Szeged and Mostar root-indices of graphs

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CroCoDays, September, 2024

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The Szeged polynomial

- G connected graph with at least two vertices.
- For $e = uv \in E(G)$:

$$\begin{aligned} N_u(e|G) &= \{x \in V(G) \mid d_G(u,x) < d_G(v,x)\}, \\ N_v(e|G) &= \{x \in V(G) \mid d_G(v,x) < d_G(u,x)\}. \end{aligned}$$

- $n_u(e) = |N_u(e|G)|$,
  $n_v(e) = |N_v(e|G)|$.
- The **Szeged index** of G (Gutman, 1994):

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e).$$

- The **Szeged polynomial** of G (Ashrafi, et. al., 2007):

$$Sz(G,x) = \sum_{e=uv \in E(G)} x^{n_u(e) n_v(e)}.$$

Weighted-product and weighted-plus Szeged polynomial

- **weighted-product Szeged polynomial** (Ashrafi, et. al., 2007):

$$wSz_1(G,x) = \sum_{e=uv\in E(G)} \deg(u)\deg(v)x^{n_u(e)n_v(e)}.$$

- **weighted-plus Szeged polynomial** (B., et. al., 2023):

$$wSz_2(G,x) = \sum_{e=uv\in E(G)} (\deg(u)+\deg(v))x^{n_u(e)n_v(e)}.$$

- **Mostar polynomial** (Ali, Došlić, 2021):

$$Mo(G,x) = \sum_{e=uv\in E(G)} x^{|n_u(e)-n_v(e)|}.$$

Polynomials vs. indices

Note, that

$$Sz(G) = Sz'(G,1), \qquad wSz_1(G) = wSz_1'(G,1),$$
$$wSz_2(G) = wSz_2'(G,1), \qquad Mo(G) = Mo'(G,1).$$

Some known families

Proposition (Szeged: A. R. Ashrafi et. al., 2007)

If C_n is a cycle on $n \geq 3$ vertices, then

$$
\begin{aligned}
Sz(C_n, x) &= \begin{cases} nx^{\frac{n^2}{4}}; & n \text{ even} \\ nx^{\frac{(n-1)^2}{4}}; & n \text{ odd} \end{cases}, \\
wSz_1(C_n, x) = wSz_2(C_n, x) &= \begin{cases} 4nx^{\frac{n^2}{4}}; & n \text{ even} \\ 4nx^{\frac{(n-1)^2}{4}}; & n \text{ odd} \end{cases}, \\
Mo(C_n, x) &= n.
\end{aligned}
$$

Some known families

Proposition (Szeged: A. R. Ashrafi et. al., 2007)

If S_n is a star on $n+1$ vertices, where $n \geq 1$, then

$$\begin{aligned} Sz(S_n, x) &= nx^n, \\ wSz_1(S_n, x) &= n^2 x^n, \\ wSz_2(S_n, x) &= n(n+1)x^n, \\ Mo(S_n, x) &= nx^{n-1}. \end{aligned}$$

Some known families

Proposition (Szeged: A. R. Ashrafi et. al., 2007)

If K_n is a complete graph on $n \geq 2$ vertices, then

$$\begin{aligned} Sz(K_n, x) &= \binom{n}{2} x, \\ wSz_1(K_n, x) &= \binom{n}{2}(n-1)^2 x, \\ wSz_2(K_n, x) &= 2\binom{n}{2}(n-1)x, \\ Mo(K_n, x) &= \binom{n}{2}. \end{aligned}$$

Some known families

Proposition (Szeged: A. R. Ashrafi et. al., 2007 - wrong)

If W_n is a wheel on $n+1$ vertices, where $n \geq 3$, then

$$\begin{aligned} Sz(W_n, x) &= nx^{n-2} + nx^4, \\ wSz_1(W_n, x) &= 3n^2x^{n-2} + 9nx^4, \\ wSz_2(W_n, x) &= n(n+3)x^{n-2} + 6nx^4, \\ Mo(W_n, x) &= n + nx^{n-3}. \end{aligned}$$

Some known families

Proposition (Szeged: A. R. Ashrafi et. al., 2007)

If P_n is a path on $n \geq 3$ vertices, then

$$Sz(P_n, x) = \begin{cases} 2\left(x^{1\cdot(n-1)} + x^{2\cdot(n-2)} + \cdots + x^{\left(\frac{n}{2}-1\right)\left(\frac{n}{2}+1\right)} + \frac{1}{2}x^{\frac{n^2}{4}}\right); & n \text{ even} \\ 2\left(x^{1\cdot(n-1)} + x^{2\cdot(n-2)} + \cdots + x^{\frac{n-1}{2}\frac{n+1}{2}}\right); & n \text{ odd} \end{cases},$$

$$wSz_1(P_n, x) = \begin{cases} 8\left(\frac{1}{2}x^{1\cdot(n-1)} + x^{2\cdot(n-2)} + \cdots + x^{\left(\frac{n}{2}-1\right)\left(\frac{n}{2}+1\right)} + \frac{1}{2}x^{\frac{n^2}{4}}\right); & n \text{ even} \\ 8\left(\frac{1}{2}x^{1\cdot(n-1)} + x^{2\cdot(n-2)} + \cdots + x^{\frac{n-1}{2}\frac{n+1}{2}}\right); & n \text{ odd} \end{cases},$$

$$wSz_2(P_n, x) = \begin{cases} 8\left(\frac{3}{4}x^{1\cdot(n-1)} + x^{2\cdot(n-2)} + \cdots + x^{\left(\frac{n}{2}-1\right)\left(\frac{n}{2}+1\right)} + \frac{1}{2}x^{\frac{n^2}{4}}\right); & n \text{ even} \\ 8\left(\frac{3}{4}x^{1\cdot(n-1)} + x^{2\cdot(n-2)} + \cdots + x^{\frac{n-1}{2}\frac{n+1}{2}}\right); & n \text{ odd} \end{cases},$$

$$Mo(P_n, x) = \begin{cases} 1 + 2x^2(1 + x^2 + x^4 + \cdots + x^{n-4}); & n \text{ even} \\ 2x(1 + x^2 + x^4 + \cdots x^{n-3}); & n \text{ odd} \end{cases}.$$

Roots of polynomials

$$\begin{aligned} Sz^*(G,x) &= 1 - Sz(G,x), \\ wSz_1^*(G,x) &= 1 - wSz_1(G,x), \\ wSz_2^*(G,x) &= 1 - wSz_2(G,x), \\ Mo^*(G,x) &= 1 - xMo(G,x). \end{aligned}$$

Lemma (Dehmer et. al., 2020)

*If $P(x) = p_1x + p_2x^2 + \cdots + p_nx^n$ is a polynomial where $n \in \mathbb{N}$, $p_i \in [0,\infty)$ for any $i \in \{1,\ldots,n\}$, and $p_1 + p_2 + \cdots + p_n \geq 1$, then the polynomial $Q(x) = 1 - P(x)$ has **exactly one** positive root. Moreover, the unique positive root δ of $Q(x)$ belongs to the interval $(0,1]$. Furthermore, $\delta = 1$ if and only if $p_1 + p_2 + \cdots + p_n = 1$.*

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Lemma (Dehmer et. al., 2020)

*If $P(x) = p_1 x + p_2 x^2 + \cdots + p_n x^n$ is a polynomial where $n \in \mathbb{N}$, $p_i \in [0, \infty)$ for any $i \in \{1, \ldots, n\}$, and $p_1 + p_2 + \cdots + p_n \geq 1$, then the polynomial $Q(x) = 1 - P(x)$ has **exactly one** positive root. Moreover, the unique positive root δ of $Q(x)$ belongs to the interval $(0, 1]$. Furthermore, $\delta = 1$ if and only if $p_1 + p_2 + \cdots + p_n = 1$.*

Proof: $\forall x \in (0, \infty]$, $Q'(x) < 0$, $1 - P(0) > 0, 1 - P(1) \leq 0$.

Analytical results

Another way to write down the polynomials

$$\begin{aligned} E_k^a(G) &= \{e = uv \in E(G) \mid n_u(e)n_v(e) = k\}, \\ E_k^d(G) &= \{e = uv \in E(G) \mid |n_u(e) - n_v(e)| = k - 1\}. \end{aligned}$$

Moreover, for any $k \geq 1$ let

$$\begin{aligned} a_k(G) &= \left|E_k^a(G)\right|, \\ b_k(G) &= \sum_{e=uv \in E_k^a(G)} (\deg(u)\deg(v)), \\ c_k(G) &= \sum_{e=uv \in E_k^a(G)} (\deg(u) + \deg(v)), \\ d_k(G) &= \left|E_k^d(G)\right|. \end{aligned}$$

Another way to write down the polynomials

Then, the polynomials can be defined as:

$$Sz(G,x) = \sum_{k\geq 1} a_k(G)x^k, \qquad wSz_1(G,x) = \sum_{k\geq 1} b_k(G)x^k,$$
$$wSz_2(G,x) = \sum_{k\geq 1} c_k(G)x^k, \qquad Mo(G,x) = \sum_{k\geq 1} d_k(G)x^{k-1}.$$

Lower bounds

$$A(G) = \max\{a_k(G) \mid k \geq 1\}, \qquad B(G) = \max\{b_k(G) \mid k \geq 1\},$$
$$C(G) = \max\{c_k(G) \mid k \geq 1\}, \qquad D(G) = \max\{d_k(G) \mid k \geq 1\}.$$

Theorem

If G is a connected graph with at least two vertices, then

$$\delta(Sz^*(G,x)) > \frac{1}{A(G)+1}, \qquad \delta(wSz_1^*(G,x)) > \frac{1}{B(G)+1},$$
$$\delta(wSz_2^*(G,x)) > \frac{1}{C(G)+1}, \qquad \delta(Mo^*(G,x)) > \frac{1}{D(G)+1}.$$

Proof for $\delta(Sz^*(G,x)) = \delta$:

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$$1 = Sz(G,\delta) = \sum_{k\geq 1} a_k(G)\delta^k$$

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$$1 = Sz(G,\delta) = \sum_{k\geq 1} a_k(G)\delta^k < \sum_{k\geq 1} A(G)\delta^k$$

Proof for $\delta(Sz^*(G,x)) = \delta$:

$$1 = Sz(G,\delta) = \sum_{k\geq 1} a_k(G)\delta^k < \sum_{k\geq 1} A(G)\delta^k = A(G)\sum_{k=1}^{\infty}\delta^k$$

Proof for $\delta(Sz^*(G,x)) = \delta$**:**

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which gives the claimed inequality.

Example

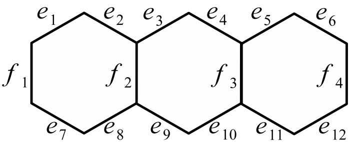

Figure: Molecular graph G of anthracene.

$$\begin{aligned} E_9^d(G) &= \{e_1, e_2, e_5, e_6, e_7, e_8, e_{11}, e_{12}\}, \\ E_1^d(G) &= \{f_1, f_2, f_3, f_4, e_3, e_4, e_9, e_{10}\}. \end{aligned}$$

$$d_9(G) = 8, d_1(G) = 8$$

$$Mo(G, x) = 8 + 8x^8$$

Then

$$\delta(Mo^*(G, x)) \doteq 0.12500.$$

On the other hand, $D(G) = 8$, therefore, $\delta(Mo^*(G, x)) \geq \frac{1}{9}$.

Root-indices of basic graph families

Proposition

If K_n is a complete graph on $n \geq 2$ vertices, then

$$\begin{aligned}
\delta(Sz^*(K_n, x)) &= \frac{2}{n(n-1)}, \\
\delta(wSz_1^*(K_n, x)) &= \frac{2}{n(n-1)^3}, \\
\delta(wSz_2^*(K_n, x)) &= \frac{1}{n(n-1)^2}, \\
\delta(Mo^*(K_n, x)) &= \frac{2}{n(n-1)}.
\end{aligned}$$

Root-indices of basic graph families

Proposition

If C_n is a cycle on $n \geq 3$ vertices, then

$$\begin{aligned}
\delta(Sz^*(C_n,x)) &= \begin{cases} n^{-\frac{4}{n^2}}; & n \text{ even} \\ n^{-\frac{4}{(n-1)^2}}; & n \text{ odd} \end{cases}, \\
\delta(wSz_1^*(C_n,x)) = \delta(wSz_2^*(C_n,x)) &= \begin{cases} (4n)^{-\frac{4}{n^2}}; & n \text{ even} \\ (4n)^{-\frac{4}{(n-1)^2}}; & n \text{ odd} \end{cases}, \\
\delta(Mo^*(C_n,x)) &= \frac{1}{n}.
\end{aligned}$$

Root-indices of basic graph families

Proposition

If S_n is a star on $n+1$ vertices, where $n \geq 1$, then

$$\begin{aligned}
\delta(Sz^*(S_n,x)) &= n^{-\frac{1}{n}}, \\
\delta(wSz_1^*(S_n,x)) &= n^{-\frac{2}{n}}, \\
\delta(wSz_2^*(S_n,x)) &= (n(n+1))^{-\frac{1}{n}}, \\
\delta(Mo^*(S_n,x)) &= n^{-\frac{1}{n}}.
\end{aligned}$$

Root-indices of basic graph families

Theorem

Let $n \geq 3$ *and* $c_n = \delta(P(W_n, x))$, *where* $P^* \in \{Sz^*, wSz_1^*, wSz_2^*, Mo^*\}$. *Then the sequence* (c_n) *converges to 0.*

Root-indices of basic graph families

Theorem

Let $n \geq 2$ be an even number and let $c_n = \delta(Mo^*(P_n, x))$. Then $c_2 = 1$, $c_4 \doteq 0.58975$, the sequence (c_n) is strictly decreasing, and the limit $c = \lim_{n\to\infty} c_n$ is

$$c = \frac{1}{3}\left(-1 - \frac{2}{\sqrt[3]{17+3\sqrt{33}}} + \sqrt[3]{17+3\sqrt{33}}\right) \doteq 0.54369.$$

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Proof:

$$\begin{aligned} c_n &+ 2c_n^3(1 + c_n^2 + \cdots + c_n^{n-4}) = 1, \\ c_{n+2} &+ 2c_{n+2}^3(1 + c_{n+2}^2 + \cdots + c_{n+2}^{n-4} + c_{n+2}^{n-2}) = 1. \end{aligned}$$

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Theorem

Let $n \geq 2$ be an even number and let $c_n = \delta(Mo^*(P_n, x))$. Then $c_2 = 1$, $c_4 \doteq 0.58975$, the sequence (c_n) is strictly decreasing, and the limit $c = \lim_{n\to\infty} c_n$ is

$$c = \frac{1}{3}\left(-1 - \frac{2}{\sqrt[3]{17 + 3\sqrt{33}}} + \sqrt[3]{17 + 3\sqrt{33}}\right) \doteq 0.54369.$$

Proof:

$$\begin{aligned}
c_n &+ 2c_n^3(1 + c_n^2 + \cdots + c_n^{n-4}) = 1, \\
c_{n+2} &+ 2c_{n+2}^3(1 + c_{n+2}^2 + \cdots + c_{n+2}^{n-4} + c_{n+2}^{n-2}) = 1. \\
\Rightarrow & \ \forall n, \quad c_{n+2} < c_n \text{ and } (c_n) \text{ is bounded} \Rightarrow (c_n) \text{ convergent.} \\
c_n &+ 2c_n^3(1 + c_n^2 + \cdots + c_n^{n-4}) = c_n + 2c_n^3 \frac{1 - c_n^{n-2}}{1 - c_n^2} = \\
c &+ 2c^3 \frac{1}{1 - c^2} = 1, \text{ where } c = \lim_{n\to\infty} c_n)
\end{aligned}$$

Root-indices of basic graph families

Theorem

Let $n \geq 3$ *be an odd number and let* $c_n = \delta(Mo^*(P_n, x))$*. Then* $c_3 \doteq 0.707107$*, the sequence* (c_n) *is strictly decreasing, and the limit* $c = \lim_{n\to\infty} c_n$ *is*

$$c = \frac{\sqrt{3}}{3} \doteq 0.57735.$$

Computational results

Correlation coefficients between indices and root-indices

- N_r, T_r ... the sets of all connected graphs and all trees on r vertices, respectively.

graph class	index	root-index	correlation coefficient
4* N_7	Sz	$\delta(Sz^*)$	0.4904
	wSz_1	$\delta(wSz_1^*)$	-0.3419
	wSz_2	$\delta(wSz_2^*)$	-0.0619
	Mo	$\delta(Mo^*)$	0.6711
4* T_{13}	Sz	$\delta(Sz^*)$	0.9138
	wSz_1	$\delta(wSz_1^*)$	-0.7815
	wSz_2	$\delta(wSz_2^*)$	-0.6162
	Mo	$\delta(Mo^*)$	0.8866

Correlation coefficients between root-indices

graph class	root-index	$\delta(Sz^*)$	$\delta(wSz_1^*)$	$\delta(wSz_2^*)$	$\delta(Mo^*)$
3*N_7	$\delta(Sz^*)$	3*	0.8408	0.8728	0.4628
	$\delta(wSz_1^*)$			0.9921	0.4645
	$\delta(wSz_2^*)$				0.4343
3*T_{13}	$\delta(Sz^*)$	3*	0.9366	0.9450	-0.5333
	$\delta(wSz_1^*)$			0.9987	-0.3955
	$\delta(wSz_2^*)$				-0.3965

Discrimination

- $\mathcal{C}$ ... any finite family of pairwise non-isomorphic graphs
- TI a topological index.
- $\mathcal{N} \subseteq \mathcal{C}$ is the family of graphs that TI cannot discriminate.
- $N = |\mathcal{N}|$.

Definition (E.V. Konstantinova, 1996)

The **discrimination** D of TI is

$$D(TI) = \frac{|\mathcal{C}| - N}{|\mathcal{C}|}.$$

Discrimination for the root-indices.

		$\delta(Sz^*)$		$\delta(wSz_1^*)$		$\delta(wSz_2^*)$		$\delta(Mo^*)$	
graph class	no. of graphs	N	D	N	D	N	D	N	D
all connected graphs									
N_5	21	0	1.0000	0	1.0000	2	0.9048	0	1.0000
N_6	112	0	1.0000	0	1.0000	0	1.0000	14	0.8750
N_7	853	30	0.9648	0	1.0000	0	1.0000	245	0.7128
N_8	11117	419	0.9623	44	0.9960	44	0.9960	6234	0.4392
all tree structures									
T_8	23	6	0.7391	0	1.0000	0	1.0000	6	0.7391
T_9	47	25	0.4681	0	1.0000	2	0.9574	25	0.4681
T_{10}	106	59	0.4434	0	1.0000	6	0.9434	59	0.4434
T_{11}	235	178	0.2426	4	0.9830	32	0.8638	179	0.2383
T_{12}	551	445	0.1924	12	0.9782	94	0.8294	445	0.1924
T_{13}	1301	1154	0.1130	74	0.9431	344	0.7356	1154	0.1130
T_{14}	3159	2884	0.0871	217	0.9313	975	0.6914	2884	0.0871
T_{15}	7741	7425	0.0408	870	0.8876	3140	0.5944	7426	0.0407
T_{16}	19320	18650	0.0347	2474	0.8719	8626	0.5535	18650	0.0347

Discrimination for the corresponding indices

		Sz		wSz_1		wSz_2		Mo	
graph class	no. of graphs	N	D	N	D	N	D	N	D
all connected graphs									
N_5	21	14	0.3333	7	0.6667	10	0.5238	20	0.0476
N_6	112	97	0.1339	25	0.7768	71	0.3661	108	0.0357
N_7	853	837	0.0188	510	0.4021	749	0.1219	849	0.0047
N_8	11117	11095	0.0020	10572	0.0490	11000	0.0105	11116	0.0001
all tree structures									
T_8	23	6	0.7391	4	0.8261	12	0.4783	19	0.1739
T_9	47	39	0.1702	21	0.5532	28	0.4043	43	0.0851
T_{10}	106	83	0.2170	47	0.5566	80	0.2453	102	0.0377
T_{11}	235	221	0.0596	163	0.3064	214	0.0894	231	0.0170
T_{12}	551	528	0.0417	378	0.3140	522	0.0526	547	0.0073
T_{13}	1301	1286	0.0115	1205	0.0738	1258	0.0331	1297	0.0031
T_{14}	3159	3131	0.0089	2910	0.0788	3113	0.0146	3155	0.0013
T_{15}	7741	7724	0.0022	7608	0.0172	7693	0.0062	7737	0.0005
T_{16}	19320	19289	0.0016	18985	0.0173	19257	0.0033	19316	0.0002

Structure sensitivity and abruptness

- $G \in \mathcal{C}$ and $\mathcal{H}(G)$ is the set of all pairwise non-isomorphic graphs that can be obtained from G by inserting exactly one edge.
- The **structure sensitivity** of a TI for G, $SS_G^1(TI)$ (B. Furtula et. al., 2013):

$$SS_G^1(TI) = \frac{1}{|\mathcal{H}(G)|} \sum_{H \in \mathcal{H}(G)} \left| \frac{TI(G) - TI(H)}{TI(G)} \right| .$$

- The **abruptness** of a TI for G, $Abr_G^1(TI)$ (B. Furtula et. al., 2013):

$$Abr_G^1(TI) = \max_{H \in \mathcal{H}(G)} \left| \frac{TI(G) - TI(H)}{TI(G)} \right| .$$

Modified structure sensitivity and modified abruptness

The **modified structure sensitivity** and the **modified abruptness** of TI for G (M. Rakić, B. Furtula, 2019):

$$SS^2_G(TI) = \sqrt{\frac{1}{|\mathcal{H}(G)|}\sum_{H\in\mathcal{H}(G)}(TI(G)-TI(H))^2},$$

$$Abr^2_G(TI) = \max_{H\in\mathcal{H}(G)}|TI(G)-TI(H)|.$$

Modified structure sensitivity and modified abruptness

Finally, for $i \in \{1,2\}$:

$$
\begin{aligned}
SS^i_{\mathcal{C}}(TI) &= \frac{1}{|\mathcal{C}|}\sum_{G\in\mathcal{C}} SS^i_G(TI),\\
Abr^i_{\mathcal{C}}(TI) &= \frac{1}{|\mathcal{C}|}\sum_{G\in\mathcal{C}} Abr^i_G(TI).
\end{aligned}
$$

Structure sensitivity and abruptness of root-indices

root-index	graph class ($\mathcal{C}$)	$SS^1_{\mathcal{C}}$	$SS^2_{\mathcal{C}}$	$Abr^1_{\mathcal{C}}$	$Abr^2_{\mathcal{C}}$
4*$\delta(Sz^*)$	T_8	0.0788	0.0767	0.1697	0.1351
	T_9	0.0637	0.0657	0.1556	0.1263
	T_{10}	0.0512	0.0560	0.1441	0.1188
	T_{11}	0.0426	0.0491	0.1348	0.1126
4*$\delta(wSz_1^*)$	T_8	0.2630	0.2329	0.6311	0.4283
	T_9	0.2289	0.2245	0.6439	0.4536
	T_{10}	0.1941	0.2115	0.6545	0.4751
	T_{11}	0.1698	0.2025	0.6629	0.4930
4*$\delta(wSz_2^*)$	T_8	0.2405	0.2110	0.6194	0.4076
	T_9	0.2075	0.2044	0.6340	0.4345
	T_{10}	0.1747	0.1929	0.6457	0.4571
	T_{11}	0.1521	0.1851	0.6551	0.4760
4*$\delta(Mo^*)$	T_8	0.1838	0.1456	0.4360	0.2778
	T_9	0.1610	0.1322	0.4162	0.2775
	T_{10}	0.1632	0.1379	0.4684	0.3078
	T_{11}	0.1431	0.1241	0.4267	0.2911

Conclusion

- Focusing on the family of trees, **novel root-indices correlate well** with the corresponding indices.
- Novel descriptors possess **significantly better discrimination power** than the corresponding indices.
- The **correlations** between different versions of Szeged root-indices **are quite high**.
- The best performance was found for the **weighted-product Szeged root-index.**
- The Mostar root-index **is weakly correlated** to Szeged root-indices.

Axioms - Special Issue

axioms

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IMPACT FACTOR 1.9

Aims and Scope

Axioms is an international, peer-reviewed, open access journal of **mathematics**, **mathematical logic** and **mathematical physics**, published monthly online by MDPI.

Editor-in-Chief

Prof. Dr. Humberto Bustince
Public University of Navarr, Spain

Sections

- Algebra and Number Theory
- Geometry and Topology
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SCIE
JCR-Q1 66/331
(Mathematics, Applied)

IF: 1.9 2023
5-Year Impact Factor : 1.7

Founded in 2012
(Volumes: 13)

43 days
Submission to Publication
(According to data from the second half of 2023)

MDPI

Axioms Editorial Office
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4052, Basel, Switzerland

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https://www.mdpi.com/journal/axioms/special_issues/560T7U3LML

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