Journal of Contemporary Applied Mathematics
V. 18, No 1, 2028, January-June
ISSN 2222-5498, E-ISSN 3006-3183
https://doi.org/10.62476/jcam181.2

Sharp Bounds and Extremal Properties of a Degree-Based Graph Irregularity Index

Mythili V, Dhanalakshmi S.*

Abstract. We study the degree-contrast index $\mathrm{DCI}(G) = \sum_{uv\in E(G)}(d(u) - d(v))^2/(d(u)+d(v))$, an irregularity measure that vanishes on a connected graph exactly when the graph is regular. The identity $\mathrm{DCI} = M_1 - 4\,\mathrm{ISI}$ shows that it is a derived combination of the first Zagreb and inverse sum indeg indices; our contribution is the theory built on it. We prove the sigma-index bounds $\sigma/(2\Delta) \le \mathrm{DCI} \le \sigma/(2\delta)$, strict for non-regular graphs with asymptotically optimal constants, and the sharp bounds $\sigma/(2\Delta-1) \le \mathrm{DCI} \le \sigma/(2\delta+1)$, characterising all equality cases. We give closed forms for fourteen standard graph families, indexed by their order n. For complete split graphs we prove $c_*n^3 - \frac{3}{2}n^2 \le \max_k \mathrm{DCI}(\mathrm{CS}(n,k)) < c_*n^3$ with $c_* = (632-238\sqrt{7})/27 \approx 0.0856$, whereas stars, wheels and friendship graphs grow only quadratically, and we show that the maximum of DCI over connected graphs of order n is $\Theta(n^3)$. Exhaustive enumeration in exact arithmetic shows that the unique maximiser is the star for $4 \le n \le 7$ and the complete split graph $\mathrm{CS}(n,2)$ for $8 \le n \le 10$.

Key Words and Phrases: Topological index, degree-based index, irregularity measure, Zagreb index, inverse sum indeg index, extremal graphs.

2010 Mathematics Subject Classifications: 05C09, 05C92.

1. Introduction

In chemical graph theory a topological index attaches to a molecular graph drawn with its hydrogens suppressed a single number that tends to track measured physical, chemical or biological behaviour, giving an inexpensive and repeatable numerical fingerprint of structure [7, 28, 17, 24]. Among such invariants, those defined purely from vertex degrees form the longest-established and most intensively examined class; it originates with the Zagreb indices [17] and Randić's

*Corresponding author.

 © *2010 jcam* All rights reserved.

branching index [24] and continues to draw interest both in applied structure–property studies [23] and in the bounds and extremal problems it poses [3, 14].

A prominent subclass, the irre,gularity indices, records how far a graph is from being regular. Its two archetypes are Albertson's index $\mathrm{irr}(G) = \sum_{uv\in E(G)} |d(u) - d(v)|$ [4] and the squared version known as the sigma index $\sigma(G) = \sum_{uv\in E(G)} (d(u) - d(v))^2$, for which $\sigma(G) = F(G) - 2M_2(G)$ [16].

Irregularity measures have been studied intensively in recent years. The Albertson index has been generalised to a one-parameter family [20]; Furtula and Oz introduced a "complementary" construction that substitutes $d(u), d(v)$ by $d(u) + d(v)$ and $|d(u) - d(v)|$ in existing definitions [14]; and further variants such as the total irregularity measure [6], the reciprocal irregularity [8], and the σ_t-irregularity [10] have appeared. For the extremal problems relevant here the literature is quite precise. Albertson [4] proved that $\mathrm{irr}(G) < 4n^3/27$ for every graph of order n, and Abdo, Cohen and Dimitrov [1] showed that the exact maximum of irr over all graphs of order n is $\lfloor n/3 \rfloor \lceil 2n/3 \rceil (\lceil 2n/3 \rceil - 1)$, attained only by complete split (clique–star) graphs with a clique of about $n/3$ vertices. Abdo, Dimitrov and Gutman [2] characterised the general graphs of order n with maximal σ-irregularity, while sharp results for the sigma index are also known on chemical trees [19], on trees with fixed degree sequence [11], and on k-cyclic graphs [5]. Thus, for irregularity measures whose summands grow with the degree difference, the maximisers over general graphs are dense and highly inhomogeneous rather than tree-like; we shall see that the same phenomenon occurs for the descriptor studied here, although for DCI the global extremal problem remains open (Conjecture 1).

The descriptor we study combines the sigma numerator with a degree-sum denominator. That denominator is the signature of the sum-connectivity, harmonic and inverse sum indeg (ISI) indices [27], an invariant whose bounds and extremal behaviour are themselves the subject of much current work: bounds under graph operations [18, 9], the structure of trees with maximal ISI [29], variable generalisations [22], and sharp bounds for tricyclic graphs [30]. Because our main structural result expresses the new descriptor exactly through M_1 and ISI, this body of results transfers to it directly.

Concretely, the present work studies the descriptor

$$\mathrm{DCI}(G) = \sum_{uv\in E(G)} \frac{(d(u) - d(v))^2}{d(u) + d(v)}, \tag{1}$$

to which we give the name degree-contrast index.

Its numerator is that of the sigma index, whereas its denominator $d(u)+d(v)$ is the degree-sum weighting shared by the sum-connectivity, harmonic and inverse-

sum-indeg indices. Its motivation is structural: an edge whose endpoints have very different degrees—a highly branched vertex bonded to a terminal one—signals local heterogeneity, and (1) weights such contrasts by the reciprocal of the local connectivity $d(u) + d(v)$. We stress that this weighting is *not* a normalisation in the usual sense: DCI is unbounded and, as shown in Section 6, its maximum over graphs of order n grows like n^3. Throughout the paper the word "normalised" is reserved for the index NDCI of Section 6, whose values lie in $[0, 1)$.

Scope and novelty. We state at the outset that DCI is *not* a new algebraically independent invariant. The exact identity $\mathrm{DCI} = M_1 - 4\,\mathrm{ISI}$ (Theorem 1) shows that it is a fixed linear combination of the first Zagreb index and the inverse sum indeg index, and any statistical or structural information it carries is already contained in the pair (M_1, ISI). Its interest lies in the fact that this particular combination is a natural degree-sum-weighted irregularity measure: it retains the sigma numerator but divides each edge contribution by the local connectivity $d(u) + d(v)$. The new contributions of the paper are therefore mathematical results *about* this derived descriptor, namely (i) sharp inequalities relating DCI to the sigma index, with a complete characterisation of the equality cases; (ii) exact closed forms for fourteen standard graph families, indexed by their true order; and (iii) an extremal analysis: explicit bounds for the cubic growth of complete split graphs, the correct order of growth $\Theta(n^3)$ of the maximum, the correction of a natural but false conjecture that the star is the maximiser, documented exhaustive computations for $n \leq 10$, and a precisely stated conjecture for the remaining cases. The generalisation DCI_α, the bond-order-weighted variant BDCI and the normalised companion index NDCI are introduced to fix notation; BDCI in particular is presented here purely as a mathematical construction.

Contributions. The specific contributions of the paper are the following.

- **Reduction identity and sharp bounds.** We prove that DCI is a genuine irregularity measure (Proposition 1) and establish the exact reduction $\mathrm{DCI} = M_1 - 4\,\mathrm{ISI}$ (Theorem 1). This yields the sigma-sandwich $\sigma/(2\Delta) \leq \mathrm{DCI} \leq \sigma/(2\delta)$ (Theorem 2), which is strict for every non-regular graph but has asymptotically optimal constants, and the refined bounds $\sigma/(2\Delta - 1) \leq \mathrm{DCI} \leq \sigma/(2\delta + 1)$ (Theorem 3), which are attained, with a complete characterisation of the equality cases; we also give the exact value on biregular graphs.

- **Closed forms for fourteen graph families.** We derive explicit closed forms for the path, cycle, complete, cocktail-party, star, complete bipartite, complete tripartite, complete split, double star, friendship, wheel, pan, barbell and lollipop graphs (Table 1), each established by a dedicated propo-

sition, with every family indexed so that its order is stated explicitly (the wheel W_n and pan graph Pan_n both have exactly n vertices).

- **Growth and extremal analysis.** We show that the star, wheel and friendship graphs have DCI $\sim n^2$, whereas optimised complete split graphs satisfy the explicit estimate $c_* n^3 - \frac{3}{2} n^2 \le \max_k \mathrm{DCI}(\mathrm{CS}(n,k)) < c_* n^3$ (Proposition 12), and that the maximum of DCI over all connected graphs of order n is $\Theta(n^3)$ (Theorem 4). The star is the unique maximiser for $4 \le n \le 7$, $\mathrm{CS}(n,2)$ beats the star for every $n \ge 8$ (Propositions 13–14), and $\mathrm{CS}(n,2)$ is the unique maximiser for $8 \le n \le 10$; the computations behind these uniqueness statements are summarised in Table 2 and described in the Appendix. Global extremality of complete split graphs, and the value of the leading constant of $\mathrm{DCI}_{\max}(n)$, are *not* claimed; they are posed as Conjecture 1.

- **A normalised companion index.** We introduce the edge-averaged index NDCI and prove $\mathrm{NDCI}(G) \in [0,1)$, with equality to 0 exactly for regular graphs and with $\sup \mathrm{NDCI} = 1$ (Proposition 15); it replaces the star-based ratio, which exceeds 1 once $n \ge 8$.

Throughout, these results place DCI precisely within the irregularity-index literature: it is a fixed linear combination of the first Zagreb and inverse sum indeg indices, hence an interpretable, complementary heterogeneity descriptor rather than an independent new invariant.

Organisation. Section 2 collects preliminaries, Section 3 gives the definitions and Section 4 the basic properties and bounds. The closed forms for the fourteen families and their growth rates are collected in Section 5, and the extremal behaviour and the normalised index in Section 6, followed by concluding remarks. The Appendix describes the exhaustive computations.

2. Preliminaries

Throughout, every graph is finite, simple and connected. Given $G = (V, E)$, set $n = |V|$ (the *order*) and $m = |E|$, let $d(v)$ be the degree of a vertex v, and write $\Delta = \Delta(G)$ and $\delta = \delta(G)$ for the largest and smallest degrees. The degree-based invariants we shall need are

$$M_1(G) = \sum_{v \in V} d(v)^2 = \sum_{uv \in E} \big(d(u) + d(v)\big) \qquad \text{(first Zagreb)},$$

$$M_2(G) = \sum_{uv \in E} d(u) d(v) \qquad \text{(second Zagreb)},$$

$$F(G) = \sum_{v \in V} d(v)^3 \qquad \text{(forgotten) [13]},$$

$$\sigma(G) = \sum_{uv \in E} (d(u) - d(v))^2 = F(G) - 2M_2(G) \qquad \text{(sigma)},$$

$$\mathrm{irr}(G) = \sum_{uv \in E} |d(u) - d(v)| \qquad \text{(Albertson irregularity) [4]},$$

$$\mathrm{ISI}(G) = \sum_{uv \in E} \frac{d(u)d(v)}{d(u) + d(v)} \qquad \text{(inverse sum indeg)},$$

$$H(G) = \sum_{uv \in E} \frac{2}{d(u) + d(v)} \qquad \text{(harmonic) [12]}.$$

An edge uv is called *balanced* if $d(u) = d(v)$ and *unbalanced* otherwise. Let $\Delta > \delta$. We say that G is (Δ, δ)-*biregular* if every edge has one endpoint of degree Δ and the other of degree δ. In that case no two vertices of equal degree are adjacent, so G is necessarily bipartite with colour classes V_Δ and V_δ consisting of the vertices of degree Δ and δ respectively, and $\Delta|V_\Delta| = \delta|V_\delta| = m$; such graphs are also called semiregular bipartite graphs. We warn that some authors use "biregular" for any graph with exactly two distinct vertex degrees; that weaker notion (which allows balanced edges, e.g. in the complete split graphs) is *not* the one used here. The complete bipartite graphs $K_{a,b}$ with $a \neq b$ are the familiar examples.

3. The degree-contrast index and its generalisations

Definition 1. *For a graph G we define*

$$\mathrm{DCI}(G) = \sum_{uv \in E(G)} \frac{(d(u) - d(v))^2}{d(u) + d(v)},$$

$$\mathrm{DCI}_\alpha(G) = \sum_{uv \in E(G)} \frac{|d(u) - d(v)|^{2+\alpha}}{(d(u) + d(v))^{1+\alpha/2}}, \quad \alpha \geq 0.$$

For an edge-weighted molecular graph (G, w), *i.e. a hydrogen-suppressed molecular graph G together with a weight function $w : E(G) \to \{1, \frac{3}{2}, 2, 3\}$ recording the bond order of the chemical bond represented by each edge (*1 *single,* $\frac{3}{2}$ *aromatic,* 2 *double,* 3 *triple), we define the* bond-order-weighted degree-contrast index

$$\mathrm{BDCI}(G, w) = \sum_{uv \in E(G)} w(uv)\, \frac{(d(u) - d(v))^2}{d(u) + d(v)}.$$

Here $d(u)$ always denotes the graph degree of u in the simple graph G (the number of non-hydrogen neighbours), not its valence; the bond order enters only through the edge weight.

The exponents of DCI_α are chosen so that (a) $\mathrm{DCI}_0 = \mathrm{DCI}$; (b) each summand equals $t_{uv}^{1+\alpha/2}$, where $t_{uv} = (d(u) - d(v))^2/(d(u) + d(v))$ is the corresponding summand of DCI, so that increasing α amplifies large contrasts relative to small ones; and (c) the degree-sum weighting of DCI is retained. BDCI is an invariant of the weighted graph (G, w) rather than of G alone, and $\mathrm{BDCI}(G, \mathbf{1}) = \mathrm{DCI}(G)$ when all bonds are single ($w \equiv 1$).
The generalisations DCI_α and BDCI are introduced here for completeness and to fix notation. In particular, BDCI is presented in this paper purely as a mathematical construction on edge-weighted graphs: the choice of weights $1, \frac{3}{2}, 2, 3$ is a convention, and no claim is made here about its chemical or predictive meaning, which would require independent validation against experimental data. The structural theory below is developed for DCI. We record only the immediate comparison that follows from the definition: since $w(uv) \geq 1$ for every edge, $\mathrm{BDCI}(G, w) \geq \mathrm{DCI}(G)$, with equality if and only if every unbalanced edge carries weight 1.

4. Basic properties

Proposition 1 (Non-negativity and regularity)**.** *For every graph G, $\mathrm{DCI}(G) \geq 0$. If G is connected, then $\mathrm{DCI}(G) = 0$ if and only if G is regular. The same holds for DCI_α ($\alpha \geq 0$) and for* BDCI *with positive weights.*

Proof. Every term of (1) is a ratio with a non-negative numerator and strictly positive denominator, so the total is at least 0. For the total to vanish, $(d(u) - d(v))^2$ must be 0 on each edge, i.e. $d(u) = d(v)$ throughout E; in a connected graph this equalises all degrees, which is precisely regularity. The same argument applies verbatim to DCI_α, and, as each weight $w(uv)$ is positive, to BDCI.

Theorem 1 (Reduction identity)**.** *For every finite simple graph G,*

$$\mathrm{DCI}(G) = M_1(G) - 4\,\mathrm{ISI}(G). \tag{2}$$

Proof. Fix an edge uv. Then

$$\frac{(d(u) - d(v))^2}{d(u) + d(v)} = \frac{(d(u) + d(v))^2 - 4d(u)d(v)}{d(u) + d(v)} = (d(u) + d(v)) - \frac{4d(u)d(v)}{d(u) + d(v)}.$$

Adding these edge contributions and applying $\sum_{uv\in E}(d(u)+d(v)) = M_1(G)$ leaves $\mathrm{DCI}(G) = M_1(G) - 4\sum_{uv\in E} d(u)d(v)/(d(u)+d(v))$, which is exactly $M_1(G) - 4\,\mathrm{ISI}(G)$.

Relation (2) says that DCI is fully determined by M_1 and ISI and adds nothing they do not jointly encode; the compensating benefit is that the extensive literature on those two invariants transfers at once to DCI.

Theorem 2 (Sigma sandwich)**.** *Let G be a connected simple graph of order $n \geq 2$, with minimum degree δ (≥ 1) and maximum degree Δ. Then*

$$\frac{\sigma(G)}{2\Delta} \leq \mathrm{DCI}(G) \leq \frac{\sigma(G)}{2\delta} = \frac{F(G) - 2M_2(G)}{2\delta}. \tag{3}$$

If G is regular, all three members vanish and both inequalities hold with equality. If G is non-regular, both inequalities are strict. Moreover, if G is (Δ,δ)-biregular then $\mathrm{DCI}(G) = \sigma(G)/(\Delta+\delta)$ exactly, a value lying strictly between the two bounds.

Proof. Every edge satisfies $2\delta \leq d(u)+d(v) \leq 2\Delta$, so $(d(u)-d(v))^2/(2\Delta) \leq (d(u)-d(v))^2/(d(u)+d(v)) \leq (d(u)-d(v))^2/(2\delta)$; summing over $E(G)$ and substituting $\sigma = F - 2M_2$ produces (3). If G is regular, every edge is balanced and $\sigma(G) = \mathrm{DCI}(G) = 0$. If G is connected and non-regular, it has at least one unbalanced edge (otherwise the degree would be constant along every path), and on every unbalanced edge $2\delta < d(u)+d(v) < 2\Delta$ with a strictly positive numerator; hence both summed inequalities are strict. If G is (Δ,δ)-biregular, every edge has degree sum $\Delta+\delta$, whence $\mathrm{DCI}(G) = \frac{1}{\Delta+\delta}\sum_{uv}(d(u)-d(v))^2 = \sigma(G)/(\Delta+\delta)$, which lies strictly inside $\big(\sigma(G)/(2\Delta), \sigma(G)/(2\delta)\big)$ since $\Delta > \delta$ and $\sigma(G) > 0$.

Remark 1 (In what sense (3) is sharp)**.** *Since* (3) *is strict for every connected non-regular graph, its bounds are never attained and* (3) *is* not *sharp in the sense of equality. Its constants are nevertheless best possible asymptotically. For $p \geq 1$ the graph $K_{p,p+1}$ is $(p+1,p)$-biregular with $\sigma = p(p+1)$ and* $\mathrm{DCI} = p(p+1)/(2p+1)$*, so*

$$\frac{\mathrm{DCI}(K_{p,p+1})}{\sigma/(2\delta)} = \frac{2p}{2p+1} \longrightarrow 1, \qquad \frac{\mathrm{DCI}(K_{p,p+1})}{\sigma/(2\Delta)} = \frac{2p+2}{2p+1} \longrightarrow 1 \qquad (p\to\infty).$$

Hence neither factor $1/(2\delta)$ nor $1/(2\Delta)$ can be replaced by a smaller, respectively larger, constant multiple valid for all graphs. The following refinement is sharp in the strict sense.

Theorem 3 (Sharp sigma bounds)**.** *Let G be a connected simple graph of order $n \geq 2$, with minimum degree δ and maximum degree Δ. Then*

$$\frac{\sigma(G)}{2\Delta - 1} \leq \mathrm{DCI}(G) \leq \frac{\sigma(G)}{2\delta + 1}. \tag{4}$$

If G is regular, both inequalities hold with equality ($\sigma(G) = \mathrm{DCI}(G) = 0$). If G is non-regular, equality holds on the right if and only if every unbalanced edge of G joins a vertex of degree δ to a vertex of degree $\delta+1$, and equality holds on the left if and only if every unbalanced edge joins a vertex of degree $\Delta - 1$ to a vertex of degree Δ. In particular, both bounds are attained by $K_{p,p+1}$ for every $p \geq 1$, the upper bound by every path P_n ($n \geq 3$), and the lower bound by $K_n - e$ ($n \geq 3$).

Proof. Balanced edges contribute 0 to all three members of (4). On an unbalanced edge uv the degrees are two *distinct* integers in $[\delta, \Delta]$, so

$$2\delta + 1 \leq d(u) + d(v) \leq 2\Delta - 1,$$

and therefore $(d(u) - d(v))^2/(2\Delta - 1) \leq (d(u) - d(v))^2/(d(u) + d(v)) \leq (d(u) - d(v))^2/(2\delta + 1)$. Summing over all edges gives (4). If G is regular, all members vanish. If G is non-regular, the set of unbalanced edges is non-empty and each of them has a strictly positive numerator, so equality in a summed inequality holds if and only if the corresponding edgewise inequality is an equality on every unbalanced edge. On the right this means $d(u) + d(v) = 2\delta + 1$, and since both degrees are integers $\geq \delta$ this forces $\{d(u), d(v)\} = \{\delta, \delta + 1\}$; on the left it means $d(u) + d(v) = 2\Delta - 1$, which forces $\{d(u), d(v)\} = \{\Delta - 1, \Delta\}$. In $K_{p,p+1}$ every edge joins degrees $p = \delta$ and $p+1 = \Delta$; in P_n every unbalanced edge joins degrees $1 = \delta$ and 2; in $K_n - e$ every unbalanced edge joins degrees $n - 2 = \Delta - 1$ and $n - 1 = \Delta$.

Because $2\delta < 2\delta+1$ and $2\Delta-1 < 2\Delta$, Theorem 3 strictly improves Theorem 2 for every non-regular graph, which explains why (3) is never attained.

Corollary 1 (Order-only bounds)**.** *Let G be a connected simple graph of order $n \geq 3$. Then*

$$\frac{\sigma(G)}{2n - 3} \leq \mathrm{DCI}(G) \leq \frac{\sigma(G)}{3} = \frac{F(G) - 2M_2(G)}{3}.$$

If G is regular, both inequalities hold with equality (all members vanish). If G is non-regular, equality holds on the right if and only if every unbalanced edge joins a vertex of degree 1 to a vertex of degree 2 (this forces $\delta = 1$; examples are the paths P_n), and equality holds on the left if and only if every unbalanced edge joins a vertex of degree $n - 2$ to a vertex of degree $n - 1$ (this forces $\Delta = n - 1$; an example is $K_n - e$).

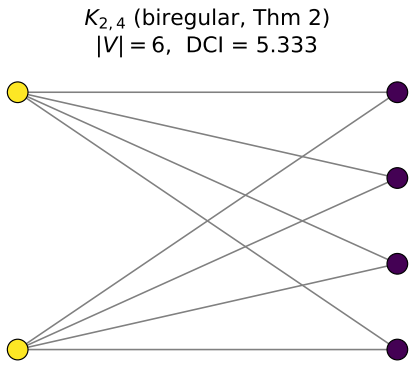


Figure 1: A biregular instance for Theorem 2: on $K_{2,4}$ every edge joins degrees $\Delta = 4$ and $\delta = 2$, so $\mathrm{DCI} = \sigma/(\Delta + \delta)$ exactly. Vertices are coloured by degree.

Proof. Since G is connected and $n \geq 3$, we have $1 \leq \delta \leq \Delta \leq n - 1$, so $2\delta + 1 \geq 3$ and $2\Delta - 1 \leq 2n - 3$, and the inequalities follow from (4); the last expression uses $\sigma = F - 2M_2$. If G is regular, all members vanish. Let G be non-regular, so $\sigma(G) > 0$. Equality on the right requires $\sigma(G)/(2\delta + 1) = \sigma(G)/3$, i.e. $\delta = 1$, together with equality on the right of (4); by Theorem 3 this means that every unbalanced edge has degree pair $\{1, 2\}$. Conversely, if every unbalanced edge has degree pair $\{1, 2\}$, then $\delta = 1$ (an unbalanced edge exists and has an endpoint of degree 1) and Theorem 3 gives equality. The left-hand case is identical, with $\Delta = n - 1$ and the degree pair $\{n - 2, n - 1\}$.

We shall also use the elementary comparison with Albertson's index. For an unbalanced edge, $|d(u) - d(v)| < d(u) + d(v)$ gives $(d(u) - d(v))^2/(d(u) + d(v)) < |d(u) - d(v)|$, whence

$$\mathrm{DCI}(G) \leq \mathrm{irr}(G), \tag{5}$$

with equality if and only if G is regular (both sides then being 0).

5. Closed forms for standard graph families

Using (1) directly (equivalently, Theorem 1) we obtain the closed forms in Table 1. To avoid any ambiguity, the table lists the order $|V(G)|$ of every family explicitly; in particular the wheel $W_n = C_{n-1} \vee K_1$ and the pan graph Pan_n are indexed so that they have exactly n vertices, and all figures comparing families plot DCI against the true order $n = |V(G)|$. Three qualitative points stand out: DCI vanishes on the regular families (Proposition 3); it is bounded on near-constant degree sequences ($\mathrm{DCI}(P_n) = \frac{2}{3}$ and $\mathrm{DCI}(\mathrm{Pan}_n) = \frac{7}{5}$, independent of n);

and on the high-contrast families it grows at two different rates. The star, the wheel and the friendship graph satisfy DCI $\sim n^2$ as $n \to \infty$, whereas complete split graphs whose clique contains a fixed proportion of the vertices grow *cubically* in n (Proposition 12, Figure 3). Figure 2 displays a representative instance of each of the fourteen families, with vertices coloured by degree so that the degree contrast measured by DCI is visible directly.

Table 1: Degree-contrast index of fourteen standard graph families. The column "Order" gives $|V(G)|$; the last column cites the proposition that establishes the closed form.

Family	Condition	Order $\lvert V(G)\rvert$	DCI(G)	Established in
Path P_n	$n \geq 3$	n	$\frac{2}{3}$	Prop. 4
Cycle C_n	$n \geq 3$	n	0	Prop. 3
Complete K_n	$n \geq 2$	n	0	Prop. 3
Cocktail party $K_{p\times 2}$	$p \geq 2$	$2p$	0	Prop. 3
Star $K_{1,n-1}$	$n \geq 2$	n	$\frac{(n-1)(n-2)^2}{n}$	Prop. 2
Complete bipartite $K_{a,b}$	$a, b \geq 1$	$a+b$	$\frac{ab(a-b)^2}{a+b}$	Prop. 5(b)
Complete tripartite $K_{a,b,c}$	$a, b, c \geq 1$	$a+b+c$	$\frac{ab(a-b)^2}{a+b+2c} + \frac{ac(a-c)^2}{a+2b+c} + \frac{bc(b-c)^2}{2a+b+c}$	Prop. 5(a)
Complete split CS(n,k)	$1 \leq k \leq n-1$	n	$\frac{k(n-k)(n-1-k)^2}{n-1+k}$	Prop. 2
Double star $S_{p,q}$	$p, q \geq 1$	$p+q+2$	$\frac{p^3}{p+2} + \frac{q^3}{q+2} + \frac{(p-q)^2}{p+q+2}$	Prop. 6
Friendship F_k	$k \geq 1$	$2k+1$	$\frac{4k(k-1)^2}{k+1}$	Prop. 7
Wheel $W_n = C_{n-1} \vee K_1$	$n \geq 4$	n	$\frac{(n-1)(n-4)^2}{n+2}$	Prop. 8
Pan Pan$_n$ (C_{n-1} + pendant)	$n \geq 4$	n	$\frac{7}{5}$	Prop. 9
Barbell B_n	$n \geq 2$	$2n$	$\frac{2(n-1)}{2n-1}$	Prop. 10
Lollipop $L_{n,k}$	$n \geq 3$, $k \geq 2$	$n+k$	$\frac{n-1}{2n-1} + \frac{(n-2)^2}{n+2} + \frac{1}{3}$	Prop. 11

Proposition 2 (Complete split, incl. star)**.** *For the complete split graph* $\mathrm{CS}(n,k) = K_k \vee \overline{K_{n-k}}$ *of order* n*,*

$$\mathrm{DCI}\big(\mathrm{CS}(n,k)\big) = \frac{k(n-k)(n-1-k)^2}{n-1+k}.$$

Proof. In $\mathrm{CS}(n,k)$ the k clique vertices have degree $n-1$ and the $n-k$ independent vertices have degree k. Edges inside the clique join two degree-$(n-1)$ vertices and add nothing. The $k(n-k)$ edges between the clique and the independent set each join a degree-$(n-1)$ vertex to a degree-k vertex, contributing $\big((n-1)-k\big)^2/\big((n-1)+k\big)$. Summing gives the stated value. (Setting $k=1$ recovers the star formula $(n-1)(n-2)^2/n$.)

Proposition 3 (Regular families)**.** $\mathrm{DCI}(C_n) = \mathrm{DCI}(K_n) = \mathrm{DCI}(K_{p\times 2}) = 0$.

Proof. Each graph is regular: C_n is 2-regular, K_n is $(n-1)$-regular, and $K_{p\times 2}$ (that is, K_{2p} with a perfect matching deleted, of order $2p$) is $(2p-2)$-regular. By Proposition 1 a connected graph has $\mathrm{DCI} = 0$ iff it is regular.

Proposition 4 (Path)**.** *For the path P_n with $n \geq 3$,* $\mathrm{DCI}(P_n) = \frac{2}{3}$*, independent of n.*

Proof. The two pendant vertices have degree 1 and all interior vertices degree 2. The two end edges join degrees $(1, 2)$, each contributing $1^2/3 = \frac{1}{3}$; every interior edge joins two degree-2 vertices and contributes 0. Hence $\mathrm{DCI}(P_n) = 2 \cdot \frac{1}{3} = \frac{2}{3}$.

Proposition 5 (Complete tripartite and complete bipartite graphs)**.** (a) *For integers $a, b, c \geq 1$,*

$$\mathrm{DCI}(K_{a,b,c}) = \frac{ab(a-b)^2}{a+b+2c} + \frac{ac(a-c)^2}{a+2b+c} + \frac{bc(b-c)^2}{2a+b+c}.$$

(b) *For integers $a, b \geq 1$,*

$$\mathrm{DCI}(K_{a,b}) = \frac{ab(a-b)^2}{a+b}.$$

Proof. (a) The three parts A, B, C of sizes a, b, c carry degrees $b + c$, $a + c$, $a + b$ respectively. An A–B edge joins degrees $b + c$ and $a + c$, contributing $(b-a)^2/(a+b+2c)$; there are ab such edges. Likewise the ac edges of class A–C each supply $(c-a)^2/(a+2b+c)$ and the bc edges of class B–C each contribute $(c-b)^2/(2a+b+c)$. Adding the contributions gives the claimed expression; for $a = b = c$ it gives the regular graph $K_{a,a,a}$ with $\mathrm{DCI} = 0$. (b) In $K_{a,b}$ the a vertices of one part have degree b and the b vertices of the other part have degree a. Each of the ab edges joins degrees b and a and contributes $(a-b)^2/(a+b)$, which gives the formula directly. (Part (b) is proved separately because it is not a specialisation of part (a): the value $c = 0$ lies outside the domain $a, b, c \geq 1$.)

Proposition 6 (Double star)**.** *For the double star $S_{p,q}$ (two adjacent centres of degree $p + 1$ and $q + 1$ carrying p and q leaves; order $p + q + 2$),* $\mathrm{DCI}(S_{p,q}) = \frac{p^3}{p+2} + \frac{q^3}{q+2} + \frac{(p-q)^2}{p+q+2}$.

Proof. The p leaves of the first centre give edges of degrees $(p + 1, 1)$, each contributing $p^2/(p + 2)$, for a total $p^3/(p + 2)$; symmetrically the second centre

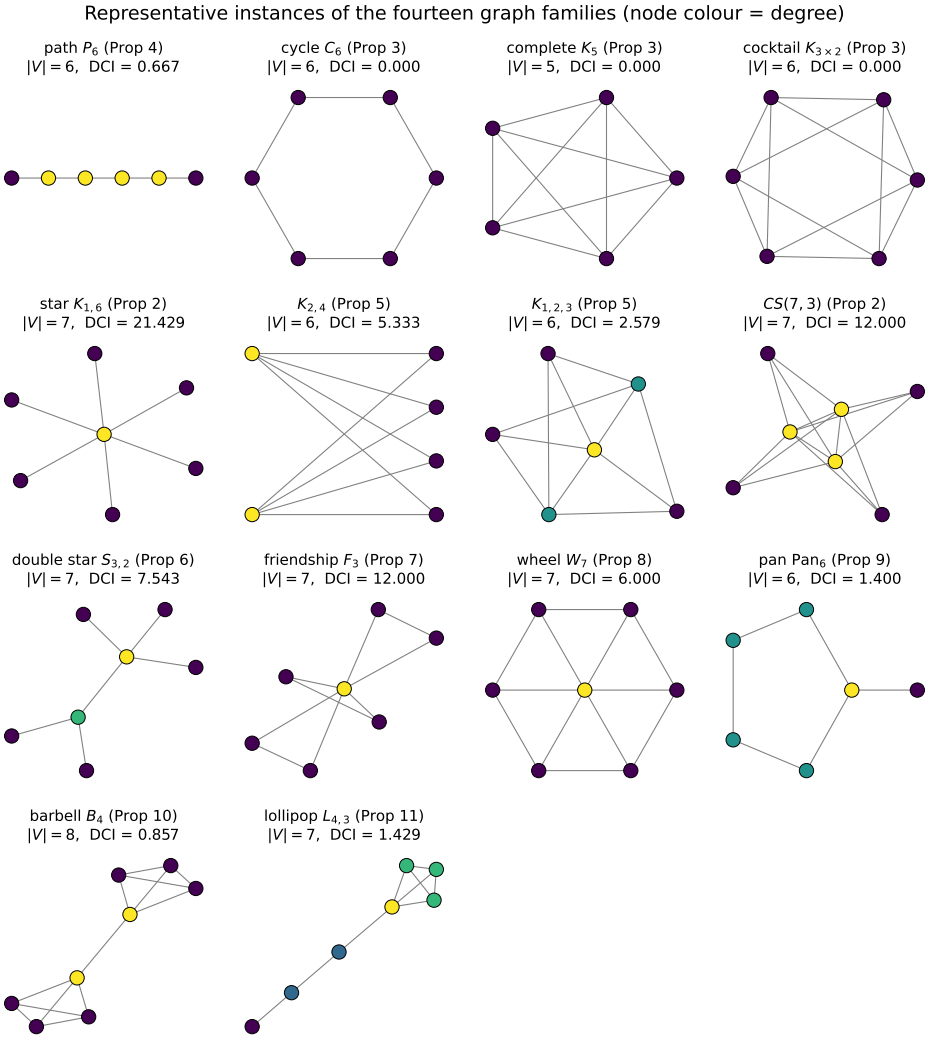


Figure 2: Representative instances of the fourteen graph families of Table 1, each labelled with the establishing proposition, its order $|V|$, and its degree-contrast index value; vertices are coloured by degree. In the order-consistent notation the wheel shown is W_7 (hub and 6 rim vertices) and the pan graph is Pan_6 (C_5 with one pendant vertex). The regular families (C_6, K_5, $K_{3\times 2}$) have $\mathrm{DCI} = 0$ (Proposition 3), while the high-contrast families (star, friendship, wheel, complete split) attain large values.

gives $q^3/(q+2)$. The single central edge joins degrees $p+1$ and $q+1$, contributing $(p-q)^2/(p+q+2)$. Adding the three terms gives the claim. (With $p=q=1$ this reduces to $\mathrm{DCI}(P_4)=\frac{2}{3}$, consistent with Proposition 4.)

Proposition 7 (Friendship graph)**.** *For the friendship graph F_k (k triangles sharing one common vertex, on $2k+1$ vertices),* $\mathrm{DCI}(F_k)=\frac{4k(k-1)^2}{k+1}$.

Proof. The central vertex has degree $2k$ and the $2k$ outer vertices have degree 2. The $2k$ spoke edges each join degrees $2k$ and 2, contributing $(2k-2)^2/(2k+2)=2(k-1)^2/(k+1)$; summed over the $2k$ spokes this is $4k(k-1)^2/(k+1)$. The k triangle edges join two degree-2 vertices and contribute 0. (For $k=1$, $F_1=K_3$ is regular and the value is 0.)

Proposition 8 (Wheel)**.** *For $n\geq 4$ let $W_n=C_{n-1}\vee K_1$ be the wheel of order n: a hub of degree $n-1$ joined to every vertex of a cycle C_{n-1}, whose vertices then have degree 3. Then*

$$\mathrm{DCI}(W_n)=\frac{(n-1)(n-4)^2}{n+2},\qquad n\geq 4.$$

Proof. The $n-1$ spoke edges join the degree-$(n-1)$ hub to a degree-3 rim vertex, each contributing $(n-4)^2/(n+2)$; the $n-1$ rim edges join two degree-3 vertices and make no contribution. Adding the spoke terms gives $(n-1)(n-4)^2/(n+2)$. (At $n=4$, $W_4=K_4$ is regular and the value is 0, matching the formula.)

Proposition 9 (Pan graph)**.** *For $n\geq 4$ let Pan_n be the pan graph of order n, obtained from the cycle C_{n-1} by attaching a single pendant vertex. Then* $\mathrm{DCI}(\mathrm{Pan}_n)=\frac{7}{5}$*, independent of n.*

Proof. The attachment vertex has degree 3; its two incident cycle edges join degrees $(3,2)$ and each contribute $1/5$. The remaining $n-3$ cycle edges join degree-2 vertices and contribute 0. The pendant edge joins degrees $(3,1)$ and contributes $2^2/4=1$. Thus $\mathrm{DCI}(\mathrm{Pan}_n)=2\cdot\frac{1}{5}+1=\frac{7}{5}$.

Proposition 10 (Barbell)**.** *For the barbell graph B_n (two disjoint copies of K_n joined by a single bridge edge; order $2n$),* $\mathrm{DCI}(B_n)=\frac{2(n-1)}{2n-1}$, $n\geq 2$.

Proof. Each bridge endpoint has degree n ($n-1$ clique neighbours and one bridge neighbour); all other vertices have degree $n-1$. Inside one clique, the $n-1$ edges from the bridge endpoint join degrees $(n,n-1)$ and each contribute

$1/(2n-1)$, giving $(n-1)/(2n-1)$ per clique; the remaining clique edges and the bridge edge contribute 0. Summing over the two cliques gives $2(n-1)/(2n-1)$. (Note $\mathrm{DCI}(B_n) \to 1$ as $n \to \infty$.)

Proposition 11 (Lollipop)**.** *For the lollipop graph $L_{n,k}$ (K_n with a path on $k \geq 2$ new vertices attached to one clique vertex; order $n+k$),* $\mathrm{DCI}(L_{n,k}) = \frac{n-1}{2n-1} + \frac{(n-2)^2}{n+2} + \frac{1}{3}$, *$n \geq 3$, independent of the path length k.*

Proof. The junction (the clique vertex carrying the path) has degree n; the other clique vertices have degree $n-1$, the path-interior vertices degree 2, and the path end vertex degree 1. Inside the clique, the $n-1$ edges from the junction join degrees $(n, n-1)$ and contribute $(n-1)/(2n-1)$ in total, while the remaining clique edges contribute 0. The junction-to-path edge joins degrees $(n, 2)$ and contributes $(n-2)^2/(n+2)$. Every interior path edge joins two degree-2 vertices and contributes 0; the final path edge joins degrees $(2, 1)$ and contributes $1/3$. Summing gives the stated value, which does not depend on k. (For $k = 1$, a single pendant on K_n, the last two terms are replaced by the single term $(n-1)^2/(n+1)$.)

Remark 2. *Every closed form in Table 1 can also be obtained from the reduction identity* $\mathrm{DCI} = M_1 - 4\,\mathrm{ISI}$ *together with published values of M_1 and the inverse sum indeg index for these families.*

Growth rates: quadratic versus cubic

For the three single-hub families the closed forms give, as $n = |V(G)| \to \infty$,

$$\mathrm{DCI}(K_{1,n-1}) = \frac{(n-1)(n-2)^2}{n} \sim n^2, \qquad \mathrm{DCI}(W_n) = \frac{(n-1)(n-4)^2}{n+2} \sim n^2,$$
$$\mathrm{DCI}\big(F_{(n-1)/2}\big) = \frac{(n-1)(n-3)^2}{n+1} \sim n^2, \tag{6}$$

the last for odd n, so these families grow quadratically. Complete split graphs behave differently.

Proposition 12 (Cubic growth of complete split graphs)**.** *Let $g(c) = c(1-c)^3/(1+c)$ for $c \in [0, 1]$, and put*

$$\gamma = \frac{\sqrt{7}-2}{3} \approx 0.2153, \qquad c_* = g(\gamma) = \frac{632 - 238\sqrt{7}}{27} \approx 0.0856.$$

(a) (Uniform estimate.) *For every $n \geq 2$ and every $1 \leq k \leq n-1$,*

$$g\Big(\frac{k}{n}\Big) - \frac{1}{n} \;\leq\; \frac{\mathrm{DCI}(\mathrm{CS}(n,k))}{n^3} \;<\; g\Big(\frac{k}{n}\Big). \tag{7}$$

In particular, if $k = k(n)$ satisfies $k/n \to c \in (0,1)$, then $\mathrm{DCI}(\mathrm{CS}(n,k)) = g(c)\, n^3\,(1 + o(1))$.

(b) γ is the unique maximiser of g on $[0,1]$, and for every $n \geq 3$

$$c_*\, n^3 - \tfrac{3}{2}\, n^2 \;\leq\; \max_{1 \leq k \leq n-1} \mathrm{DCI}\big(\mathrm{CS}(n,k)\big) \;<\; c_*\, n^3. \tag{8}$$

(c) Every maximising clique size $k^*(n)$ satisfies $g(k^*(n)/n) \geq c_* - \frac{3}{2n}$; consequently $k^*(n)/n \to \gamma$.

Proof. Step 1 (exact rescaled formula). By Proposition 2, writing $x = k/n \in [\frac{1}{n}, 1 - \frac{1}{n}]$ and $t = \frac{1}{n}$,

$$H_n(k) := \frac{\mathrm{DCI}(\mathrm{CS}(n,k))}{n^3} = \frac{k(n-k)(n-1-k)^2}{n^3(n-1+k)} = x(1-x)\,\psi_x(t),$$
$$\psi_x(s) := \frac{(1-x-s)^2}{1+x-s},$$

while $g(x) = x(1-x)\,\psi_x(0)$.

Step 2 (derivative of ψ_x). For $0 \leq s \leq t$ we have $0 \leq 1-x-s \leq 1$ (because $x \leq 1 - \frac{1}{n}$) and $1 \leq 1+x-s \leq 2$ (because $x \geq \frac{1}{n}$). Differentiation gives

$$\psi_x'(s) = \frac{(1-x-s)\big[-2(1+x-s) + (1-x-s)\big]}{(1+x-s)^2} = -\frac{(1-x-s)(1+3x-s)}{(1+x-s)^2}.$$

Since $1 + 3x - s > 0$, we get $\psi_x'(s) \leq 0$, with strict inequality for $0 \leq s < 1 - x$ (a non-trivial interval because $1 - x \geq t > 0$); and $|\psi_x'(s)| \leq 1 \cdot (1+3x)/1 \leq 4$.

Step 3 (proof of (7)). By Step 2, ψ_x is strictly decreasing on $[0,t]$, so $\psi_x(t) < \psi_x(0)$ and $H_n(k) < g(x)$. By the mean value theorem, $\psi_x(0) - \psi_x(t) \leq 4t$, and with $x(1-x) \leq \frac{1}{4}$ we obtain $g(x) - H_n(k) \leq \frac{1}{4} \cdot 4t = \frac{1}{n}$. This proves (7), uniformly in k. The asymptotic statement follows because g is continuous.

Step 4 (maximiser of g). For $c \in (0,1)$ we have $g(c) > 0$ and

$$\frac{g'(c)}{g(c)} = \frac{1}{c} - \frac{3}{1-c} - \frac{1}{1+c} = \frac{1 - 4c - 3c^2}{c(1-c)(1+c)},$$
$$\text{i.e.} \qquad g'(c) = \frac{(1-c)^2(1-4c-3c^2)}{(1+c)^2}.$$

The quadratic $1 - 4c - 3c^2$ is positive on $[0,\gamma)$ and negative on $(\gamma,1]$, where $\gamma = (-4 + \sqrt{28})/6 = (\sqrt{7} - 2)/3$ is its only root in $[0,1]$. Hence g increases on

$[0,\gamma]$, decreases on $[\gamma,1]$, and γ is its unique maximiser. With $1-\gamma=(5-\sqrt{7})/3$ and $1+\gamma=(1+\sqrt{7})/3$,

$$c_* = g(\gamma) = \frac{(\sqrt{7}-2)(5-\sqrt{7})^3}{27(1+\sqrt{7})} = \frac{(\sqrt{7}-2)(230-82\sqrt{7})}{27(1+\sqrt{7})}$$
$$= \frac{394\sqrt{7}-1034}{27(1+\sqrt{7})} = \frac{632-238\sqrt{7}}{27}.$$

We also need the Lipschitz bound $|g'(c)|\le 1$ on $[0,1]$. On $[0,\gamma]$, $0\le g'(c)\le (1-c)^2/(1+c)^2\le 1$. On $[\gamma,1]$, $|g'(c)|=(1-c)^2(3c^2+4c-1)/(1+c)^2\le (1-c)(3c^2+4c-1)/(1+c)^2$, and $(1+c)^2-(1-c)(3c^2+4c-1)=3c^3+2c^2-3c+2\ge 2c^2-3c+2>0$ (the last quadratic has negative discriminant), so again $|g'(c)|<1$.

Step 5 (proof of (8)*).* The upper bound follows from (7) and $g\le c_*$: $H_n(k)<g(k/n)\le c_*$ for every k. For the lower bound let k_n be the integer nearest to γn. For $n\ge 3$ we have $\gamma n\ge 0.64$, so $1\le k_n\le n-1$, and $|k_n/n-\gamma|\le \frac{1}{2n}$. By $|g'|\le 1$ and (7),

$$\max_k H_n(k)\ge H_n(k_n)\ge g(k_n/n)-\frac{1}{n}\ge c_*-\frac{1}{2n}-\frac{1}{n}=c_*-\frac{3}{2n}.$$

Multiplying by n^3 gives (8).

Step 6 (proof of (c)). If $k^*(n)$ maximises H_n, then by (7) and Step 5, $g(k^*(n)/n) > H_n(k^*(n))\ge c_*-\frac{3}{2n}$. Let c be any limit point of $k^*(n)/n$ in the compact interval $[0,1]$; by continuity $g(c)\ge c_*$, so $c=\gamma$ by uniqueness of the maximiser. Hence $k^*(n)/n\to\gamma$.

Thus the optimised complete split family has *cubic*, not quadratic, growth; the numerically optimal clique sizes $k^*(n)=1,2,3,4,5,6$ for $n\le 7$, $8\le n\le 12$, $13\le n\le 16$, $17\le n\le 21$, $22\le n\le 26$ and $27\le n\le 30$ respectively are consistent with $k^*(n)\approx 0.2153\,n$. By comparison, the maximum of Albertson's index is attained by complete split graphs with clique fraction $1/3$ [1]; the degree-sum weighting in DCI shifts the optimum towards smaller cliques.

6. Extremal behaviour and normalisation

Since $\mathrm{DCI}(G)=0$ characterises regular graphs (the minimisers), the natural extremal question is the maximiser over all connected graphs of order n. The star is a tempting candidate, and indeed:

Proposition 13 (Small orders)**.** *For $4\le n\le 7$, the star $K_{1,n-1}$ is the unique connected graph of order n maximising* DCI.

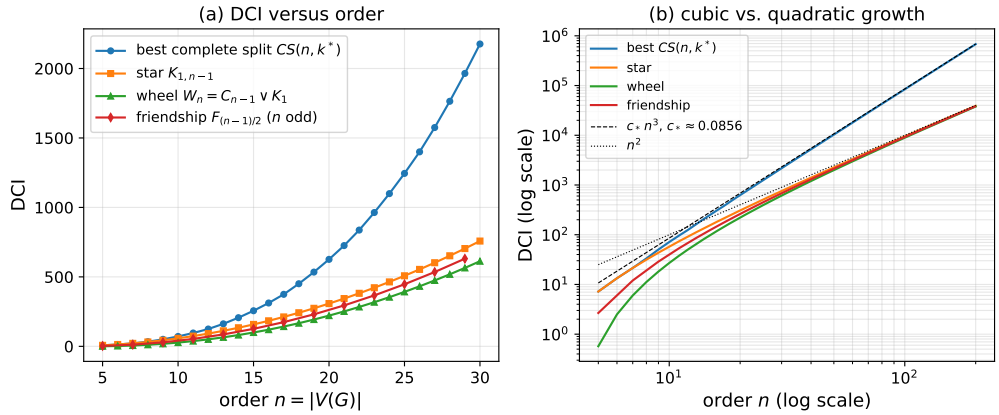


Figure 3: DCI as a function of the order $n = |V(G)|$ for four high-contrast families: the star $K_{1,n-1}$, the wheel $W_n = C_{n-1} \vee K_1$ (order n), the friendship graph $F_{(n-1)/2}$ (odd n only), and the best complete split graph $\mathrm{CS}(n, k^*)$. (a) Linear scale. (b) Log–log scale up to $n = 200$: the star, wheel and friendship graphs grow quadratically ($\sim n^2$), while the optimised complete split graph grows cubically, $\sim c_* n^3$ with $c_* \approx 0.0856$ (Proposition 12).

Proof (computer-assisted). For each $n \in \{4, 5, 6, 7\}$ all non-isomorphic connected graphs of order n were generated with the program `geng` of the `nauty` package [21], version 2.8.8, using the command `geng -c` n; `geng` outputs every isomorphism class exactly once, so the enumeration is exhaustive and free of duplicates. For each graph, DCI was evaluated in *exact* rational arithmetic (Algorithm 1 in the Appendix), and the maximum and the number of isomorphism classes attaining it were recorded. The numbers of connected graphs are 6, 21, 112 and 853, in agreement with the known counts [26]. In each case exactly one isomorphism class attains the maximum, namely the star, with $\mathrm{DCI}(K_{1,n-1}) = (n-1)(n-2)^2/n = 3,\ \frac{36}{5},\ \frac{40}{3},\ \frac{150}{7}$; the second-largest values are $\frac{7}{5},\ \frac{74}{15},\ \frac{74}{7},\ 20$, respectively (Table 2). For these orders the result was confirmed independently of `nauty` on the atlas of all graphs with at most seven vertices [25]. □

Proposition 14 (Failure for $n \geq 8$)**.** *For every $n \geq 8$ there is a connected graph of order n with strictly larger* DCI *than the star. In particular,* $\mathrm{CS}(n, 2)$ *satisfies*

$$\mathrm{DCI}\big(\mathrm{CS}(n,2)\big) = \frac{2(n-2)(n-3)^2}{n+1} > \frac{(n-1)(n-2)^2}{n} = \mathrm{DCI}\big(K_{1,n-1}\big) \quad (n \geq 8).$$

For instance $\mathrm{DCI}(\mathrm{CS}(8,2)) = \frac{100}{3} \approx 33.3 > 31.5 = \mathrm{DCI}(K_{1,7})$.

Proof. Both closed forms are instances of Proposition 2 ($k = 2$ and $k = 1$). Since $n - 2 > 0$ for $n \geq 3$, dividing the desired inequality by $n - 2$ and clearing

the positive denominators $n(n+1)$ shows it is equivalent to

$$2n(n-3)^2 > (n-1)(n-2)(n+1), \quad \text{i.e.} \quad f(n) := n^3 - 10n^2 + 19n - 2 > 0.$$

The derivative $f'(n) = 3n^2 - 20n + 19$ has larger root $(10+\sqrt{43})/3 \approx 5.52 < 8$, so f is strictly increasing on $[8, \infty)$; and $f(8) = 512 - 640 + 152 - 2 = 22 > 0$. Hence $f(n) \geq f(8) > 0$ for every real $n \geq 8$, proving the inequality for all integers $n \geq 8$. (At $n = 7$, $f(7) = -16 < 0$: the star is still extremal there, consistent with Proposition 13.)

Proposition 14 shows only that the star is not extremal for $n \geq 8$; it does *not* show that complete split graphs are extremal among all connected graphs. What can be proved for all n is the correct order of magnitude of the maximum.

Theorem 4 (Order of magnitude of the maximum)**.** *Let* $\mathrm{DCI}_{\max}(n)$ *denote the maximum of* DCI *over all connected graphs of order* n*. Then, for every* $n \geq 3$*,*

$$c_*\, n^3 - \tfrac{3}{2}\, n^2 \;\leq\; \mathrm{DCI}_{\max}(n) \;<\; \left\lfloor \frac{n}{3} \right\rfloor \left\lceil \frac{2n}{3} \right\rceil \left(\left\lceil \frac{2n}{3} \right\rceil - 1 \right) \;\leq\; \frac{4n^3}{27},$$

with $c_* = (632 - 238\sqrt{7})/27 \approx 0.0856$*. In particular* $\mathrm{DCI}_{\max}(n) = \Theta(n^3)$*,*

$$0.0856 \approx c_* \;\leq\; \liminf_{n\to\infty} \frac{\mathrm{DCI}_{\max}(n)}{n^3} \;\leq\; \limsup_{n\to\infty} \frac{\mathrm{DCI}_{\max}(n)}{n^3} \;\leq\; \frac{4}{27} \approx 0.148,$$

and no family with $\mathrm{DCI} = O(n^2)$ *(such as stars, wheels or friendship graphs) is extremal for large* n*.*

Proof. The lower bound follows from Proposition 12(b), since complete split graphs are connected. For the upper bound, a maximising graph is non-regular for $n \geq 3$ (the star already has positive DCI), so by (5) $\mathrm{DCI}(G) < \mathrm{irr}(G)$, and Abdo, Cohen and Dimitrov [1] proved $\mathrm{irr}(G) \leq \lfloor n/3 \rfloor \lceil 2n/3 \rceil (\lceil 2n/3 \rceil - 1)$ for every graph of order n; this quantity is at most $4n^3/27$ (Albertson's bound [4]).

Remark 3 (What is proved and what is not)**.** *Theorem 4 determines the* order *of* $\mathrm{DCI}_{\max}(n)$ *but not its leading constant: it does not prove that* $\mathrm{DCI}_{\max}(n)/n^3 \to c_*$*, nor that complete split graphs are maximisers. Both statements would follow from Conjecture 1 below (via Proposition 12(b)), and both remain open.*

Exhaustive computations for $n = 8, 9, 10$**.** We extended the computation in the proof of Proposition 13, with exactly the same protocol (generator `geng -c` n of `nauty` 2.8.8 and exact arithmetic; see the Appendix), to the orders $n = 8, 9, 10$. The results are listed in Table 2. Among all 11 117, 261 080 and 11 716 571

connected graphs of these orders (the known counts [26]), the maximum of DCI is attained by exactly one isomorphism class, which in each case is $\mathrm{CS}(n,2)$, with $\mathrm{DCI}_{\max}(8)=\frac{100}{3}$, $\mathrm{DCI}_{\max}(9)=\frac{252}{5}$ and $\mathrm{DCI}_{\max}(10)=\frac{784}{11}$. This is a statement about a finite, completely enumerated set of graphs and is *not* inferred from the family values; the family curves in Figure 4 serve only as a comparison. Among the three plotted families the complete split graph is the largest for every $n \geq 8$, and it coincides with the exhaustive maximum for all $n \leq 10$. Whether this persists for larger n is open, and we state it separately as a conjecture.

Problem 1. *Determine the connected graph(s) of order n maximising* DCI*, and the value* $\mathrm{DCI}_{\max}(n)$*.*

Conjecture 1. *For every $n \geq 8$,*

$$\mathrm{DCI}_{\max}(n) = \max_{1\leq k\leq n-1} \mathrm{DCI}\big(\mathrm{CS}(n,k)\big),$$

and every connected graph of order n attaining $\mathrm{DCI}_{\max}(n)$ *is isomorphic to a complete split graph* $\mathrm{CS}(n,k^*(n))$ *with a maximising clique size $k^*(n)$.*

If Conjecture 1 holds, Proposition 12 gives $c_*n^3-\frac{3}{2}n^2 \leq \mathrm{DCI}_{\max}(n) < c_*n^3$, hence $\mathrm{DCI}_{\max}(n)/n^3 \to c_*$ and $k^*(n)/n \to (\sqrt{7}-2)/3$; these consequences are conditional and are not used elsewhere in the paper. The evidence for Conjecture 1 is (i) the exhaustive computations for $n \leq 10$ (Table 2); (ii) the analogous theorem for Albertson's irregularity, whose maximisers over all graphs of order n are exactly complete split graphs [1]; and (iii) the closely related complementary second Zagreb index $cM_2(G)=\sum_{uv}|d(u)^2-d(v)^2| = \sum_{uv}|d(u)-d(v)|\,(d(u)+d(v))$, for which Furtula and Oz [14] conjectured that the maximisers over all graphs of order n are complete split graphs, a conjecture since proved by Gao [15]. We emphasise that, apart from these computations and Theorem 4, Conjecture 1 is unproved; in particular the statements of this section concerning complete split graphs refer to comparisons among explicit families or to the completely enumerated orders $n \leq 10$, not to global extremality.

A normalised companion index. A ratio of the form $\mathrm{DCI}(G)/\big((n-1)(n-2)^2/n\big)$—dividing by the star value—does not take values in $[0,1]$, because by Proposition 14 the star is not the maximiser for $n \geq 8$; the ratio exceeds 1 for such n and, by Proposition 12, is even unbounded as $n \to \infty$. Dividing by $\mathrm{DCI}_{\max}(n)$ is not an option either, since this quantity is unknown (Problem 1). We therefore do not rescale DCI itself but introduce the edge-averaged companion index

$$\mathrm{NDCI}(G) = \frac{1}{m}\sum_{uv\in E(G)} \frac{(d(u)-d(v))^2}{(d(u)+d(v))^2}, \tag{9}$$

Table 2: Exhaustive maximisation of DCI over all connected graphs of order n, computed in exact arithmetic (see the Appendix). "Graphs" is the number of non-isomorphic connected graphs produced by `geng -c n`; "#max" is the number of isomorphism classes attaining the maximum.

n	Graphs	$\mathrm{DCI}_{\max}(n)$	#max	Unique maximiser	Second-largest value
4	6	3	1	$K_{1,3} = \mathrm{CS}(4,1)$	$7/5$
5	21	$36/5$	1	$K_{1,4} = \mathrm{CS}(5,1)$	$74/15$
6	112	$40/3$	1	$K_{1,5} = \mathrm{CS}(6,1)$	$74/7$
7	853	$150/7$	1	$K_{1,6} = \mathrm{CS}(7,1)$	20
8	11 117	$100/3$	1	$\mathrm{CS}(8,2)$	$63/2$ (star $K_{1,7}$)
9	261 080	$252/5$	1	$\mathrm{CS}(9,2)$	$496/11$
10	11 716 571	$784/11$	1	$\mathrm{CS}(10,2)$	$720/11$

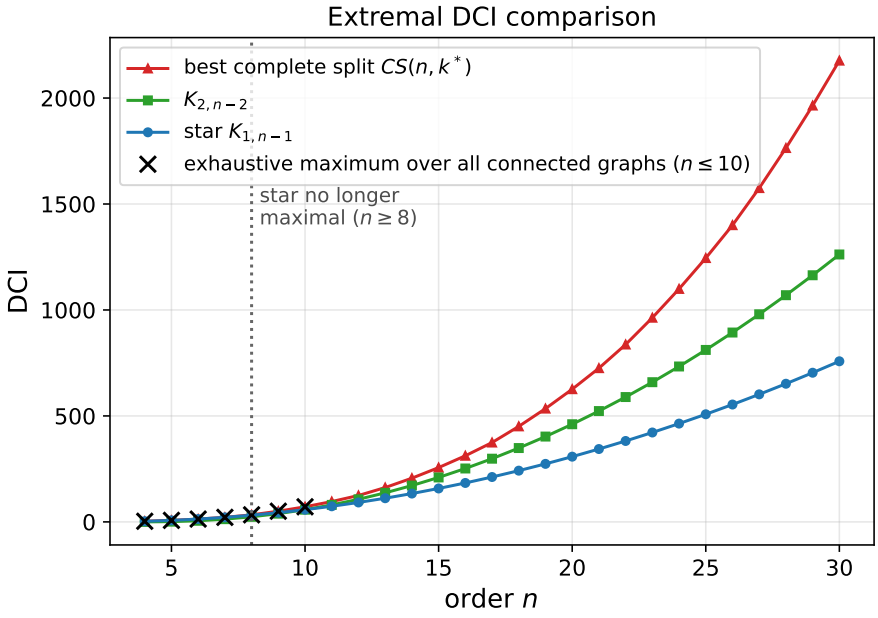


Figure 4: Maximum DCI attained by the star $K_{1,n-1}$, by $K_{2,n-2}$, and by the best complete split graph $\mathrm{CS}(n,k^*)$, as a function of the order n. Crosses mark the exhaustive maximum over all connected graphs of order $n \le 10$. The star is overtaken at $n = 8$ (Proposition 14); global extremality of complete split graphs for $n > 10$ is conjectural (Conjecture 1).

obtained by averaging over the edges the squared relative contrast $\big((d(u) - d(v))/(d(u) + d(v))\big)^2$; equivalently, it is the edge-average of $t_{uv}/(d(u) + d(v))$, where t_{uv} is the summand of DCI. It is an irregularity measure in its own right (not a scalar multiple of DCI) and is provably well behaved.

Proposition 15. *For every graph G with at least one edge,* $\mathrm{NDCI}(G) \in [0, 1)$*, and, for connected G,* $\mathrm{NDCI}(G) = 0$ *iff G is regular. The interval is best possible:* $\sup_G \mathrm{NDCI}(G) = 1$*, approached by the stars,* $\mathrm{NDCI}(K_{1,n-1}) = \big((n-2)/n\big)^2 \to 1$.

Proof. For any edge, $0 \le (d(u) - d(v))^2 < (d(u) + d(v))^2$ (strict because $d(u), d(v) \ge 1$ implies $4d(u)d(v) > 0$), so each summand lies in $[0, 1)$; their average lies in $[0, 1)$. It is 0 iff every summand is 0, i.e. iff all edges are balanced, which for connected G means that G is regular. In $K_{1,n-1}$ every edge joins degrees $n - 1$ and 1, giving the stated value.

Representative values: $\mathrm{NDCI}(K_{1,9}) = 0.64$, $\mathrm{NDCI}(K_{2,8}) = 0.36$, $\mathrm{NDCI}(C_n) = 0$; for $n = 20$, $\mathrm{NDCI}(K_{1,19}) = 0.81$ and $\mathrm{NDCI}(K_{2,18}) = 0.64$.

7. Conclusion

We studied the degree-contrast index DCI, a degree-sum-weighted irregularity measure. By the exact identity $\mathrm{DCI} = M_1 - 4\,\mathrm{ISI}$ it is a derived descriptor, a fixed linear combination of the first Zagreb and inverse sum indeg indices, and not an algebraically independent invariant; the contribution of the paper is the body of results established for it. On the inequality side, we proved the strict sigma-sandwich $\sigma/(2\Delta) \le \mathrm{DCI} \le \sigma/(2\delta)$ with asymptotically optimal constants, the sharp bounds $\sigma/(2\Delta - 1) \le \mathrm{DCI} \le \sigma/(2\delta + 1)$ and their order-only consequences, with all equality cases characterised and the regular and non-regular cases separated. We derived closed forms, indexed by the true order, for fourteen standard graph families, each established by an explicit proposition (Table 1). On the extremal side we corrected a natural but false maximiser conjecture—the star is extremal only for $n \le 7$ and is beaten by $\mathrm{CS}(n, 2)$ for every $n \ge 8$—proved the explicit estimate $c_* n^3 - \frac{3}{2}n^2 \le \max_k \mathrm{DCI}(\mathrm{CS}(n, k)) < c_* n^3$, showed that stars, wheels and friendship graphs grow only quadratically, proved that $\mathrm{DCI}_{\max}(n) = \Theta(n^3)$, and verified by a fully documented exhaustive enumeration in exact arithmetic that the maximiser is unique for $4 \le n \le 10$ (the star for $n \le 7$ and $\mathrm{CS}(n, 2)$ for $8 \le n \le 10$). Whether complete split graphs are the maximisers for all $n \ge 8$, and hence whether c_* is the true leading constant of $\mathrm{DCI}_{\max}(n)$, remains open (Conjecture 1); settling it, together with the optimal clique size $k^*(n)$, is the most promising direction for further work. Finally, we supplied a companion index NDCI with values in $[0, 1)$, the interval being

best possible. The bond-order-weighted variant BDCI was introduced only as a mathematical construction; assessing its chemical usefulness requires a separate validation against experimental data.

References

[1] Abdo, H., Cohen, N., & Dimitrov, D. (2014). Graphs with maximal irregularity. *Filomat, 28*(7), 1315–1322.

[2] Abdo, H., Dimitrov, D., & Gutman, I. (2018). Graphs with maximal σ irregularity. *Discrete Applied Mathematics, 250*, 57–64.

[3] Abdo, H., Dimitrov, D., & Gutman, I. (2019). Graph irregularity and its measures. *Applied Mathematics and Computation, 357*, 317–324.

[4] Albertson, M. O. (1997). The irregularity of a graph. *Ars Combinatoria, 46*, 219–225.

[5] Ali, A., Albalahi, A. M., Alanazi, A. M., Bhatti, A. A., & Hamza, A. E. (2023). On the maximum sigma index of k-cyclic graphs. *Discrete Applied Mathematics, 325*, 58–62.

[6] Ali, A., Dimitrov, D., Réti, T., Albalahi, A. M., & Hamza, A. E. (2025). Bounds and optimal results for the total irregularity measure. *MATCH Communications in Mathematical and in Computer Chemistry, 94*, 5–29.

[7] Annasagaram, G., & G. P. L. (2027). Rainbow dynamic coloring in fan and star-fan graphs. *Journal of Contemporary Applied Mathematics, 17*(1), 133–142. https://doi.org/10.62476/jcam171.8

[8] Chen, X., & Liu, X. (2026). The reciprocal irregularity of a graph. *Discrete Applied Mathematics, 378*, 348–357.

[9] Deng, H., Balachandran, S., Elumalai, S., & Venkatesh, S. G. (2024). Bounds on inverse sum indeg index of graph operations. *Ars Combinatoria, 163*.

[10] Dimitrov, D., & Stevanović, D. (2023). On the σ_t-irregularity and the inverse irregularity problem. *Applied Mathematics and Computation, 441*, Article 127709.

[11] Dimitrov, D., Gao, W., Lin, W., & Chen, J. (2023). Extremal trees with fixed degree sequence for σ-irregularity. *Discrete Mathematics Letters, 12*, 166–172.

[12] Fajtlowicz, S. (1987). On conjectures of Graffiti—II. *Congressus Numerantium, 60*, 187–197.

[13] Furtula, B., & Gutman, I. (2015). A forgotten topological index. *Journal of Mathematical Chemistry, 53*, 1184–1190.

[14] Furtula, B., & Oz, M. S. (2025). Complementary topological indices. *MATCH Communications in Mathematical and in Computer Chemistry, 93*(1), 247–263. https://doi.org/10.46793/match.93-1.247F

[15] Gao, H. (2025). *Extremal graphs with maximum complementary second Zagreb index* [Preprint]. arXiv. https://arxiv.org/abs/2503.01343

[16] Gutman, I., Togan, M., Yurttas, A., Cevik, A. S., & Cangul, I. N. (2018). Inverse problem for sigma index. *MATCH Communications in Mathematical and in Computer Chemistry, 79*, 491–508.

[17] Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals: Total π-electron energy of alternant hydrocarbons. *Chemical Physics Letters, 17*, 535–538.

[18] Jamal, F., & Imran, M. (2024). Bounds on Sombor index and inverse sum indeg (ISI) index of graph operations. *Communications in Combinatorics and Optimization, 9*(4), 785–798.

[19] Kovijanić Vukićević, Z., Popivoda, G., Vujošević, S., Škrekovski, R., & Dimitrov, D. (2024). The σ-irregularity of chemical trees. *MATCH Communications in Mathematical and in Computer Chemistry, 91*, 267–282.

[20] Lin, Z., Zhou, T., Wang, X., & Miao, L. (2022). The general Albertson irregularity index of graphs. *AIMS Mathematics, 7*(1), 25–38.

[21] McKay, B. D., & Piperno, A. (2014). Practical graph isomorphism, II. *Journal of Symbolic Computation, 60*, 94–112.

[22] Molina, E. D., Bosch, P., Sigarreta, J. M., & Tourís, E. (2023). On the variable inverse sum deg index. *Mathematical Biosciences and Engineering, 20*(5), 8800–8813.

[23] Mythili, V., Shenbaga Devi, S., Arthi, P., & Dhanalakshmi, S. (2026). Predicting dual-target antibacterial activity and SARS-CoV-2 docking affinity of pendant-armed copper(II) metallodrugs: A neighborhood topological and graph entropy approach. *Natural Resources for Human Health, 6*(7s), 517–529.

[24] Randić, M. (1975). Characterization of molecular branching. *Journal of the American Chemical Society, 97*, 6609–6615.

[25] Read, R. C., & Wilson, R. J. (1998). *An atlas of graphs*. Oxford University Press.

[26] Sloane, N. J. A. (Ed.). (n.d.). Number of connected graphs with n nodes (Sequence A001349). In *The On-Line Encyclopedia of Integer Sequences*. https://oeis.org/A001349

[27] Vukičević, D., & Gašperov, M. (2010). Bond additive modeling 1: Adriatic indices. *Croatica Chemica Acta, 83*, 243–260.

[28] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of the American Chemical Society, 69*, 17–20.

[29] Wu, Y., Hong, C., Fu, P., & Lin, W. (2025). Large trees with maximal inverse sum indeg index have no vertices of degree 2 or 3. *Discrete Applied Mathematics, 360*, 131–138.

[30] Zhang, Q., Zaman, S., Ullah, A., Ali, P., & Mahmoud, E. E. (2025). The sharp lower bound of tricyclic graphs with respect to the ISI index. *The European Physical Journal E, 48*(2–3).

Appendix: Computational protocol for the exhaustive searches

Generation. For each order $n = 4, \dots, 10$ all non-isomorphic connected graphs were generated with `geng` from `nauty` version 2.8.8 [21], using the command `geng -c` n. The program outputs every isomorphism class exactly once (in `graph6` format), so the enumeration is exhaustive and free of duplicates. The resulting counts, 6, 21, 112, 853, 11 117, 261 080 and 11 716 571, agree with the known numbers of connected graphs [26].

Algorithm 1 (exact evaluation of DCI and exhaustive maximisation).
Input: order n; the list of all connected graphs of order n.
Output: number of graphs; largest and second-largest values of DCI; number of maximisers.

1. Set $L = \operatorname{lcm}(2, 3, \dots, 2n-2)$. Every edge degree sum lies in $\{2, \dots, 2n-2\}$, so $L \cdot \mathrm{DCI}(G)$ is an integer for every graph of order n.
2. For each graph G, compute the degrees and the integer $S(G) = \sum_{uv \in E} (d(u) - d(v))^2 \cdot \big(L/(d(u) + d(v))\big) = L \cdot \mathrm{DCI}(G)$.

3. Keep the largest value S_1, the second-largest distinct value S_2 and the number of graphs with $S(G) = S_1$. All comparisons are exact integer comparisons; no floating-point tolerance is involved.

4. Report S_1/L and S_2/L as reduced fractions, and identify each maximiser by an isomorphism test against $\mathrm{CS}(n, k)$, $1 \le k \le n-1$.

Verification. The computation was carried out with two independent implementations, one using the scaled integers of Algorithm 1 and one using exact rational arithmetic directly; for $n \le 7$ it was also repeated on the atlas of all graphs with at most seven vertices [25], which does not use `nauty`. For every $n = 4, \ldots, 10$ all computations agree on the number of graphs, the maximum, the second-largest value, the number of maximisers (always one) and the identity of the maximiser; the results are listed in Table 2.

Data availability. The programs used for these computations are available from the corresponding author on reasonable request.

V. Mythili
Department of Mathematics, SRM Institute of Science and Technology, Ramapuram Campus, Chennai, India
E-mail: mv6156@srmist.edu.in

S. Dhanalakshmi
Department of Mathematics, SRM Institute of Science and Technology, Ramapuram Campus, Chennai, India
E-mail: dhanalas1@srmist.edu.in

Received 24 February 2026
Accepted 01 November 2026