, edge toughness, and binding number [37], and to increase graph scattering number and rupture degree [36, 37]. Compression has also been shown to decrease the number of k-factors for any k [31], decrease the number of ℓ-matchings for any ℓ [40], increase the largest root of the matching polynomial [16], increase both the number of independent sets of order r and the number of cliques of order r for any r [16], decrease the smallest real root of the independence polynomial [16], decrease the magnitude of the i^{th} coefficient of the Laplacian polynomial for any i [16], decrease the magnitude of the i^{th} coefficient of the chromatic polynomial for any i [16, 47], increase the spectral radius [17], and increase the number of homomorphisms into certain target graphs [18, 19]. Most recently a wide variety of parameters associated with the Tutte polynomial have been shown to decrease, or in rare cases increase, after graph compression [38].

We recently became aware that a number of results in the mathematical chemistry literature also appear to use the compression operation, although as far as we can tell without realizing it, and almost always only in a partial or limited form. To give one example, in the recent paper [26] a number of graph transformations from a tree T to a new tree T' are examined, two of which are pictured in Figure 2. Both of the transformations pictured—although considered separately in [26]—are in fact simply examples of some graph compressions limited to trees. In the upper transformation in Figure 2 the tree T' is the compression of the tree T from vertex v to vertex u, and in the second transformation T' is the result of two compressions of T, first from u to v and then from u_1 to v.

Similarly, threshold graphs seem to have arisen quite often in the mathematical chemistry literature, particularly as extremal graphs for particular topological indices, although when they

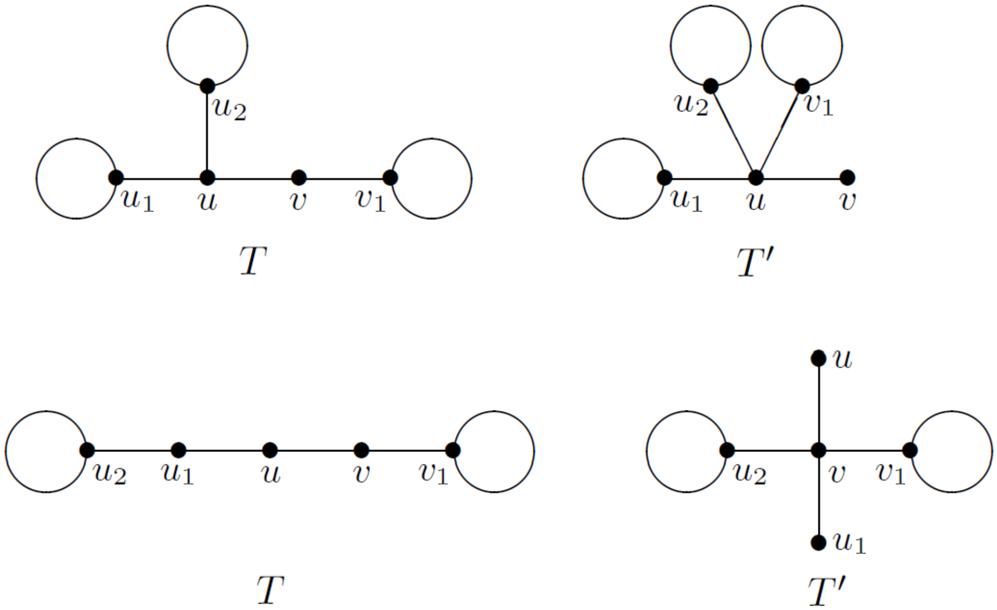

Figure 2: Two graph transformations, each of which is an example of graph compression.

have arisen they have not been recognized as such. (We use the term *topological index* here as it has been used in the mathematical chemistry literature, to mean a graph parameter that has been shown to have some relationship with a chemical parameter when graphs are used to model molecular chemicals.) To give one example, in [35] it was determined that extremal graphs of a particular index must come from "the family $\mathcal{F}$" of graphs; it turns out that the class $\mathcal{F}$ is just the class of threshold graphs, but defined in [35] in a non-standard (and somewhat complicated) way. Later we will see many instances of threshold graphs as extremal graphs for topological indices as well as much simpler and more useful definitions for them.

The purpose of this paper is twofold. First, we will demonstrate that a variety of topological indices are uniformly affected by compression. This work on compression and topological indices appears in Sections 2 and 3. Secondly, in conjunction with Theorem 1.1, we will discuss extremal results on the topological indices considered. Since graph compressions eventually produce threshold graphs, and threshold graphs possess many nice properties, we will show how these properties can be used to deduce properties of extremal graphs for a variety of topological indices. This work on extremal graphs for topological indices appears in Sections 4 and 5. Although we obtain a number of new extremal results in these sections, we also emphasize how naturally and easily the compression and threshold graph framework generates and generalizes both old and new results. This ease and directness often contrasts quite strongly with how previous results were obtained. Our hope is that by demonstrating the power, simplicity, and applicability of the compression and threshold graph machinery in the topological index arena, these techniques may become more widely known and useful.

Before we begin we first make a few brief notes about what types of compressions we will be using. First, in this paper we consider only connected graphs. Compressions when u and v are distance 3 or more apart in a graph renders u an isolate, and so throughout the paper we assume the following:

- In this paper all compressions will be assumed to involve only vertices $u, v \in V(G)$ such that $dist_G(u, v) \leq 2$, where $dist_G(u, v)$ denotes the distance between vertices u and v in the graph G.

The above assumption is also in agreement with the vast majority of the graph compression literature, which also typically deals only with connected graphs. Lastly, we note that $G_{u\to v}$ and $G_{v\to u}$ are isomorphic, with the isomorphism given by switching the labels of u and v. Hence:

- When compressing G from u to v we assume that $d_G(v) \geq d_G(u)$, where $d_G(a)$ indicates the degree of vertex a in graph G.

Notationally, when the choice of graph G is clear we may also omit the subscript and write $dist(u, v)$ for distance or $d(u), d(v)$ for degrees. For any terms or notations not defined in the body of the paper we refer the reader to a standard reference like [11].

2 Vertex-Based Topological Indices and Compression

A large number of topological indices are of one of the two forms

$$\sum_{a\in V(G)} f(d(a)) \qquad \text{or} \qquad \sum_{ab\in E(G)} f(d(a), d(b))$$

where as mentioned earlier $d(a)$ indicates the degree of vertex a, and f is some function that serves to define the topological index. We will call these forms vertex-based and edge-based to distinguish them, and discuss the two forms in turn. In this section we will discuss vertex-based topological indices.

From the viewpoint of compression, for any choice of vertices $u, v \in V(G)$ the compression of G from u to v changes only the degrees of u and v themselves, leaving the degrees of all non-u, v vertices the same. Since compression moves edges from u to v, the new degrees of u and v in $G_{u\to v}$ are respectively $d(u) - k$ and $d(v) + k$ for some non-negative k. Hence, setting $H = G_{u\to v}$ to simplify notation, for any vertex-based parameter p we have

$$\begin{aligned} p(H) - p(G) &= \sum_{a\in V(H)} f(d_H(a)) - \sum_{a\in V(G)} f(d_G(a)) \\ &= f(d_H(u)) + f(d_H(v)) - f(d_G(u)) - f(d_G(v)) \\ &= f(d_G(u) - k) + f(d_G(v) + k) - f(d_G(u)) - f(d_G(v)). \end{aligned} \tag{1}$$

Therefore determining whether compression increases or decreases a vertex-based index p is equivalent to determining whether the four terms of (1) sum to a positive or negative number. For many parameters, determining the sign of the right-hand side of (1) is fairly simple. In particular, this is true for functions f that are convex or concave. To that end, we note the following lemma on convex and concave functions (see e.g. Proposition 1.25 in [49]).

Lemma 2.1. *If f is a convex function on an interval $I \subset \mathbb{R}$, with x, y, z, w in I such that $x < y \leq z < w$, then*

$$\frac{f(y) - f(x)}{y - x} \leq \frac{f(w) - f(z)}{w - z}.$$

If f is a concave function on I then the inequality is reversed.

Name	Notation	Function
First Zagreb	$R^0_2(G)$	x^2
Forgotten	$R^0_3(G)$	x^3
Zeroth-order connectivity	$R^0_{-1/2}(G)$	$1/\sqrt{x}$
Inverse degree	$R^0_{-1}(G)$	$1/x$
Modified First Zagreb	$R^0_{-2}(G)$	$1/x^2$

Table 1: Various topological indices generalized by the zeroth-order Randić index.

(We note in passing that if $f(x)$ in the above theorem is strictly convex then the inequality is strict, and similarly when f is strictly concave the reversed inequality is strict. These stronger conditions typically lead to strict inequalities in our later compression results, but for simplicity in this paper we just treat the convex and concave cases and leave any strict versions implicit.)

Now the following result on compression and vertex-based topological indices is an immediate consequence.

Theorem 2.2. *Let p be a graph parameter defined by*

$$p(G) = \sum_{a \in V(G)} f(d(a))$$

for some function $f(x) \geq 0$ for all $x > 0$. If f is convex, then $p(G) \leq p(G_{u \to v})$ and if f is concave then $p(G) \geq p(G_{u \to v})$.

Proof. When f is convex, and taking $x = d(u) - k$, $y = d(u)$, $z = d(v)$ and $w = d(v) + k$ in Lemma 2.1 and simplifying shows that we have

$$0 \leq f(d(u) - k) + f(d(v) + k) - f(d(u)) - f(d(v))$$

and thus by equation (1) above we have $p(G) \leq p(G_{u \to v})$. When f is concave the result is entirely analogous. □

Determining when various vertex-based indices in the literature are defined by convex or concave functions f is often an easy exercise, especially since in connected graphs degrees are positive. This is even more true when the functions f are twice differentiable, since it is well-known that in this case $f''(x) \geq 0$ indicates f is a convex function, and $f''(x) \leq 0$ a concave one. We illustrate this with the zeroth-order Randić index $R^0_\alpha(G)$, which is defined as $R^0_\alpha(G) = \sum_{a \in V(G)} (d(a))^\alpha$. The zeroth-order Randić index in fact generalizes a number of different topological indices, as shown in Table 2.

Theorem 2.3. *When $\alpha \geq 1$ or $\alpha \leq 0$ we have $R^0_\alpha(G) \leq R^0_\alpha(G_{u \to v})$, and when $0 \leq \alpha \leq 1$ we have $R^0_\alpha(G) \geq R^0_\alpha(G_{u \to v})$.*

Proof. The second derivative of the function $f(x) = x^\alpha$ is $f''(x) = \alpha(\alpha - 1)x^{\alpha - 2}$ which, for positive x values, is non-negative when $\alpha \geq 1$ and $\alpha \leq 0$, and non-positive when $0 \leq \alpha \leq 1$. (We actually have $f''(x) = 0$ at $x = 0$ and $x = 1$.) Hence the defining function of the zeroth-order Randić index is convex when $\alpha \geq 1$ or $\alpha \leq 0$, and concave when $0 \leq \alpha \leq 1$. The result now follows by the previous theorem. □

Another vertex-based topological index is the *variable sum exdeg index* $SEI_\alpha(G)$, which is defined to be

$$SEI_\alpha(G) = \sum_{a \in V(G)} d(a)\alpha^{d(a)}$$

for some positive number α.

Theorem 2.4. *When $\alpha > 1$ and $0 < \alpha < e^{-1}$, we have $SEI_\alpha(G) \leq SEI_\alpha(G_{u\to v})$.*

Proof. The function $f(x) = x\alpha^x$ defines the index, and $f''(x) = 2\alpha^x \ln \alpha + x\alpha^x(\ln \alpha)^2$. The second derivative function f'' is easily seen to be positive when $\alpha > 1$. Consider now when $0 < \alpha < e^{-1}$, say $\alpha = e^{-t}$ for some $t > 1$. Then $f''(x) = te^{-tx}(tx - 2)$, which is positive for all $x \geq 2$ and so, recalling that x stands for the degree of a vertex, we have $SEI_\alpha(G) \leq SEI_\alpha(G_{u\to v})$ for all u, v of degree 2 or greater. However compressions involving vertices of degree 1 result in $G_{u\to v} = G$, and so the statement of the theorem holds in general as well. □

Multiplicative versions of some of the sum-based parameters have also appeared in the literature, for example the multiplicative first Zagreb index Π_1 is defined to be

$$\Pi_1(G) = \prod_{a \in V(G)} (d(a))^2$$

and the second multiplicative Zagreb index is

$$\Pi_2(G) = \prod_{a \in V(G)} (d(a))^{d(a)}.$$

Determining the behavior of compression for these parameters can still often be approached via convexity and concavity. Recall that a function f is *log-convex* if $\ln f$ is convex, and *log-concave* if $\ln f$ is concave. We have the following.

Theorem 2.5. *Let p be a graph parameter defined by*

$$p(G) = \prod_{a \in V(G)} f(d(a))$$

for some function $f(x) \geq 0$ for all $x > 0$. If f is log-convex, then $p(G) \leq p(G_{u\to v})$ and if f is log-concave then $p(G) \geq p(G_{u\to v})$.

Proof. Consider the sum-based parameter

$$\ln(p(G)) = \sum_{a \in V(G)} \ln(f(d(a))).$$

If f is log-convex then by Theorem 2.2 we have $\ln(p(G)) \leq \ln(p(G_{u\to v}))$. But $\ln x$ is a monotonically increasing function, and so that implies we must have $p(G) \leq p(G_{u\to v})$, as required. The result for log-concave f is entirely analogous. □

Corollary 2.6. *We have $\Pi_1(G) \geq \Pi_1(G_{u\to v})$ and $\Pi_2(G) \leq \Pi_2(G_{u\to v})$.*

Proof. It is easy to check that $f''(x) = -2/x^2$ when $f(x) = \ln(x^2)$ and that $f''(x) = 1/x$ when $f(x) = \ln(x^x)$. Thus for $x > 0$ the first function is log-concave and the second function is log-convex, and now the result follows from the definitions of $\Pi_1(G)$ and $\Pi_2(G)$ and Theorem 2.5. □

3 Edge-Based Topological Indices and Compression

We turn now to edge-based graph parameters, i.e. parameters of the form

$$\sum_{ab \in E(G)} f(d(a), d(b)).$$

The analysis here is slightly more involved. As mentioned before, only the degrees of vertices u and v change after compression from u to v, but for edge-based parameters we must take into account all edges incident to those vertices in each sum. However, since the functions f we are dealing with are invariably symmetric functions, much follows similar lines as before. For the moment let us assume that $uv \in E(G)$, and set V_u, V_v, and V_{uv} to be the vertices in $V(G)$ adjacent to u and not v, adjacent to v and not u, and adjacent to both u qnd v respectively. Taking advantage of symmetry, and again setting $H = G_{u \to v}$ for brevity, we have $p(H) - p(G)$ equal to

$$\begin{aligned}
&\sum_{ab \in E(H)} f(d_H(a), d_H(b)) - \sum_{ab \in E(G)} f(d_G(a), d_G(b)) \qquad (2)\\
&= f(d_H(v), d_H(u)) - f(d_G(v), d_G(u)) \\
&\quad + \sum_{a \in V_u} [f(d_H(v), d_H(a)) - f(d_G(u), d_G(a))] + \sum_{a \in V_v} [f(d_H(v), d_H(a)) - f(d_G(v), d_G(a))] \\
&\quad + \sum_{a \in V_{uv}} [f(d_H(u), d_H(a)) + f(d_H(v), d_H(a)) - f(d_G(u), d_G(a)) - f(d_G(v), d_G(a)] \\
&= f(d_G(v) + k, d_G(u) - k) - f(d_G(v), d_G(u)) \\
&\quad + \sum_{a \in V_u} [f(d_G(v) + k, d_G(a)) - f(d_G(u), d_G(a))] + \sum_{a \in V_v} [f(d_G(v) + k, d_G(a)) - f(d_G(v), d_G(a))] \\
&\quad + \sum_{a \in V_{uv}} [f(d_G(u) - k, d_G(a)) + f(d_G(v) + k, d_G(a)) - f(d_G(u), d_G(a)) - f(d_G(v), d_G(a))]
\end{aligned}$$

where as earlier k is the number of edges that were moved from u to v by the compression. A careful examination of the terms of $p(G_{u \to v}) - p(G)$ listed above yields the following.

Theorem 3.1. *Let p be a graph parameter defined by*

$$p(G) = \sum_{ab \in E(G)} f(d(a), d(b))$$

for some symmetric function $f(x, y) \geq 0$ for $x, y > 0$. Let $F(x) = f(x, y)$ with y considered to be fixed (and positive). If

1. *$F(x)$ is increasing,*
2. *$F(x)$ is convex, and*
3. *$f(x + k, y - k) \geq f(x, y)$*

holds for all $x \geq y > k \geq 1$, then $p(G) \leq p(G_{u \to v})$ for all u, v such that $dist(u, v) \leq 2$.

Name	Function
First hyper-Zagreb index	$(x+y)^2$
Sombor index	$\sqrt{x^2+y^2}$
Reduced Sombor index	$\sqrt{(x-1)^2+(y-1)^2}$
Extended index	$\frac{1}{2}\left(\frac{x}{y}+\frac{y}{x}\right)$
Albertson irregularity index	$\lvert x-y\rvert$
Sigma index	$(x-y)^2$

Table 2: Various topological indices satisfying the conditions of Theorem 3.1. Exponential versions of these topological indices also satisfy the same conditions.

Proof. Examining the expressions in square brackets in the final lines of equation (2) above, we see that the terms corresponding to V_u and V_v, namely

$$f(d_G(v)+k, d_G(a)) - f(d_G(u), d_G(a))$$

and

$$f(d_G(v)+k, d_G(a)) - f(d_G(v), d_G(a)),$$

are non-negative since F is increasing. Furthermore, the terms corresponding to V_{uv}, namely

$$f(d_G(u)-k, d_G(a)) + f(d_G(v)+k, d_G(a)) - f(d_G(u), d_G(a)) - f(d_G(v), d_G(a))$$

are non-negative since F is convex. When $uv \in E(G)$ then the third condition implies that the terms corresponding to that edge, namely $f(d_G(v)+k, d_G(u)-k) - f(d_G(v), d_G(u))$, are non-negative as well. Taken together, these imply that $p(G) \leq p(G_{u\to v})$.

It only remains to note that the three conditions of the theorem need only hold for the range $x \geq y > k \geq 1$ given. Recall from the Introduction that it suffices to consider compressions from u to v for pairs of vertices u, v such that $dist_G(u,v) \leq 2$ and $d_G(v) \geq d_G(u)$. The latter condition implies $x \geq y$ in this setting, and since k represents the number of edges moved from u to v after the compression, we have $y \geq k$. Now with $dist_G(u,v) \leq 2$, then at least one edge incident to u must remain unchanged during compression: the edge uv if $dist_G(u,v) = 1$ and all edges of the form ux for $x \in N_G(u) \cap N_G(v)$ if $dist_G(u,v) = 2$. This implies that in fact $y > k$. Finally if $k = 0$ then no edges were moved in the compression and $G_{u\to v} = G$, in which case the conclusion $p(G) \leq p(G_{u\to v})$ holds trivially. Thus the conditions of the theorem holding for all $x \geq y > k \geq 1$ will ensure $p(G) \leq p(G_{u\to v})$. $\square$

Some prominent topological indices which satisfy all three conditions of Theorem 3.1, and so are uniformly decreased by compression, are given in Table 2. Verifying that these indices satisfy Theorem 3.1 are simple calculus and calculation exercises which are omitted (although for the Sombor indices it may be helpful to recall that, since degrees are non-negative and the square root function is monotonically increasing, then $s \leq t$ implies $\sqrt{s} \leq \sqrt{t}$).

In a similar fashion we may obtain sufficient conditions that imply compression decreases a topological index, although there seem to be few topological indices to which these pertain. The following theorem is analogous to Theorem 3.1 and the proof is omitted.

Theorem 3.2. *Let p be a graph parameter defined by*

$$p(G) = \sum_{ab \in E(G)} f(d(a), d(b))$$

for some symmetric function $f(x, y) \geq 0$ for $x, y > 0$. Let $F(x) = f(x, y)$ with y considered to be fixed (and positive). If

1. *$F(x)$ is decreasing,*
2. *$F(x)$ is concave, and*
3. *$f(x + k, y - k) \leq f(x, y)$*

holds for all $x \geq y > k \geq 1$, then $p(G) \geq p(G_{u \to v})$ for all u, v such that $dist(u, v) \leq 2$.

Recently exponential topological indices, which are of the form

$$\sum_{a,b \in E(G)} e^{f(d(a),d(b))}$$

have also been studied. Since the exponential function is monotonically increasing $e^{f(x,y)}$ satisfies the conditions of Theorem 3.1 whenever $f(x, y)$ does, and so we have the following.

Theorem 3.3. *Let p be a graph parameter of the form*

$$p(G) = \sum_{ab \in E(G)} e^{f(d(a),d(b))}$$

for some symmetric function $f(x, y) \geq 0$ for $x, y > 0$. Let $F(x) = f(x, y)$ with y considered to be fixed (and positive). If

1. *$F(x)$ is increasing,*
2. *$F(x)$ is convex, and*
3. *$f(x + k, y - k) \geq f(x, y)$*

holds for all $x \geq y > k \geq 1$, then $p(G) \leq p(G_{u \to v})$ for all u, v such that $dist(u, v) \leq 2$.

The theorem above implies that compression works in the same way for the exponential version $e^{f(x,y)}$ of the topological indices listed in Table 2—the exponential first Zagreb index, the exponential Sombor index, and so on—as it does for the non-exponential version.

For nearly all of the topological indices mentioned in both this section and the previous section, the compression results given here generalize previous graph transformations on trees or unicycles or other limited classes of graphs in the topological index literature. Rather than list those transformations here we refer the reader to the references given in the following section, where we discuss the extremal results that are a natural extension of the compression results just seen.

4 Compression and Threshold Graphs

Threshold graphs are a well-known and much-studied class of graphs which have appeared in a number of different mathematical contexts, and as a consequence there are many equivalent ways to define them. A good reference for these definitions and many more properties of threshold graphs is the book [43]. We will make use of a number of these definitions, the first of which is the following. Note that $N_G[u]$ indicates the closed neighborhood $N_G[u] = N_G(u) \cup u$.

Definition 4.1. *A* threshold graph *is a graph in which, for any pair of vertices $u, v \in V(G)$, either $N_G(u) \subseteq N_G[v]$ or $N_G(v) \subseteq N_G[u]$.*

When $G_{u \to v} \neq G$ then the compression operation has taken two vertices $u, v \in V(G)$ for which neither $N_G(u) \subseteq N_G[v]$ nor $N_G(v) \subseteq N_G[u]$ holds, and produced a new graph $G_{u \to v} = H$ in which $N_H(u) \subseteq N_H[v]$. After compression, then, a graph is "more threshold" and continued applications of compression to different pairs of vertices can only increase this. Therefore repeated compressions will eventually result in a threshold graph, a fact noted in the Introduction as Theorem 1.1. Furthermore, a threshold graph G is essentially incompressible: if $N_G(u) \subseteq N_G[v]$ then $G_{u \to v} = G$ (indeed, no edges are moved in the transformation) and if $N_G(v) \subseteq N_G[u]$ then $G_{u \to v}$ is isomorphic to G, with the isomorphism given by switching the labels of u and v. So threshold graphs are the "end result" of repeated applications of compression. These facts have important consequences for extremal problems, as first noted by Satyanarayana, Schoppmann, and Suffel [48] in the context of network reliability but also noted by a number of authors since. In the rest of the paper we let $\mathcal{G}_{n,m}$ denote the class of simple connected graphs with n vertices and m edges.

Theorem 4.2. *Let p be a graph parameter such that $p(G) \leq p(G_{u \to v})$ (respectively, $p(G) \geq p(G_{u \to v})$) for all $G \in \mathcal{G}_{n,m}$ and all $u, v \in V(G)$ such that $dist(u, v) \leq 2$. Then there exists a connected threshold graph $H \in \mathcal{G}_{n,m}$ such that $p(G) \leq p(H)$ (resp., $p(G) \geq p(H)$) for all $G \in \mathcal{G}_{n,m}$. In other words, there is a simple connected threshold graph that maximizes (resp., minimizes) the parameter p over all simple connected graphs with the same number of vertices and edges.*

As we saw in the two previous sections, many topological indices are parameters that satisfy Theorem 4.2, and therefore there are threshold graphs that either maximize or minimize those parameters. How can we easily identify those threshold graphs? Another of the key structural properties of threshold graphs that may be helpful here is the following, which is an alternative definition of threshold graphs.

Definition 4.3. *A* split graph *is a graph whose vertex set may be partitioned into two sets, one of which induces a clique and the other of which induces an independent set. A* threshold graph *is a split graph in which the neighborhoods of the independent set are nested, in other words, there exists an ordering of the vertices $v_1, v_2, \ldots, v_k$ of the independent set such that*

$$N(v_1) \subseteq N(v_2) \subseteq \cdots \subseteq N(v_k).$$

A significant number of papers in the topological indices literature have sought to identify the extremal graphs of various topological indices in the classes of trees, unicyclic graphs, and bicyclic graphs. With the above definition it is simple to see that in each of the classes $\mathcal{G}_{n,n-1}$ (trees), $\mathcal{G}_{n,n}$ (unicyclic graphs), and $\mathcal{G}_{n,n+1}$ (bicyclic graphs) there is only one threshold graph. Those graphs are the star, the star with one additional edge added, and the star with two additional and adjacent

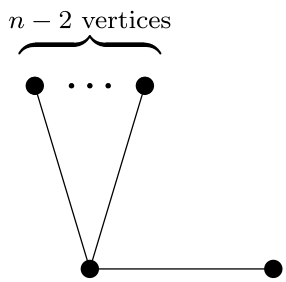

Figure 3: From left to right, the only threshold graphs in the $\mathcal{G}_{n,n-1}$, $\mathcal{G}_{n,n}$, and $\mathcal{G}_{n,n+1}$ classes, respectively.

edges added. These graphs are pictured in Figure 3. (We have drawn them in order to emphasize their relationship to Definition 4.3 above, with a clique on the bottom and an independent set at the top of each graph.)

Since the graphs in Figure 3 are the only threshold graphs in their classes, and compression produces threshold graphs, for these classes showing that compression uniformly increases a parameter is sufficient to identify the relevant maximal graph directly, and showing that compression decreases a parameter is sufficient to identify the relevant minimal graph. Thus, by utilizing compression and threshold graph techniques one can often significantly eliminate the tedious calculations and reduce the long case analyses that have frequently been seen in these efforts. Indeed, in these classes knowledge of compression and threshold graph techinques can render these tasks almost trivial. For example, regarding vertex-based topological indices, the following is now an elementary and immediate consequence of Theorems 2.3 and 4.2.

Theorem 4.4. *The three graphs pictured in Figure 3 are*

- *maximal graphs for $R_0^\alpha(G)$ when $\alpha \leq 0$ or $\alpha \geq 1$, and*
- *minimal graphs for $R_0^\alpha(G)$ when $0 \leq \alpha \leq 1$.*

in their respective graph classes.

Theorem 4.4 generalizes some of the extremal results for these parameters previously obtained in [21] (first Zagreb index), [1] (forgotten index for trees), [5] (forgotten index for unicyclic and bicyclic graphs), [53] (inverse degree index for trees), [44] (inverse degree index for unicyclic graphs) [24] (zeroth order Randić index for trees), [41] (general α for trees), [56] (general α for unicyclic graphs), [13, 54] (general α for bicyclic graphs). Moreover, using the compression and threshold graph machinery Theorem 4.4 is obtained almost instantly and with very little calculation required, which stands in stark contrast to how the results were typically obtained in the works listed. To highlight some examples, the original proof in [44] finding the maximal unicyclic graphs used not one but four distinct graph transformations, while finding the maximal bicyclic graphs in [13] used a case analysis that stretched over four sections of that paper. Using the compression and threshold graph machinery here, the task is accomplished using only a convexity/concavity check to verify that compression increases the Randić index, as in Theorem 2.2, and then noting the uniqueness of the threshold graph in the relevant class.

Similarly by Theorems 2.6 and 4.2, the following are also immediate.

Theorem 4.5. *For the multiplicative Zagreb indices $\Pi_1(G)$ and $\Pi_2(G)$ the variable sum exdeg index $SEI_\alpha(G)$, the three graphs given in Figure 3 are*

- *maximal for the variable sum exdeg index $SEI_\alpha(G)$ when $\alpha > 1$ and when $0 \leq \alpha < e^{-2}$,*
- *minimal for the first multiplicative Zagreb index $\Pi_1(G)$, and*
- *maximal for the second multiplicative Zagreb index $\Pi_2(G)$*

in the respective graph classes.

Theorem 4.5 generalizes some of the results of [32] (first and second multiplicative Zagreb index for trees) and [30] (second multiplicative Zagreb index for unicyclic and bicyclic graphs), and encompasses some of the results from [22, 46] (variable sum exdeg index). Again, by using some knowledge of compression and threshold graphs our results are obtained much more simply and naturally than previous results. As far as we can tell, the results in Theorem 4.5 on minimum graphs for the first multiplicative Zagreb index in classes $\mathcal{G}_{n,n}$ and $\mathcal{G}_{n,n+1}$ are new.

Of course, for the earlier edge-based topological indices that satisfy the conditions of Theorem 3.1 we can obtain similar results equally easily.

Theorem 4.6. *The three graphs pictured in Figure 3 are maximal graphs for all of the topological indices given in Table 2, as well as their exponential variants, in the $\mathcal{G}_{n,n-1}, \mathcal{G}_{n,n}$, and $\mathcal{G}_{n,n+1}$ classes.*

Theorem 4.6 generalizes some of the results of [28] (first hyper-Zagreb index), [14] (Sombor index for trees), [15, 20] (Sombor index for unicyclic and bicyclic graphs), [55] (reduced Sombor index for trees and unicycles), [23] (reduced Sombor index for bicyclic graphs), [52] (symmetric division index for trees and unicycles), [34] (Albertson irregularity index), [2] (sigma index). Again, comparing the proof method involving compression and threshold graphs presented here to the proofs of the results just listed often reveals stark differences in difficulty. As an example, the proof published in [20] that determined the maximal graph for the Sombor index in $\mathcal{G}_{n,n+1}$ stretched over 5 pages and featured 11 cases and subcases of algebraic inequality analysis. The maximal graph in that class is, of course, the rightmost graph in Figure 3, and this is an immediate consequence of Theorem 4.6.

Regarding exponential variants, Theorem 4.6 generalizes some of the results of Gao [25] and Gao and Gao [27] for trees. To the best of our knowledge, the results on unicyclic and bicyclic graphs for these exponential topological indices are new.

5 Other graph classes

What about more edge-dense graph classes? In the graph classes immediately beyond $\mathcal{G}_{n,n+1}$ things can of course still be reasonably straightforward since there are still relatively few threshold graphs. For example, Figure 4 shows the only two threshold graphs in the next class $\mathcal{G}_{n,n+2}$. It is not difficult to determine that there are only two threshold graphs in $\mathcal{G}_{n,n+3}$ as well, and then three threshold graphs in $\mathcal{G}_{n,n+4}$. Thus when compression uniformly increases or decreases a topological index, then finding maximal or minimal graphs in these classes is just a matter of comparing the values of the topological indices of two or three graphs.

Even this knowledge may be a significant help. We note for instance that in [22] the authors sought to find the maximal graphs in $\mathcal{G}_{n,n+2}$ and $\mathcal{G}_{n,n+3}$ for the variable sum exdeg index $SEI(G)$,

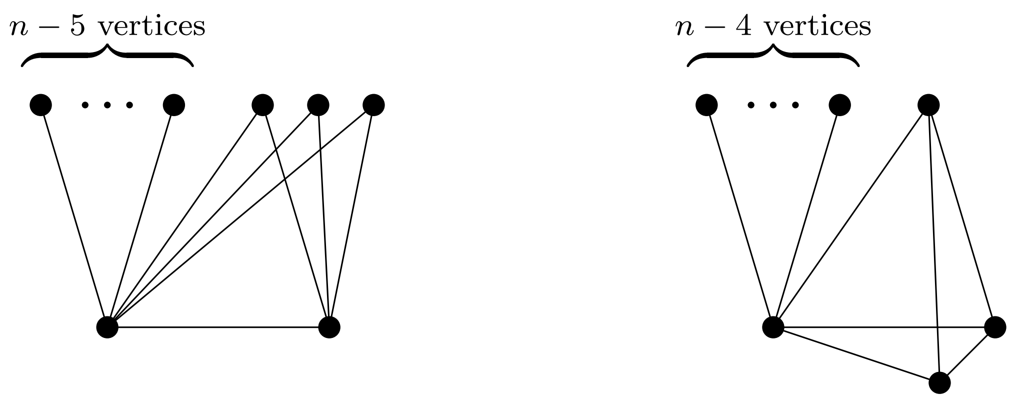

Figure 4: The only two threshold graphs in the $\mathcal{G}_{n,n+2}$ graph class.

but were only able to determine such a graph must have a *universal vertex*, that is, a vertex that is adjacent to every other vertex in the graph. This still left 5 graphs in the $\mathcal{G}_{n,n+2}$ class and 11 graphs in the $\mathcal{G}_{n,n+3}$ class, all of which had to be examined in order to discover the maximal graphs in those classes. Of course, as necessitated by Theorems 2.4 and 4.2, it was eventually determined that the two threshold graphs in each of the classes were the maximal graphs. (Which threshold graph is maximal depends upon the value of α, see [22].)

An even more striking example involves a topological index not mentioned yet, the general sum-connectivity index $\chi_\alpha(G)$, an edge-based topological index which is defined by the function

$$\chi_\alpha(G) = \sum_{ab\in E(G)} (d(a) + d(b))^\alpha$$

for various values of α. The general sum-connectivity index generalizes other well-known indices, including the sum-connectivity index $\chi_{-1/2}$, the first hyper-Zagreb index χ_2, and the harmonic index $2\chi_{-1}$. In [57], the entire 12-page paper was spent gradually eliminating candidate graphs in $\mathcal{G}_{n,n+2}$ until only the two graphs in Figure 4 remained as possible maximal graphs for the $\alpha \geq 1$ case of the general sum-connectivity index. Here is an alternative method of proving that result using compression and threshold graph machinery.

Theorem 5.1 ([57])**.** *Let $\alpha \geq 1$. Then at least one of the two graphs in Figure 4 are maximal graphs for the general sum-connectivity index $\chi_\alpha(G)$ in the class $\mathcal{G}_{n,n+2}$.*

Proof. It is straightforward to check, using derivatives for the first two conditions and direct calculation for the third condition, that $f(x, y) = (x + y)^\alpha$ satisfies all three conditions of Theorem 3.1 when $\alpha \geq 1$. By Theorem 4.2 then, there are threshold graphs that maximize $\chi_\alpha(G)$ for these values in $\mathcal{G}_{n,n+2}$ (or indeed any of the $\mathcal{G}_{n,m}$ classes). The only two threshold graphs in $\mathcal{G}_{n,n+2}$ are the two graphs in Figure 4, and this completes the proof. □

We note in passing that, since Theorem 3.1 only requires $x \geq y \geq 1$, that similar results can be obtained equally easily for the variable Platt index $P_\alpha(G)$ (when $\alpha \geq 1$), which is defined by the function $f(x, y) = (x + y - 2)^\alpha$, and similar results can also be easily obtained for the generalized

Albertson index $A_p(G)$ (when $p \geq 1$) which is defined as

$$A_p(G) = \left(\sum_{ab \in E(G)} |d(a) - d(b)|^p \right)^{1/p}.$$

(As mentioned earlier with square roots, it may be helpful with the generalized Albertson index to recall that $s \leq t$ implies $s^{1/p} \leq t^{1/p}$ for $p \geq 1$.) These encompass some of the results of [4] on the Platt index and some of the results on the generalized Albertson index for trees [42], but to the best of our knowledge the other results implied for the generalized Albertson index (e.g., the graphs of Figure 3 are maximal in their classes) are new.

Edge-sparse graph classes have relatively few graphs and thus, as we have seen, relatively few threshold graphs to consider, but larger graph classes will also have correspondingly more threshold graphs. Thus if the goal is to find extremal graphs for all $\mathcal{G}_{n,m}$ then some other perspective is needed. What else can be said about threshold graphs in general that may be helpful in extremal problems? We will mention a few other facts about threshold graphs that relate to what we have seen in the mathematical chemistry literature. Another alternative definition of threshold graphs is the following.

Definition 5.2. *A graph G is a threshold graph if and only if the vertices of G can be ordered so that each vertex is either adjacent to all of the vertices or to none of the vertices that precede it in the order.*

From the definition above it is immediate that every connected threshold graph G must have a universal vertex, a vertex of degree $n-1$ that is adjacent to every other vertex of G. As we saw earlier, this fact was proved separately in the analysis of the variable sum exdeg index. In fact from what we have seen in the topological index literature the existence of a universal vertex has been proved separately for a wide variety of extremal graphs for topological indices. This ubiquity was noted in [3] for example, where conditions much like the conditions of Theorem 3.1 were shown to imply universal vertices in extremal graphs for a wide variety of topological indices. Definition 5.2 shows that universal vertices are a definitional feature of connected threshold graphs, and so come "for free" as a consequence of compression techniques with no additional proof required. In other work some effort has also been taken to show that when the universal vertex is deleted then another similarly-structured graph (i.e., a connected threshold graph with possibly some additional isolated vertices) results, for some examples see [50, 51]. This fact too is an automatic consequence of the first definition above. Perhaps worth noting here is the more general fact that deleting any vertex of a threshold graph (not necessarily a universal vertex) produces another threshold graph. This is also an immediate implication of Definition 5.2.

Another defintion of threshold graphs, this time involving forbidden subraphs, is the following.

Definition 5.3. *G is a threshold graph if and only if G is $\{P_4, C_4, 2K_2\}$-free, that is, G has none of the graphs listed as induced subgraphs.*

We observe variants of this definition have also been proven to be true for the extremal graphs of various topological indices; in [50, 51] for example it is proven the extremal graphs there are $\{P_4, C_p\}$-free for all $p \geq 4$, a fact that is a simple consequence of Definition 5.3 above.

Somewhat more generally, we can say the following.

Theorem 5.4. *Let p be a graph parameter. If $p(G) \leq p(G_{u \to v})$ (resp., $p(G) \geq p(G_{u \to v})$) for all $u, v \in V(G)$ such that $dist(u, v) \leq 2$, then for each n and m, there is a maximal (resp., minimal) graph $G \in \mathcal{G}_{n,m}$ for p such that*

1. *for any pair of vertices $u, v \in V(G)$, either $N_G(u) \subseteq N_G[v]$ or $N_G(v) \subseteq N_G[u]$,*
2. *the vertex set of G may be partitioned into two sets, one of which induces a clique and the other of which induces an independent set in which the neighborhoods of the independent set are nested,*
3. *the vertices of G can be ordered so that each vertex is either adjacent to all of the vertices or to none of the vertices that precede it in the order,*
4. *G has a universal vertex, and deleting this vertex results in a connected threshold graph plus (possibly) additional isolated vertices, and*
5. *G is $\{P_4, C_4, 2K_2\}$-free.*

Properties along the lines of those mentioned above are the ones we have seen most often prove useful in the topological index literature but threshold graphs have many more interesting properties that are not mentioned here, see [43].

6 Majorization and Threshold Graphs

Before concluding we briefly note one other method, besides compression, that also commonly reveals when threshold graphs are extremal graphs. We let S denote a sequence of length n, and we assume that S is listed in decreasing order, i.e. if $S = (x_1, x_2, \ldots, x_n)$ then $x_1 \geq x_2 \geq \ldots x_n$. We say a sequence S *majorizes* the sequence S', and write $S \preccurlyeq S'$ if

$$\sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} x_i'$$

for all $1 \leq k \leq n$, and $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} x_i'$. Majorization is a well-known and much-studied topic, see for example the textbook [45]. As suggested by the notation, majorization induces a partial order on finite sequences of the same length and sum. Threshold graphs, and their degree sequences, arise naturally in this context.

Theorem 6.1 ([43])**.** *Let d_G be the degree sequence of $G \in \mathcal{G}_{n,m}$. Then there exists a threshold graph $H \in \mathcal{G}_{n,m}$ such that $d_G \preccurlyeq d_H$. In other words, the maximal degree sequences in the poset of degree sequences of $\mathcal{G}_{n,m}$ under the majorization order are the degree sequences of threshold graphs.*

Importantly, a number of multivariate functions obey the majorization order, in the sense that if $S \preccurlyeq S'$ then $f(S) \leq f(S')$. Such functions are called *Schur-convex*. There is also the natural and analogous idea of *Schur-concave*, see e.g. [45]. Many vertex-based topological indices are Schur-convex functions of the degree sequence of a graph, and in a number of papers majorization has been applied to find extremal degree sequences for a given topological index and the extremal graphs that have those degree sequences, see for example [6, 7, 29]. However Theorem 6.1 above, which shows that majorization methods often lead directly to threshold graphs, does not seem to have been previously noted in the mathematical chemistry literature. We also mention the following fact about threshold graphs and their degree sequences, first proven by Hammer, Ibaraki, and Simeone [33].

Theorem 6.2 ([33]). *Threshold degree sequences are unique, that is, if a graph G has the same degree sequence as a threshold graph H, then G is isomorphic to H.*

Thus if a particular degree sequence is found (via majorization or some other technique) to uniquely maximize a particular vertex-based parameter, and that degree sequence is the degree sequence of a threshold graph, then that threshold graph is the unique maximum graph for that parameter. There are no other non-isomorphic graphs that maximize that parameter.

7 Conclusion

As shown in this paper compression and threshold graph techniques, when they apply, can provide a powerful method for determining structural properties of extremal graphs, or even the extremal graphs themselves. However there are limitations. The most notable limitation is probably the "unidirectional" nature of compression: while the compression operation is well-defined it does not have a well-defined inverse operation. For example, it is not difficult to find multiple non-isomorphic graphs that can all be compressed to the same graph. (See e.g., the discussion beginning the last section of [38].) Thus in Sections 3 and 4 we are careful to say that our results there can easily recapture "some" of the results from the topological index literature. Many of the works cited found both maximal and minimal graphs in the graph classes considered. Compression can be useful in finding maximal or minimal graphs, but rarely both.

We also emphasize that the conditions of the various theorems in this paper are sufficient conditions only. There exist many topological indices that do not satisfy any theorem given here that still, for example, have particular threshold graphs as extremal graphs. In future work we intend to illustrate that results that are similar in spirit but weaker than Theorems 3.1 and 3.2 can still be useful tools in discovering when threshold or "near-threshold" graphs are maximal or minimal. In the other direction, we are also aware that there exist topological indices that do not have threshold graphs as extremal graphs. Naturally compression is but one technique out of many; the number of extant topological indices is large, varied and growing, and compression will never apply to every index based on graph degrees.

On the other hand the topological indices covered here are meant to be illustrative, and are by no means exhaustive. We strongly suspect there are other (possibly many other) topological indices which we have omitted or neglected for which compression and threshold graph techniques apply and can be useful. Certainly, that is one of the hopes and intentions of this paper.

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