The Wiener index of vertex colorings

Open University Discrete Mathematics Seminar

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The Weiner index of a graph

For a set A:

- $\binom{A}{2}$ is the set of unordered pairs of elements of A.

For a graph G:

- $V(G)$ is the set of vertices of G
- $E(G)$ is the set of edges of G
- For $u, v \in V(G)$, we define $d(u, v)$, to be the length of a shortest path from u to v in G.

Definition. (Wiener, 1947)

The *Wiener index* of a graph G is the quantity

$$W(G) = \sum_{\{u,v\} \in \binom{V(G)}{2}} d(u, v).$$

The Weiner index of a set of vertices

Definition. (Bushaw, C., Leffler, 2025)

For a graph G, the Wiener index of a set of vertices $A \subseteq V(G)$ is the quantity

$$W(A) = \sum_{\{u,v\} \in \binom{A}{2}} d(u,v).$$

- In the special case of **cycle graphs**, this notion appears in the *mathematical music theory* literature; see the work of Clough and Douthett, Douthett and Krantz, Demaine and Toussaint, etc. on *maximally even sets* and *Euclidean rhythms*.
- $W(A)$ is a measure of how "spread out" the vertices of A are within the graph G.

Maximizers

Definition. (Bushaw, C., Leffler, 2025)

Suppose G is a graph and $A \subseteq V(G)$.

1. We say that A is a *maximizer of W on G* if
$$W(A) = \max\{W(B) \mid B \subseteq V(G) \text{ and } |B| = |A|\}.$$
2. We say that $B \subseteq V(G)$ is a *perturbation of A* if there is an edge $\{u, v\} \in E(G)$ with $u \in A$ and $v \in V(G) \setminus A$ such that $B = (A \setminus \{u\}) \cup \{v\}$.
3. The set A is called a *local maximizer of W on G* if
$$W(A) = \max\{W(B) \mid B \subseteq V(G) \text{ and } B \text{ is a perturbation of } A\}.$$

Maximizers on paths

The path on n vertices is denoted P_n, and we let $V(P_n) = \{1, 2, \ldots, n\}$.

Proposition. (Bushaw, C., Leffler, 2025)

Suppose A is a set of vertices in P_n, where $2 \leq |A| = m \leq n$. The following are equivalent.

1. A is a maximizer of W on P_n.
2. A is a local maximizer of W on P_n.
3. If m is even then

$$A = \left\{1, \ldots, \frac{m}{2}\right\} \cup \left\{n - \frac{m}{2} + 1, \ldots, n\right\},$$

   and if m is odd then

$$A = \left\{1, \ldots, \frac{m-1}{2}\right\} \cup \{j\} \cup \left\{n - \frac{m-1}{2} + 1, \ldots, n\right\},$$

   for some integer j with $\frac{m-1}{2} < j < n - \frac{m-1}{2} + 1$.

Maximizers on cycles

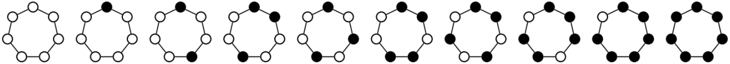


FIGURE 6. All Wiener index maximizers on C_7 up to rotations and reflections.

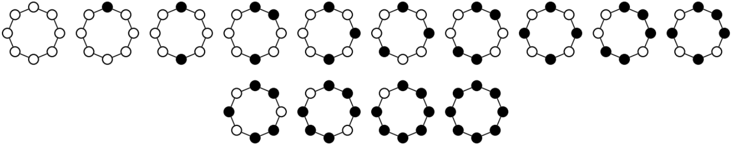
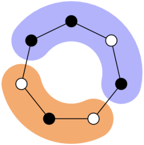


FIGURE 7. All Wiener index maximizers on C_8 up to rotations and reflections.



Maximizers on cycles

Terminology: $A \subseteq V(G)$ is *connected* if the induced subgraph $G[A]$ is connected.

Definitions.

1. A partition $\mathcal{P}$ of a set is called *equitable* if for all blocks $P, Q \in \mathcal{P}$ the cardinalities $|P|$ and $|Q|$ differ by at most one.
2. A set $A \subseteq V(G)$ is *balanced* if for every equitable 2-partition $\mathcal{P} = \{P, Q\}$ of $V(G)$ with connected blocks $|A \cap P|$ and $|A \cap Q|$ differ by at most one.
3. We say that A is *weakly balanced in G* if for every equitable 2-partition $\mathcal{P} = \{P, Q\}$ of $V(G)$ with connected blocks, $|A \cap P|$ and $|A \cap Q|$ differ by at most **two**, and furthermore, whenever $|A \cap Q| = |A \cap P| + 2$ then $|P| < |Q|$.

Maximizers on cycles

Theorem. (Bushaw, C., Leffler, 2025)

Suppose A is a set of vertices in C_n where $2 \leq |A| = m \leq n$.

1. A is a maximizer of W if and only if it is weakly balanced.
2. Suppose n is even or m is odd. Then A is a maximizer of W on C_n if and only if A is balanced.
3. Suppose n is odd and m is even. Then A is a maximizer of W on C_n if and only if A is weakly balanced. Furthermore, in this case, every maximizer of the Wiener index on C_n with cardinality m is not balanced.

From sets to colorings

For $v \in V(G)$ define $d_G(v)$ to be the $(|V(G)| - 1)$-tuple of distances from v to all other vertices in G arranged in non-decreasing order.

A graph G is called *distance degree regular* if $d_G(u) = d_G(v)$ for all $u, v \in V(G)$.

Theorem. (Bushaw, C., Leffler, 2025)

Suppose G is a distance degree regular graph. Then $A \subseteq V(G)$ is a maximizer of W if and only if $V(G) \setminus A$ is a maximizer of W.

So, for distance degree regular graphs, $A \subseteq V(G)$ is a maximizer of W if and only if

$$W(A) + W(V(G) \setminus A) \geq W(A') + W(V(G) \setminus A')$$

for all $A' \subseteq V(G)$ with $|A'| = |A|$.

The Wiener index of colorings

$$f : V(G) \longrightarrow [k] \quad \Longrightarrow \quad \mathrm{type}(f) = (|f^{-1}(i_1)|, |f^{-1}(i_2)|, \ldots)$$

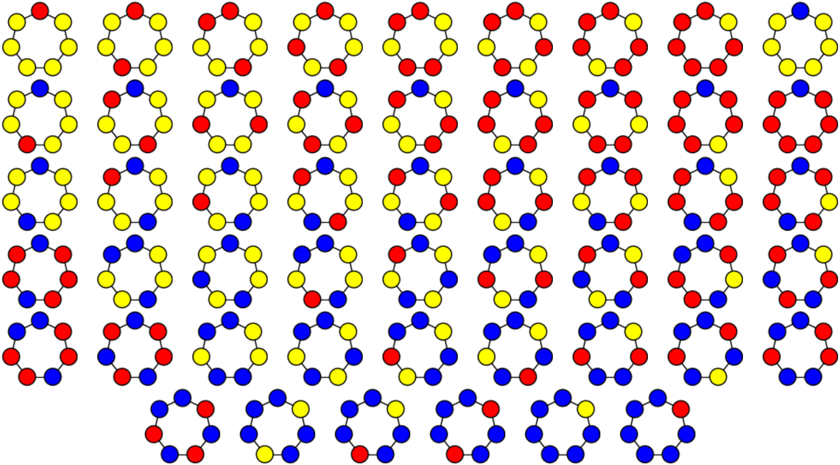
Definition. (Bushaw, C., Bardenova, Fay, Tennant, 2025)

For a graph G, suppose $f : V(G) \longrightarrow \{1, \ldots, k\}$. We define

$$W(f) = \sum_{i=1}^{k} W(f^{-1}(i)).$$

1. f is a *k-color maximizer of W on G* if f is surjective and $W(f)$ is maximal among all quantities $W(f')$ where $f' : V(G) \longrightarrow \{1, \ldots, k\}$ is surjective.
2. We say that f is a *k-color weak maximizer of W on G* if f is surjective and $W(f)$ is maximal among all quantities $W(f')$ where $f' : V(G) \longrightarrow \{1, \ldots, k\}$ is surjective and $\mathrm{type}(f') = \mathrm{type}(f)$.
3. f is a *k-color local weak maximizer of W on G* if $W(f) \geq W(S_{u,v}(f))$ for all $\{u, v\} \in E(G)$.

3-color weak maximizers of W on C_7



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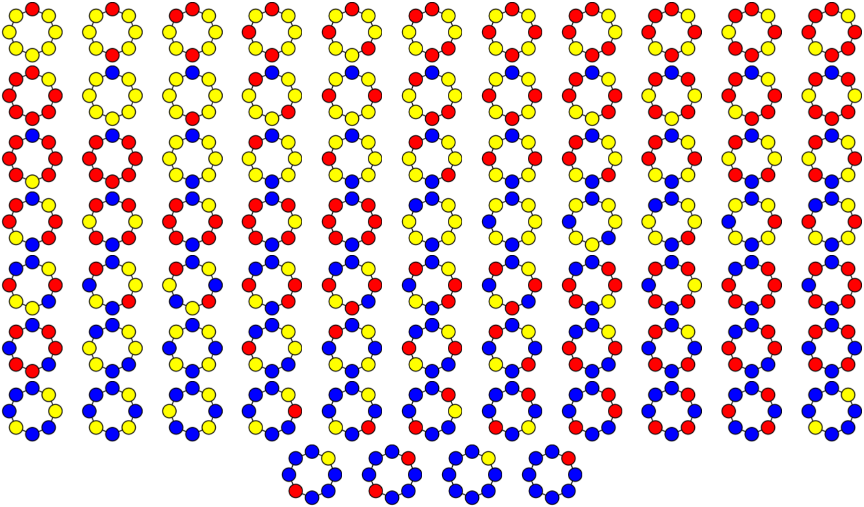

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Theorem. (Bushaw, C., Bardenova, Fay, Tennant, 2025)

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($\Longrightarrow$) Suppose $f : V(C_n) \longrightarrow \{1, \ldots, k\}$ is surjective and WLOG the set $f^{-1}(1)$ is not a maximizer of W on C_n. We must show that there is a surjective $f' : V(C_n) \longrightarrow \{1, \ldots, k\}$ with the same type as f and whose color classes are all maximizers of W.

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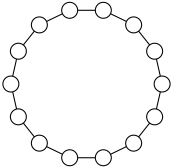
Idea: For a fixed type, say $(2, 3, 4, 5)$, how do we find such an f'?



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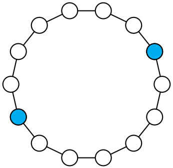

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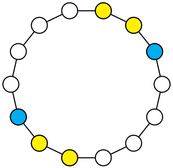

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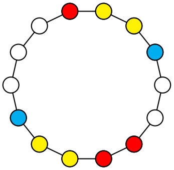

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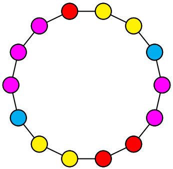
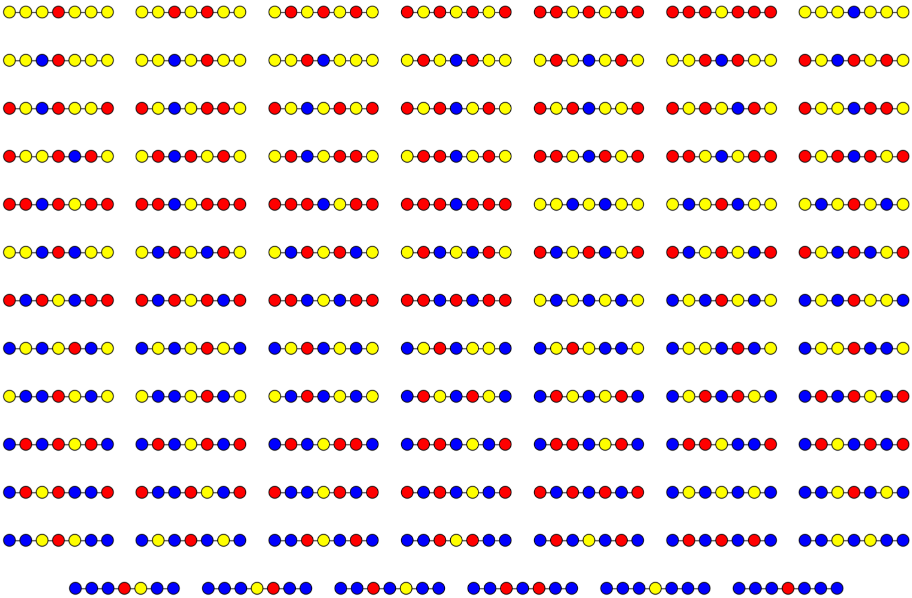


3-color weak maximizers of W on P_7



3-color weak maximizers on paths

Example.

Suppose we want to find the 3-color weak maximziers on P_{14} with type $t = (\text{blue, yellow, red}) = (2, 6, 6)$.

type	max	# maxs
$r^1 = (2, 6, 6)$	$m_1 = 6$	2
$r^2 = (2, 4, 4)$	$m_2 = 4$	2
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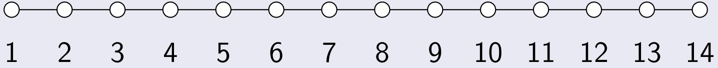
$r^4 = (0, 0, 0)$		



The collection of all such colorings is denoted $\mathcal{C}_{(2,6,6)}$.

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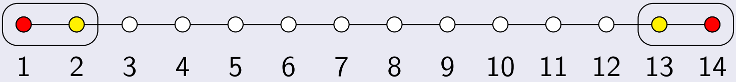

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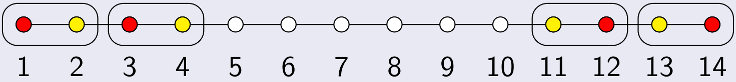

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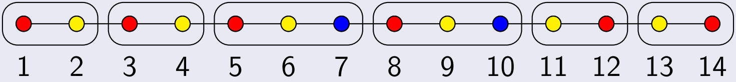

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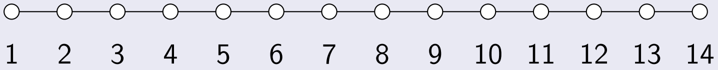

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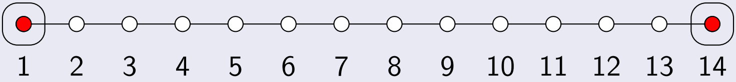

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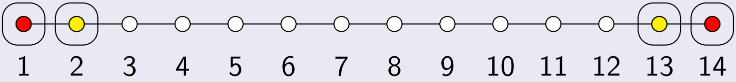

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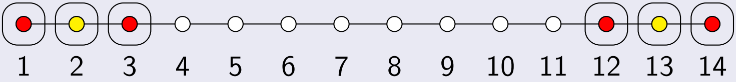

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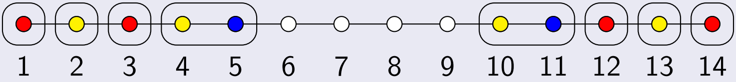

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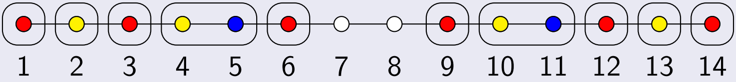

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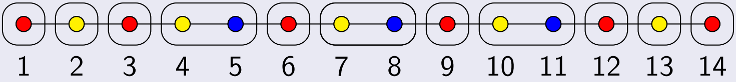
$r^7 = (0,0,0)$		



The collection of all such colorings is denoted $\mathcal{C}_{(2,6,6)}$.

k-color weak maximizers on paths

Theorem. (Bushaw, C., Bardenova, Fay, Tennant, 2025)

Suppose $1 \leq k \leq n$ are integers and $f : V(P_n) \longrightarrow [k]$ is a surjective function. The following are equivalent.

1. f is a k-color weak maximizer of W on P_n.
2. f is a k-color local weak maximizer of W on P_n.
3. $f \in \mathcal{C}_{\mathrm{type}(f)}$.

Majorization

The *majorization order* on $\mathbb{R}^k$ was introduced by Schur (1923), studied by many authors such as Hardy, Littlewood and Polya (1929), in the context of inequalities involving functions $\mathbb{R}^k \longrightarrow \mathbb{R}$.

For $x = (x_1, \ldots, x_k) \in \mathbb{R}^k$ let $x^{\downarrow} = (x_{[1]}, \ldots, x_{[k]})$ be x arranged in non-increasing order, that is $x_{[1]} \geq \cdots \geq x_{[k]}$.

$(x_1, \ldots, x_k) \prec (y_1, \ldots, y_k)$ means that:

$$
\begin{aligned}
x_{[1]} &\leq y_{[1]} \\
x_{[1]} + x_{[2]} &\leq y_{[1]} + y_{[2]} \\
&\vdots \\
x_{[1]} + \cdots + x_{[k-1]} &\leq x_{[1]} + \cdots + x_{[k-1]} \\
x_{[1]} + \cdots + x_{[k]} &= x_{[1]} + \cdots + x_{[k]}
\end{aligned}
$$

Idea: $x \prec y$ indicates that x is "more equitable" than y.

Examples of majorization

How do you compare the “equitability” of $(2, 3, 3, 4, 5)$ and $(2, 2, 4, 4, 5)$?

$$(2, 2, 4, 4, 5)$$

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Examples of majorization

How do you compare the "equitability" of $(2, 3, 3, 4, 5)$ and $(2, 2, 4, 4, 5)$?

$$\left(\frac{17}{5}, \frac{17}{5}, \frac{17}{5}, \frac{17}{5}, \frac{17}{5}\right) \prec (2, 3, 3, 4, 5) \prec (2, 2, 4, 4, 5)$$

Majorization on types of colorings

Theorem. (Bushaw, C., Bardenova, Fay, Tennant, 2025)

Suppose $G \in \{C_n, P_n\}$ and $f, f' : V(G) \longrightarrow \{1, \ldots, k\}$ are k-color weak maximizers of W on G. If $\mathrm{type}(f) \prec \mathrm{type}(f')$ and $\mathrm{type}(f) \neq \mathrm{type}(f')$ then $W(f) < W(f')$.

- So, for these two types of graphs C_n and P_n, the less equitable a k-color weak maximizer is, the larger its Wiener index will be.
- The proof uses the above characterizations of k-color weak maximizers on C_n and P_n.
- Note that if f or f' are not k-color weak maximizers of W on one of these graphs, then $\mathrm{type}(f) \prec \mathrm{type}(f')$ and $\mathrm{type}(f) \neq \mathrm{type}(f')$ does not necessarily imply $W(f) < W(f')$.

Open Question.

Can this theorem be generalized to any other graphs?

Open questions

- What are the k-color **local** weak maximizers on C_n?
  - If $f : V(C_n) \longrightarrow \{1, \dots, k\}$ is surjective and not a k-color weak maximizer of W, does there exist an edge $\{u, v\} \in E(C_n)$ such that $W(f) < W(S_{u,v}(f))$?

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- What are the k-color (local) weak maximizers on other graphs?
  - $P_n \Box P_m$ (grids)
  - $C_n \Box C_m$ (toroidal graphs)
  - $P_n \Box C_m$ (cylinders)
  - M_{2n} (Möbius ladders)

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- Other interactions:
  - For $A \subseteq V(G)$ define

$$H(A) = \sum_{\{u,v\} \in \binom{A}{2}} \frac{1}{d(u, v)}.$$

  - For $f : V(G) \longrightarrow \{1, \ldots, k\}$ define

$$H(f) = \sum_{i=1}^{k} H(f^{-1}(i)).$$

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