Directed Zagreb Indices

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Assumptions and Notation

- All (di)graphs will be simple with n vertices and m (directed) edges.
- Allow for edges in each direction in digraphs, but no duplicates.
- No isolated vertices.
- Graphs may be connected or disconnected.
- For a vertex v, $d^+(v)$ is the out-degree and $d^-(v)$ is the in-degree.

Zagreb Indices

Let $G = (V, E)$ be a graph.
Define the Zagreb indices as [Gutman and Trinajstić]:

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- Topics explored: comparing indices, upper/lower bounds, how certain classes of graphs behave
- Directed version not addressed in the literature

Zagreb Indices on Directed graphs

Let $D = (N, A)$ be a digraph. Define Zagreb indices on directed graphs as:

$$\overrightarrow{M}_1(D) = \sum_{v \in N(D)} d^+(v) d^-(v) \text{ and } \overrightarrow{M}_2(D) = \sum_{\vec{e}=(u,v) \in A(D)} d^+(u) d^-(v).$$

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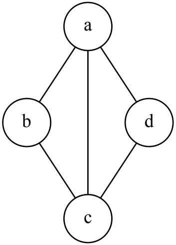

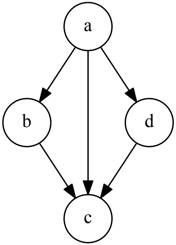

$M_1(G) = 9 + 4 + 9 + 4 = 26$ and
$M_2(G) = 6 + 6 + 6 + 6 + 9 = 33$

$\overrightarrow{M}_1(D) = 0 + 1 + 0 + 1 = 2$ and
$\overrightarrow{M}_2(D) = 3 + 3 + 3 + 3 + 9 = 21$

Some basic observations

- $\overrightarrow{M_1}$ can also be written as a sum over arcs in the digraph.

$$\overrightarrow{M_1}(D) = \frac{1}{2} \sum_{\vec{e}=(u,v)\in A(D)} (d^-(u) + d^+(v)).$$

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- Flipping the orientation of all arcs in a digraph (denoted by $\overleftarrow{D}$) does not change the directed Zagreb indices: $\overrightarrow{M}_1(D) = \overrightarrow{M}_1(\overleftarrow{D})$ and $\overrightarrow{M}_2(D) = \overrightarrow{M}_2(\overleftarrow{D})$

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- Let $D = (N, A)$ be a regular digraph with $d^+(v) = d^-(v) = k$ $\forall v \in N$. Then $\overrightarrow{M}_1(D) = nk^2$ and $\overrightarrow{M}_2(D) = mk^2$.

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- Let $D = (N, A)$ be a regular digraph with $d^+(v) = d^-(v) = k$ $\forall v \in N$. Then $\overrightarrow{M}_1(D) = nk^2$ and $\overrightarrow{M}_2(D) = mk^2$.
- The directed Zagreb indices of a disconnected graph are simply the sum of the directed Zagreb indices of the components.

Relating the Zagreb indices

For undirected Zagreb indices, $M_1 = M_2$, $M_1 > M_2$ and $M_1 < M_2$ are all possible.
Categorization provided in [Horoldagva, Das, and Selenge].

We show that for directed Zagreb indices only two are possible.

Theorem (Therorem 1)

For any directed graph D, $\overrightarrow{M}_1(D) \leq \overrightarrow{M}_2(D)$.

Proof strategy: By induction on the number of arcs in D.

Proof of Theorem 1 - Base Case

Trivially, if there are no arcs in D, then $\overrightarrow{M}_1(D) = 0 = \overrightarrow{M}_2(D)$.

For illustration, if D contains a single arc, then

$$\overrightarrow{M}_1(D) = 0 \cdot 1 + 1 \cdot 0 = 0,$$

and

$$\overrightarrow{M}_2(D) = 1 \cdot 1 = 1,$$

so

$$\overrightarrow{M}_1(D) < \overrightarrow{M}_2(D).$$

Proof of Theorem 1 - Inductive Step (Part 1)

- Inductive hypothesis: We assume that for any digraph D with k arcs, $\overrightarrow{M}_1(D) \leq \overrightarrow{M}_2(D)$. Let $D^\wedge$ be a digraph with $k+1$ arcs. We want to show that $\overrightarrow{M}_1(D^\wedge) \leq \overrightarrow{M}_2(D^\wedge)$.

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- Pick an arbitrary arc $e = (u, v) \in D^\wedge$. Removing e from $D^\wedge$ yields a digraph D' with exactly k arcs, and thus $\overrightarrow{M}_1(D') \leq \overrightarrow{M}_2(D')$ by the inductive hypothesis. Thus, by construction, $e \notin D'$.

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- Pick an arbitrary arc $e = (u, v) \in D^\wedge$. Removing e from $D^\wedge$ yields a digraph D' with exactly k arcs, and thus $\overrightarrow{M}_1(D') \leq \overrightarrow{M}_2(D')$ by the inductive hypothesis. Thus, by construction, $e \notin D'$.
- How does $\overrightarrow{M}_1$ differ between D' and $D^\wedge$?
  The only terms in the sum which are altered are the terms contributed by the nodes u and v. In $D^\wedge$, the in-degree of node u is unchanged, and its out-degree increases by 1.
  Thus, the contribution of u to $\overrightarrow{M}_1$ was previously $d^-(u) \cdot d^+(u)$, and is now $d^-(u) \cdot (d^+(u) + 1)$, a change of exactly $d^-(u)$.
  Similarly, the change from the contribution of node v is exactly $d^+(v)$.
  Thus $\overrightarrow{M}_1(D^\wedge) = \overrightarrow{M}_1(D') + d^-(u) + d^+(v)$.

Proof of Theorem 1 - Inductive Step (ctd.)

- Calculating $\overrightarrow{M}_2(D^\wedge)$, since $e \notin D'$, $\overrightarrow{M}_2(D^\wedge)$ is precisely $\overrightarrow{M}_2(D')$ plus the contribution from arc e, both to the new summand term from e, and potential increases to existing arcs in D'.

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- The new arc e generates a contribution of $(d^+(u)+1)(d^-(v)+1)$, along with additional nonnegative contributions to the terms for arcs leaving u and entering v, namely

$$\sum_{x \in N^+(u)} d^-(x) + \sum_{y \in N^-(v)} d^+(y)$$

where the in and out neighborhoods of a node u are defined, respectively, as $N^-(u) = \{v \in N(D) | (v,u) \in A(D)\}$ and $N^+(u) = \{v \in N(D) | (u,v) \in A(D)\}$

Proof of Theorem 1 - putting it all together

$$
\begin{aligned}
\overrightarrow{M}_2(D^\wedge) =& \overrightarrow{M}_2(D') + d^+(u) + d^-(v) + d^+(u)d^-(v) + 1 + \\
& \sum_{x \in N^+(u)} d^-(x) + \sum_{y \in N^-(v)} d^+(y) \\
\geq& \overrightarrow{M}_1(D') + d^+(u) + d^-(v) + d^+(u)d^-(v) + 1 + \\
& \sum_{x \in N^+(u)} d^-(x) + \sum_{y \in N^-(v)} d^+(y) \\
=& \overrightarrow{M}_1(D^\wedge) + d^+(u)d^-(v) + 1 + \\
& \sum_{x \in N^+(u)} d^-(x) + \sum_{y \in N^-(v)} d^+(y) \\
\geq& \overrightarrow{M}_1(D^\wedge)
\end{aligned}
$$

□

Connecting the Directed and Undirected Zagreb Indices

- Let G be an arbitrary undirected graph. Define G^* to be the digraph with bidirected arcs in G^* for every edge in G. Then $M_1(G) = \overrightarrow{M}_1(G^*)$ and $2 \cdot M_2(G) = \overrightarrow{M}_2(G^*)$.

Proof.

By construction of G^*, for any node $v \in G^*$ arising from a vertex $x \in G$, $d^+(v) = d^-(v) = d(x)$. The equality of $M_1(G) = \overrightarrow{M}_1(G^*)$ follows immediately, and $2 \cdot M_2(G) = \overrightarrow{M}_2(G^*)$ because there are two arcs in G^* for every edge in G. □

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- The above result, combined with Theorem 1, gives an alternative proof of the following corollary, a known result from [Fath-Tabar].

Corollary

Let G be an arbitrary undirected graph. Then, $M_1(G) \leq 2M_2(G)$.

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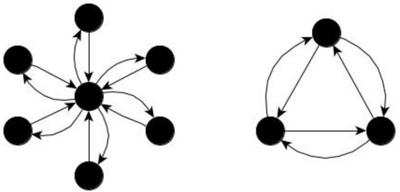
- The relationship was shown true [Hansen and Vukicević] for chemical graphs, but not true for general graphs.
- One such instance consists of a disconnected graph whose two components were a $K_{1,6}$ and C_3.
- We show that there is a natural transformation of that graph into the digraph $K^*_{1,6} \cup C^*_3$ that likewise disproves the analogous inequality for digraphs.

$K_{1,6}^* \cup C_3^*$ Disproves the Conjecture for Digraphs



Proof that $\dfrac{\overrightarrow{M}_1(D)}{n} > \dfrac{\overrightarrow{M}_2(D)}{m}$ for the above graph D.

$\overrightarrow{M}_1(D) = 36 + 6 \cdot 1 + 3 \cdot 4 = 54$, where the contributions come from the center of the star, the leaves of the star, and the nodes of the cycle.
$\overrightarrow{M}_2(D) = 6 \cdot 6 + 6 \cdot 6 + 6 \cdot 4 = 96$, with contributions from the six arcs directed out of the center of the star, the six arcs directed into the center of the star, and the six arcs in the C_3^*.
$\dfrac{\overrightarrow{M}_1(D)}{n} = \dfrac{54}{10} = 5.4 > 5.333 = \dfrac{96}{18} = \dfrac{\overrightarrow{M}_2(D)}{m}$. □

Bounds on directed Zagreb indices

Considering all orientations on a particular graph, we can create bounds on the possible values for $\overrightarrow{M}_1(D)$ and $\overrightarrow{M}_2(D)$.

Lemma

For any orientation of a $K_{1,n}$ (with no bidirectional arcs),
$0 \leq \overrightarrow{M}_1(K_{1,n}) \leq \lfloor \frac{n^2}{4} \rfloor$ *and* $\lceil \frac{n^2}{2} \rceil \leq \overrightarrow{M}_2(K_{1,n}) \leq n^2$.

Proof sketch.

Lower bound for $\overrightarrow{M}_1$: star $K_{1,n}$ where all arcs are directed into the center.
Upper bound for $\overrightarrow{M}_1$: star $K_{1,n}$ where $\lfloor \frac{n}{2} \rfloor$ of the arcs are directed into the center, and the rest ($\lceil \frac{n}{2} \rceil$ arcs) are directed out of the center. (in-degree and out-degree are as close as possible)
Lower bound for $\overrightarrow{M}_2$: one of in/out-degree is $\lfloor \frac{n}{2} \rfloor$ and the other is $\lceil \frac{n}{2} \rceil$.
Upper bound for $\overrightarrow{M}_2$: all arcs are directed into the center of the star, or all are directed out of center of the star, $\overrightarrow{M}_2 = n^2$. □

Bounds on a path digraph

Lemma

For any oriented P_n, $0 \leq \overrightarrow{M}_1(P_n) \leq n-2$ (where there is some orientation which yields each possible integral value) and $n-1 \leq \overrightarrow{M}_2(P_n) \leq 4n-8$.

Proof sketch.

Lower bound for $\overrightarrow{M}_1$: Arcs in P_n alternate directions.
Upper bound for $\overrightarrow{M}_1$: All arcs are oriented in the same direction.
Lower bound for $\overrightarrow{M}_2$: All arcs are oriented in the same direction.
Upper bound for $\overrightarrow{M}_2$: Arcs in P_n alternate directions. □

When does $\overrightarrow{M}_1(D) = 0$?

A *source* is a node with in-degree zero, and a *sink* is a node with out-degree zero.

Lemma

$\overrightarrow{M}_1(D) = 0$ *if and only if every node in* D *is either a source or a sink.*

Lemma

If a graph G *has an odd cycle, then* $\overrightarrow{M}_1(D) \neq 0$*.*

Proof idea.

By a simple parity argument, there is no possible orientation of the arcs in an odd cycle that has every such node be a sink or a source. □

Digraphs with no odd cycles

Lemma

If D contains no odd cycles, then there is an orientation of the arcs in D so that $\overrightarrow{M}_1(D) = 0$.

Proof sketch.

Since the digraph has no odd cycles, either it has no cycles, or its only cycles are even.
If no cycles, orient arcs in opposite directions on the longest path in the tree. Repeat on remaining paths, consistent with previous choices, so all nodes are either a source or a sink.
If there is an even cycle, orient its edges in opposite directions. Repeat on remaining even cycles and paths. Details omitted. □

Equality of Directed Zagreb Indices

We seek to fully characterize instances where $\overrightarrow{M}_1 = \overrightarrow{M}_2 \neq 0$.

Lemma

If a disconnected graph has $\overrightarrow{M}_1 = \overrightarrow{M}_2 \neq 0$, then each of its connected components must also have $\overrightarrow{M}_1 = \overrightarrow{M}_2 \neq 0$.

Lemma

The directed cycle C_n has $\overrightarrow{M}_1(C_n) = \overrightarrow{M}_2(C_n) \neq 0$.

Lemma

K_2^* has $\overrightarrow{M}_1(K_2^*) = \overrightarrow{M}_2(K_2^*) \neq 0$.

Conjecture: The directed cycle and K_2^* (or graphs consisting solely of directed cycles and K_2^*) are the only graphs in which $\overrightarrow{M}_1 = \overrightarrow{M}_2 \neq 0$.

Supporting the Conjecture (1)

Lemma

It is NOT true that inserting an arc will always increase $\overrightarrow{M}_2$ by more than it increases $\overrightarrow{M}_1$.

Proof.

Consider a unidirectional path, that starts at node v_0 and ends at node v_{n-1}.
Insert a directed arc from v_{n-1} to v_0.
The increase in $\overrightarrow{M}_1$ is 2, with one each contributed at v_0 and v_{n-1}.
The increase in $\overrightarrow{M}_2$ is 1, the contribution from the new arc, as the sum from the other arcs does not change. □

Supporting the Conjecture (2)

Theorem

Any digraph with a source and a sink cannot have $\overrightarrow{M}_1 = \overrightarrow{M}_2$.

Proof sketch.

Proof by contradiction.
Let D be a digraph with source u and sink v.
Suppose that $\overrightarrow{M}_1 = \overrightarrow{M}_2$.
Insert an arc from v to u.
The increase in $\overrightarrow{M}_2$ is exactly 1.
The increase in $\overrightarrow{M}_1$ is more than 1.
Since the increase in $\overrightarrow{M}_1$ is more than the increase in $\overrightarrow{M}_2$, the values $\overrightarrow{M}_1$ and $\overrightarrow{M}_2$ could not have been equal, contradicting the original assumption. □

Supporting the Conjecture (3)

Theorem

Any digraph D which consists of solely a directed cycle and one additional arc has $\overrightarrow{M}_1(D) < \overrightarrow{M}_2(D)$.

Proof Sketch.

We showed $\overrightarrow{M}_1 = \overrightarrow{M}_2$ for any directed cycle. A graph that consists of a directed cycle and one additional arc can be constructed by adding arc e:

1. as a disconnected arc,
2. as a chord in the cycle,
3. as an arc directed inward (or outward) into one node of the cycle and the other node would be a new node, or
4. an arc going in the opposite direction of one of the current arcs in the cycle.

In all cases, we verify $\overrightarrow{M}_1(D+e) > \overrightarrow{M}_2(D+e)$. □

Supporting the Conjecture (4)

Theorem

For any cycle C that is oriented but not directed, $\overrightarrow{M}_1(C) < \overrightarrow{M}_2(C)$.

Proof Sketch.

Let s be the number of maximal directed paths of length 1 in the cycle.
Let t be the number of maximal directed paths of length greater than 1, but less than n in the cycle.
To calculate $\overrightarrow{M}_1(C)$, consider when the direction on the cycle changes.
$\overrightarrow{M}_1(C) = n - (s + t) = n - s - t$.
$\overrightarrow{M}_2(C) = 4s + 4t + n - s - 2t = n + 3s + 2t$.
Since s and t are nonzero, $n + 3s + 2t > n - s - t$ which ensures that $\overrightarrow{M}_1(C) < \overrightarrow{M}_2(C)$. □

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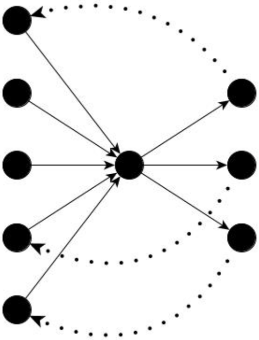
  Completely characterized by [Das, Horoldagva, and Selenge]
- Our results for Directed Zagreb Indices: $\overrightarrow{M}_2 - \overrightarrow{M}_1 \geq 0$
- In fact, we show $\overrightarrow{M}_2 - \overrightarrow{M}_1$ can equal any nonnegative integer.

Differences of Directed Zagreb Indices - Construction used

Theorem

For all $s \in \mathbb{N}$, there exists a directed graph with $\overrightarrow{M}_2 - \overrightarrow{M}_1 = s$.



A construction technique for digraphs with all possible values for the difference between the two Zagreb indices. The inclusion of any subset of the dotted edges leads to one of the digraphs in the collection.

Difference Proof

Proof Sketch.

Let D be the digraph $K_{1,n}$ with x edges directed into the center and k edges directed out of the center where $x + k = n$ and $k \leq x$. Consider the collection of $k + 1$ digraphs $\{D = D_0, D_1, D_2, \ldots, D_k\}$ where D_i is the digraph formed from D by connecting i of the arcs directed out of the center to i different arcs directed into the center.

In general, $\overrightarrow{M}_2(D_i) - \overrightarrow{M}_1(D_i) = x^2 + k^2 - xk - i$.

When $x = k$, $\overrightarrow{M}_2(D_i) - \overrightarrow{M}_1(D_i) = k^2 - i$, giving all differences in $[k^2 - k, k^2]$.

When $x = k + 1$, $\overrightarrow{M}_2(D_i) - \overrightarrow{M}_1(D_i) = k^2 + k + 1 - i$, giving all differences in $[k^2 + 1, k^2 + k + 1]$.

Continuing in this fashion gets $[k^2 + k, k^2 + 2k + 1]$, and so forth.

If we plug in $k = 1$, we see that we start the interval at $[0, 1]$ and hence can get any nonnegative integer values since these intervals line up and/or overlap and increase without bound. □

Future Work

- Resolve the conjecture regarding when the difference between $\overrightarrow{M}_1$ and $\overrightarrow{M}_2$ is zero. We believe that in all cases other than a directed cycle or K_2^* or disconnected combinations thereof, the difference between $\overrightarrow{M}_1$ and $\overrightarrow{M}_2$ is non-zero and inserting additional arcs or nodes will not result in equality of $\overrightarrow{M}_1$ and $\overrightarrow{M}_2$.

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- Is $\dfrac{\overrightarrow{M}_1}{n} \leq \dfrac{\overrightarrow{M}_2}{m}$ true for connected digraphs, or digraphs where not all arcs are bidirectional?
- Generalize other indices described on undirected graphs to digraphs.

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