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All I Really Need To Know, I Learned From Dr. Z

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All I Really Need To Know, I Learned From Dr. Z

Andrew Sills

Georgia Southern University
Opinion 60: Still Like That Old Time Blackboard Talk
Opinion 60: Still Like That Old Time Blackboard Talk

Opinion 106: Use LARGE FONTS
Opinion 60: Still Like That Old Time Blackboard Talk

Opinion 106: Use **LARGE FONTS**

Opinion 104: “For the good of future mathematics we need *generalists* and *strategians*”
A tree is a connected, acyclic graph.
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The degree sequence of a graph is the multiset of the degrees of all the vertices, arranged in nonincreasing order.
A tree is a connected, acyclic graph.

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The degree sequence of a graph is the multiset of the degrees of all the vertices, arranged in nonincreasing order.

Trees have $n$ vertices, and $n - k$ leaves.
The *Wiener Index* $W(T)$ of a tree with vertex set \( \{v_1, v_2, \ldots, v_n\} \) is given by

\[
W(T) := \sum_{1 \leq i < j \leq n} d(v_i, v_j),
\]

where $d(v_i, v_j)$ is the number of edges in the path from $v_i$ to $v_j$. 
Introduced by Harry Wiener as the path number $w$ in
Wiener Index

Among all trees with given degree sequence

\[ d_1 \geq d_2 \geq \cdots \geq d_k > 1 = d_{k+1} = d_{k+2} = \cdots = d_n, \]

find the one(s) with maximal Wiener index.
$d_1 = 3, d_2 = 2, d_3 = 2, d_4 = d_5 = d_6 = 1$
\[ d_1 = 3, \quad d_2 = 2, \quad d_3 = 2, \quad d_4 = d_5 = d_6 = 1 \]
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\[
\begin{array}{c}
2 \\
\downarrow \\
1 \quad 3 \\
\downarrow \\
2 \quad 1 \\
\downarrow \\
1 \\
\downarrow \\
31 \\
\end{array}
\]
\[d_1 = 3, \quad d_2 = 2, \quad d_3 = 2, \quad d_4 = d_5 = d_6 = 1\]
$b_1 = 2, b_2 = 1, b_3 = 1$

\[
\begin{array}{c}
2 \\
\hline
1 & 3 \\
\hline
2 & 1 \\
\hline
1 \\
\end{array}
\quad
\begin{array}{c}
1 \\
\hline
3 \\
\hline
2 & 1 \\
\hline
2 \\
\hline
1 \\
\end{array}
\]

31 32
A *caterpillar* is a tree which contains a central path $S$ (the “spine”) in which every edge is contained in, or incident to, $S$. 
If $T$ is a tree with the maximal Wiener index for a given degree sequence, then $T$ is a caterpillar.
Let $T$ be a caterpillar with nonleaf spine vertices having degrees $z_1, z_2, \ldots, z_k$ in that order. Then

$$W(T) = (n - 1)^2 + \sum_{1 \leq i < j \leq k} (j - i)(z_i - 1)(z_j - 1).$$
Theorem

Let $T$ be a caterpillar with nonleaf spine vertices having degrees

$$1 + y_1, 1 + y_2, \ldots, 1 + y_k$$

in that order. Then

$$W(T) = (n - 1)^2 + \sum_{1 \leq i < j \leq k} (j - i) y_i y_j$$
The Problem

\[ W(T) = (n - 1)^2 + \sum_{1 \leq i < j \leq k} (j - i)y_iy_j. \]

Thus we seek a permutation \( y_1, \ldots, y_k \) of the \( b_1, \ldots, b_k \) which maximizes

\[ F(y_1, y_2, \ldots, y_k) := \sum_{1 \leq i < j \leq k} (j - i)y_iy_j, \]

where \( b_i = d_i - 1 \) for all \( i \).
There are $2^{k-2}$ “candidate permutations.”
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They have a natural binary encoding from 0 to $2^{k-2} - 1$,

Let $P_j$ denote the evaluation of $F(y_1, y_2, \ldots, y_k)$,

e.g. in the case $k = 5$, we have $P_{101} = P_5 = F(b_1, b_3, b_5, b_4, b_2)$
\[ P_{101} = P_5 = F(b_1, b_3, b_5, b_4, b_2) \]
Use high school algebra!
Many candidates can be “weeded out” from consideration easily via “adjacent comparisons,” e.g.

\[ P_1 - P_0 = (b_1 + b_2 + \cdots + b_{k-2})(b_{k-1} - b_k) \geq 0 \]

\[ P_2 - P_1 = 2(b_1 + b_2 + \cdots + b_{k-3})(b_{k-2} - b_{k-1}) \geq 0 \]
Observations

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The initial weed out is a subset of

\[ \{ P_0, P_1, P_2, \ldots, P_{\lfloor \frac{2}{3} \cdot 2^{k-2} \rfloor} \} \]
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The initial weed out is a subset of

\[ \{ P_0, P_1, P_2, \ldots, P_{\left\lfloor \frac{2}{3} \cdot 2^{k-2} \right\rfloor} \} \]

\[ \ldots \text{of cardinality} \]

\[ \binom{k-2}{\left\lfloor \frac{k-2}{2} \right\rfloor} + \binom{k-3}{\left\lfloor \frac{k-2}{2} \right\rfloor}. \]
\[ \left\lfloor \frac{2}{3} \cdot 2^{k-2} \right\rfloor \] is A000975 in OEIS.
Observations

- \( \left\lfloor \frac{2}{3} \cdot 2^{k-2} \right\rfloor \) is A000975 in OEIS.

- \( \left\{ \left( \frac{k-2}{k-2} \right) + \left( \frac{k-3}{k-2} \right) \right\} \) is A050168.
Observations

- \( \{ \left\lfloor \frac{2}{3} \cdot 2^{k-2} \right\rfloor \} \) is A000975 in OEIS.

- \( \{ (\left\lfloor \frac{k-2}{k-2} \right\rfloor) + (\left\lfloor \frac{k-3}{k-2} \right\rfloor) \} \) is A050168.

Thank you, Neil Sloane!
Sometimes nonadjacent entries in the bottom of the binary tree also factor and lead to a “secondary weed out,” e.g.

\[ P_{11} - P_7 = 2(b_{k-4} - b_{k-3})(2b_1 + 2b_2 + \cdots + 2b_{k-5} - b_{k-2} + b_k) \geq 0. \]
Zhang, Liu and Han (2009)
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- $k = 4$: $P_{11}$ is always maximal.
- $k = 5$:
  - $P_{111}$ is uniquely maximal if $b_1 - b_2 - b_3 > 0$.
  - $P_{110}$ is uniquely maximal if $b_1 - b_2 - b_3 < 0$. 
Maximality Characterizations For Small $k$

Zhang, Liu and Han (2009)

- $k = 4$: $P_{11}$ is always maximal.
- $k = 5$:
  - $P_{111}$ is uniquely maximal if $b_1 - b_2 - b_3 > 0$.
  - $P_{110}$ is uniquely maximal if $b_1 - b_2 - b_3 < 0$.
  - $P_{110}$ and $P_{111}$ tie for maximality if $b_1 - b_2 - b_3 = 0$. 
Maximality Characterizations For Small $k$

Zhang, Liu and Han (2009)

- $k = 4$: $P_{11}$ is always maximal.

- $k = 5$:
  - $P_{111}$ is uniquely maximal if $b_1 - b_2 - b_3 > 0$.
  - $P_{110}$ is uniquely maximal if $b_1 - b_2 - b_3 < 0$.
  - $P_{110}$ and $P_{111}$ tie for maximality if $b_1 - b_2 - b_3 = 0$.

- $k = 6$: 11 cases.
Maximality Characterizations for Small $k$

- $P_{1111}$ is uniquely maximal if $b_1 - b_2 - b_3 - b_4 > 0$.
- $P_{1111}$ and $P_{1110}$ tie for maximality if $b_1 - b_2 - b_3 - b_4 = 0$.
- $P_{1110}$ is uniquely maximal if $b_1 - b_2 - b_3 - b_4 < 0$ and $b_1 - b_2 - b_3 > 0$.
- $P_{1110}$ and $P_{1101}$ tie for maximality if $b_1 - b_2 - b_3 = 0$.
- $P_{1101}$ is uniquely maximal if $b_1 - b_2 - b_3 < 0$ and $b_1 - b_2 - b_3 + b_4 > 0$ and $3b_1 - 3b_2 - b_5 + b_6 > 0$.
- $P_{1101}$ and $P_{1100}$ tie for maximality if $b_1 - b_2 - b_3 = 0$ and $3b_1 - 3b_2 - b_5 + b_6 > 0$.
- $P_{1101}$ and $P_{1011}$ tie for maximality if $3b_1 - 3b_2 - b_5 + b_6 = 0$ and $b_1 - b_2 - b_3 + b_4 > 0$.
- $P_{1101}$, $P_{1100}$, and $P_{1011}$ are in a three-way tie for maximality if $3b_1 - 3b_2 - b_5 + b_6 = 0$ and $b_1 - b_2 - b_3 + b_4 = 0$. 
Maximality Characterizations for Small $k$

- $P_{1100}$ is uniquely maximal if $3b_1 - 3b_2 - b_5 + b_6 \geq 0$ and $b_1 - b_2 - b_3 + b_4 < 0$; or if $3b_1 - 3b_2 - b_5 + b_6 \leq 0$ and $3b_3 - b_4 - b_5 + b_6 > 0$.

- $P_{1011}$ is uniquely maximal if $b_1 - b_2 - b_3 + b_4 \geq 0$ and $3b_1 - 3b_2 - b_5 + b_6 < 0$.

- $P_{1011}$ and $P_{1100}$ tie for maximality if $3b_1 - 3b_2 - b_5 + b_6 < 0$ and $3b_3 - 3b_4 - b_5 + b_6 = 0$. 
For $k = 7$ there are 1312 cases.
For $k < 9$, the initial and secondary weed out show that the optimal permutation cannot be on the left side of the binary tree.
Conjectures and Questions

For \( k < 9 \), the initial and secondary weed out show that the optimal permutation cannot be on the left side of the binary tree.

For \( k \geq 9 \), can there be an optimal permutation on the left side, i.e. where \( b_2 = y_2 \)?