Spectral clustering of combinatorial fullerene isomers based on their facet graph structure

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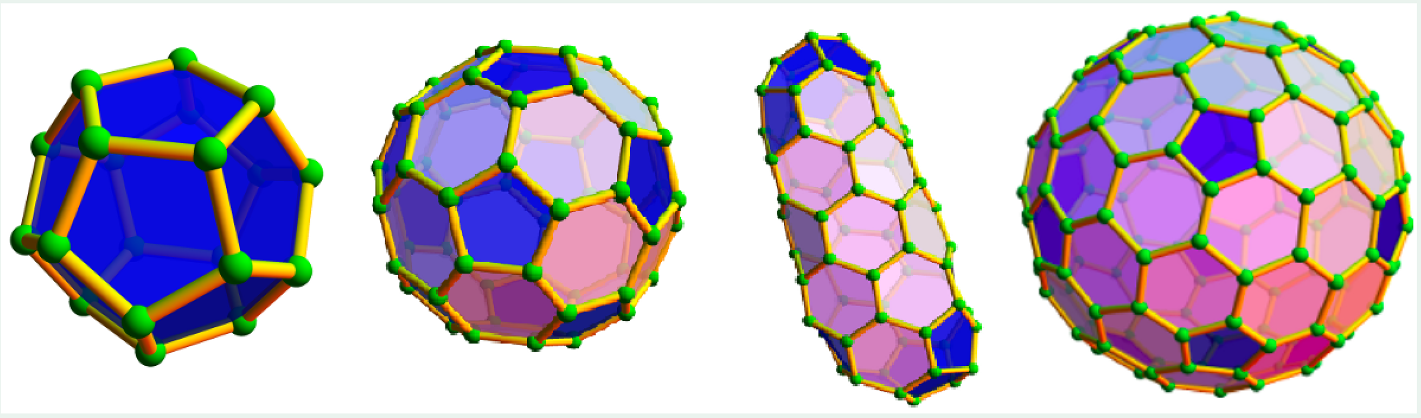
Object of Research

We call a convex polyhedron F_n in $\mathbb{R}^3$ with n vertices a **fullerene** if

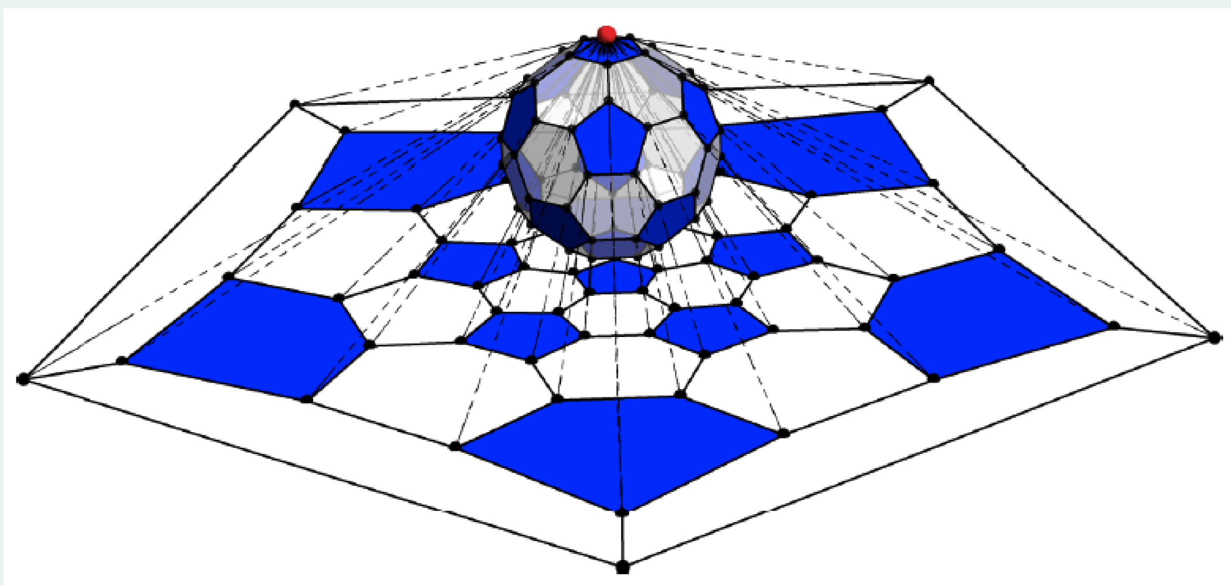
- it is simple,
- it is compact,
- it has twelve pentagonal facets and $n/2 - 10$ hexagonal facets.



By C_n we mean the set of all equivalence classes w.r.t. combinatorial equivalency of fullerenes with n vertices. These classes are called *(combinatorial) isomers*.

Basic properties:

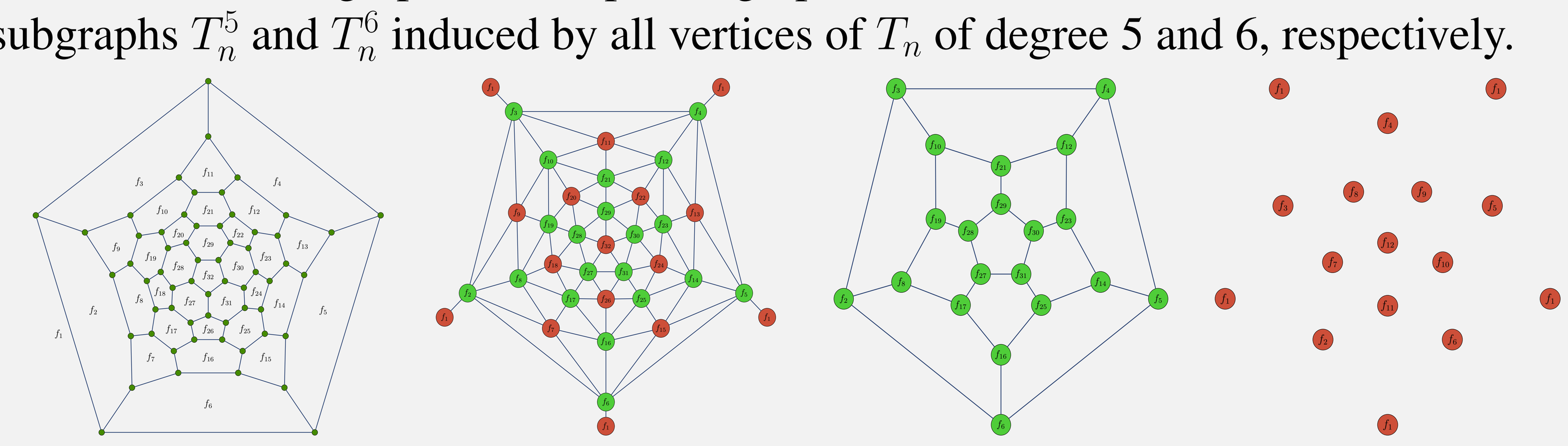
- At least one fullerene exists for every even $n \geq 20$, except for $n = 22$.
- The number of isomers grows like $\mathcal{O}(n^9)$.
- Every fullerene F_n can be mapped on a planar graph G_n s.t. vertex connectivity is preserved.



- Since F_n is simple, the **dual graph T_n** of G_n is (combinatorially) unique.

Problem Setting

Consider the dual graph T_n of a planar graph associated with a fullerene F_n, and its subgraphs T_n^5 and T_n^6 induced by all vertices of T_n of degree 5 and 6, respectively.



Main Objective

Aim: Classify fullerene isomers using the spectra of adjacency matrices of T_n, T_n^5, T_n^6, i.e., create a graph invariant which reflects the similarity of shapes between two distinct fullerenes.

Idea: Eigenvalues of adjacency matrices contain information about the arrangement of pentagons and hexagons on a fullerene's surface, and, therefore, information about the shape of a fullerene.

We use **Newton polynomials** to classify fullerenes.

Definition

For an adjacency matrix $A \in \mathbb{R}^{m \times m}$ and an integer $k \in \mathbb{N}_0$, we call

$$N(A, k) := \operatorname{tr}\left(A^k\right) = \sum_{j=1}^{m} \lambda_j^k,$$

the **Newton polynomial of A of degree k**, where $\lambda_1, \dots, \lambda_m$ are the (real) eigenvalues of A.

Newton polynomials can be interpreted as the number of closed paths.

Lemma

Let $k \leq m$ be an integer and A be the adjacency matrix of a graph G with m vertices. Then the Newton polynomials can be calculated recursively as

$$N(A,k) = -k \sum_{|H|=k} (-1)^{e(H)+c(H)} 2^{c(H)} - \sum_{j=2}^{k-2} N(A, k-j) \sum_{H:|H|=j} (-1)^{e(H)+c(H)} 2^{c(H)},$$

where the inner sum runs over all subgraphs H of G with j nodes and connected components being either edges or cycles, $e(H)$ being the numbers of edges among these components and $c(H)$ being the number of cycles.

Numerical and Theoretical Results

Number of non-unique spectra of graphs T_n, T_n^5 and T_n^6 of C_n–isomers:

n	20	24	26	28	30	32	34	36	38	40	42	44	46	48	50	52	54	56	58	60
T_n	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	3	0	0	2
T_n^5	0	0	0	0	0	0	0	0	0	3	3	15	16	43	63	95	111	147	146	177
T_n^6	0	0	0	0	1	1	2	1	1	2	0	0	0	0	0	1	0	0	0	0

This table can be extended to any $n > 60$ with positive integers in its first and second row, and zeroes in its third row. These numerical results yield to the following

Conjecture

- For all feasible n the graph T_n^6 is uniquely determined by its spectrum.
- For all feasible $n \geq 60$ at least two C_n–isomers exist having the same spectrum w.r.t. T_n.
- For all feasible $n \geq 54$ two C_n–isomers are isomorphic iff they are cospectral w.r.t. T_n^6.
- For any feasible n at least one of the spectra $\sigma(T_n), \sigma(T_n^5), \sigma(T_n^6)$ is unique for all C_n–isomers.

Theorem

Let Γ be a set of graphs with m vertices and with distinct absolute spectra such that $\lambda_{\max(G)} > 1$ for all $G \in \Gamma$. Then all graphs $G \in \Gamma$ can be uniquely characterized by at most two Newton polynomials of even degrees k_1^*, k_2^* with $m \geq k_1^* \geq k_2^*$.

This theorem applied on fullerene graphs yield

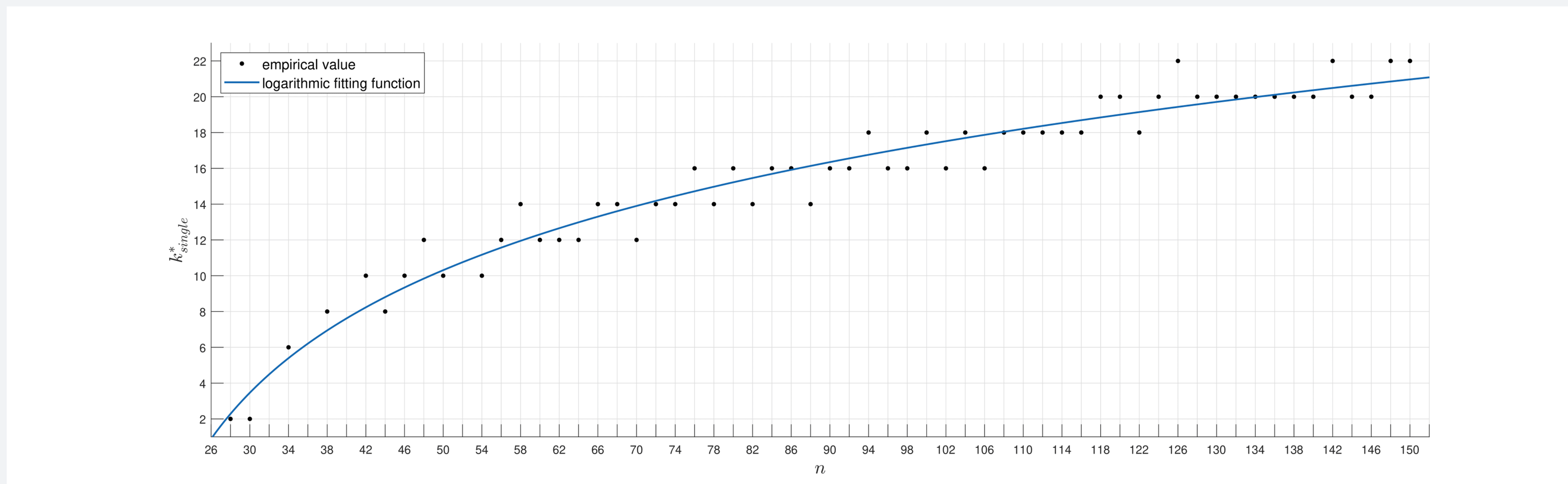
Corollary

Assuming the above Conjecture to be true, all C_n–isomers can be uniquely characterized by at most two Newton polynomials $N(A_G, k_1^*)$ and $N(A_G, k_2^*)$, $k_1^* \geq k_2^*$ even, w.r.t. at least one of the graphs $G \in \{T_n, T_n^5, T_n^6\}$.

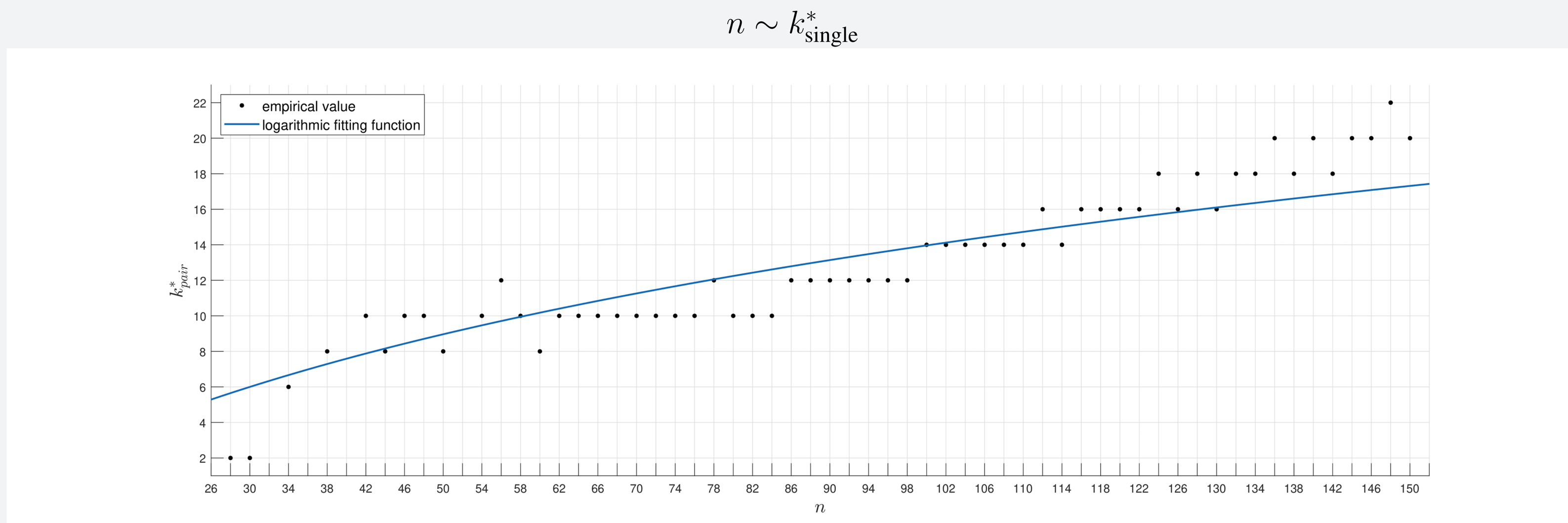
Number of clusters w.r.t. Newton polynomial $N(A_{60}^6, k)$ for even $2 \leq k \leq 100$:

k	2	4	6	8	10	12	...	100
# Clusters	18	218	1233	1784	1807	1812	...	1812
# Clusters with one element	5	47	845	1757	1802	1812	...	1812

Denote by k^*_{single} and k^*_{pair} the minimal degree k of Newton polynomials which is needed for a complete clusterization using a single and two Newton polynomials, respectively.



$n \sim k^*_{\text{single}}$



$n \sim k^*_{\text{pair}}$

Minimal degree k^*_{single} (a) and k^*_{pair} (b) needed for the complete clusterization of C_n-isomers with $28 \leq n \leq 150$

Outlook

- Prove the Conjecture.

Further Results

- Analyze the spectra of other matrices associated with a graph.
- Analyze the behavior of the spectra for infinitely large fullerenes.

References

[1] Artur Bille, Viktor Buchstaber, and Evgeny Spodarev. *Spectral clustering of combinatorial fullerene isomers based on their facet graph structure*. Journal of Mathematical Chemistry, 59 (2021), 264-288.