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

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- Opinion 106: Use LARGE FONTS

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- Opinion 106: Use LARGE FONTS
- Opinion 104: “For the good of future mathematics we need *generalists* and *strategians*”

Joint Work with HUA WANG

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- Trees have n vertices, and $n - k$ leaves.

Wiener Index

The *Wiener Index* $W(T)$ of a tree with vertex set $\{v_1, v_2, \ldots, v_n\}$ is given by

$$W(T) := \sum_{1 \le i < j \le n} d(v_i, v_j),$$

where $d(v_i, v_j)$ is the number of edges in the path from v_i to v_j.

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"Structural Determination of Paraffin Boiling Points,"
J. Am. Chem. Soc. **69** (1947) 17–20.

The Problem

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.

Example

$d_1 = 3, d_2 = 2, d_3 = 2, d_4 = d_5 = d_6 = 1$

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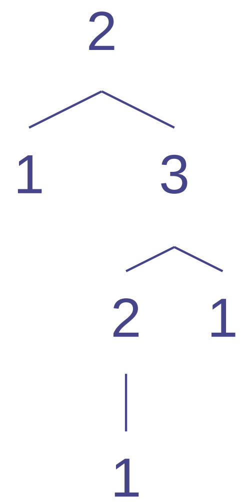

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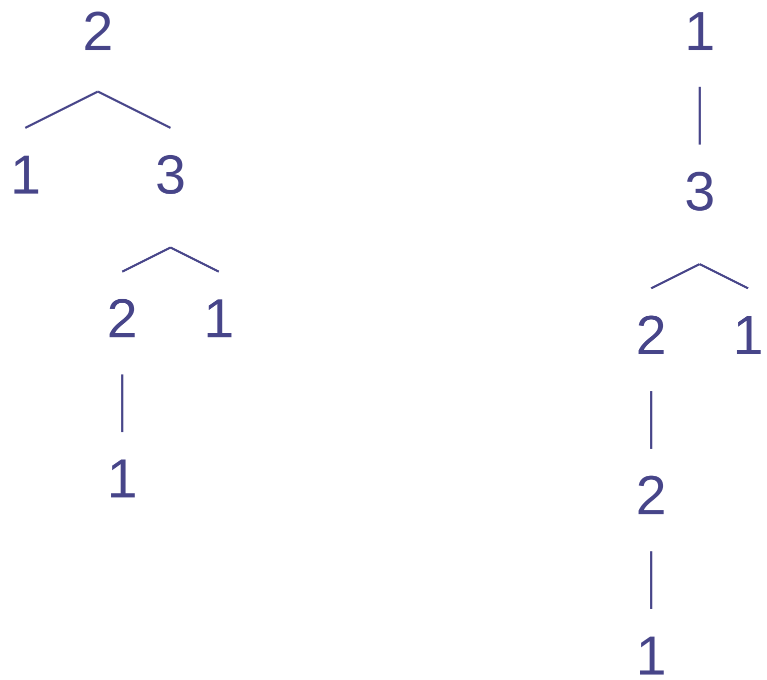

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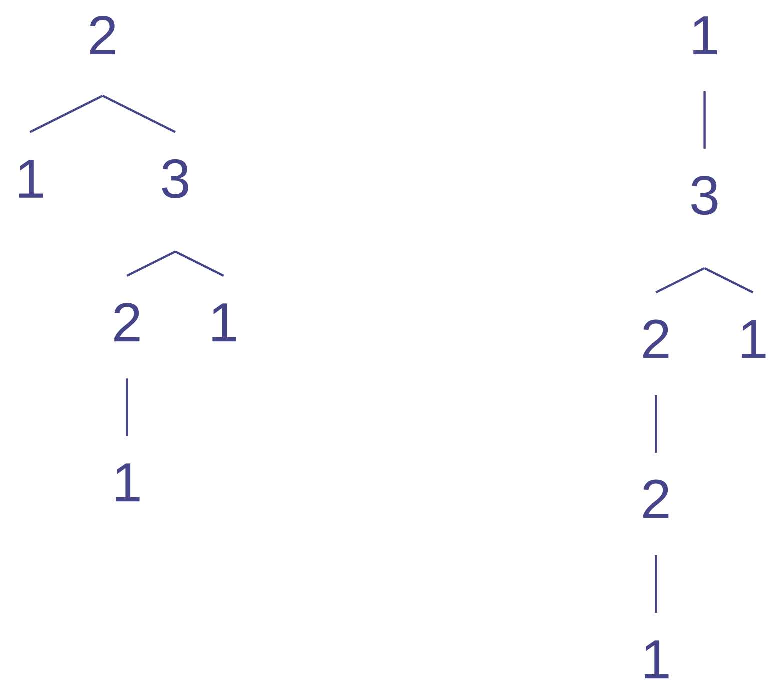

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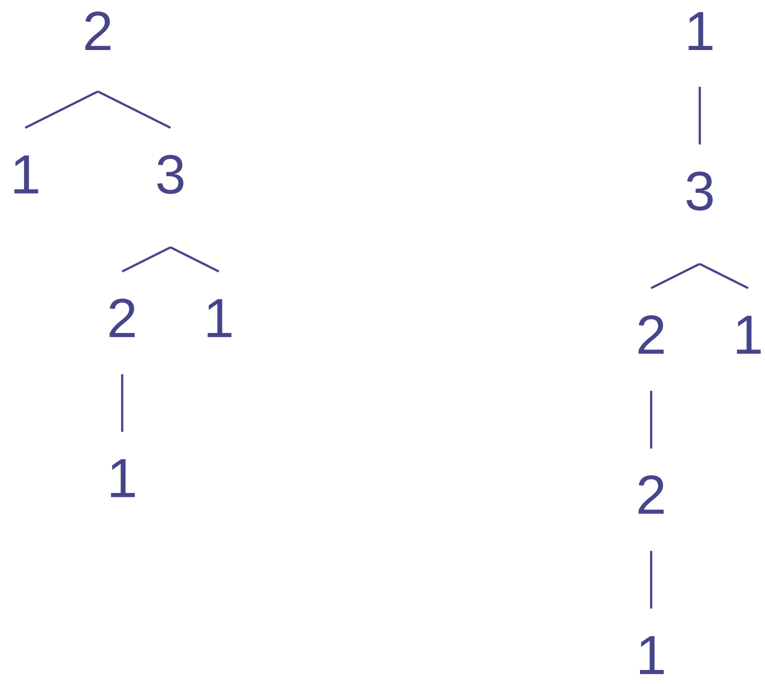
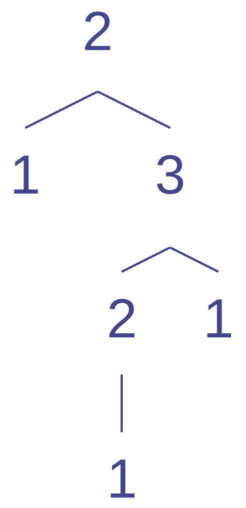


31 32

Example

$b_1 = 2, b_2 = 1, b_3 = 1$



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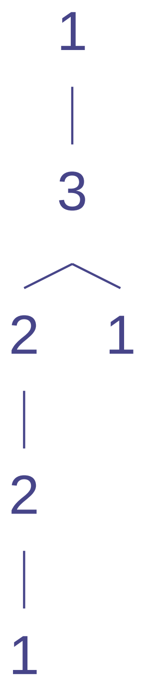

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Definition

A *caterpillar* is a tree which contains a central path S (the "spine") in which every edge is contained in, or incident to, S.

Theorem

If T is a tree with the maximal Wiener index for a given degree sequence, then T is a caterpillar.

Theorem

Let T be a caterpillar with nonleaf spine vertices having degrees

$$z_1, z_2, \ldots, z_k$$

in that order.
Then

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

Theorem

Let T be a caterpillar with nonleaf spine vertices having degrees

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The Problem

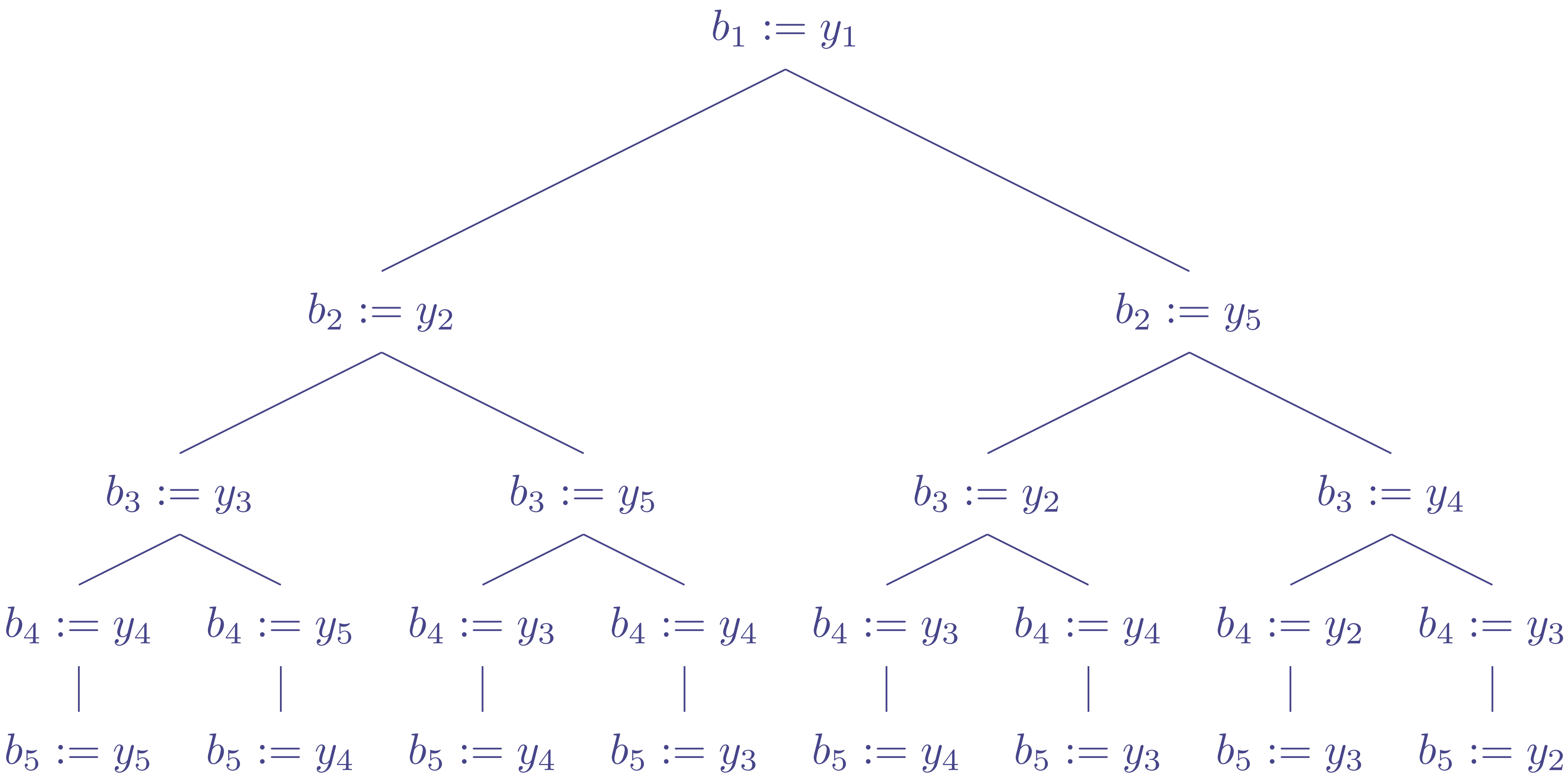
$$W(T) = (n-1)^2 + \sum_{1 \le i < j \le k} (j-i) y_i y_j .$$

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

$$F(y_1, y_2, \ldots, y_k) := \sum_{1 \le i < j \le k} (j-i) y_i y_j ,$$

where $b_i = d_i - 1$ for all i.

$k = 5$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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
  $P_{101} = P_5 = F(b_1, b_3, b_5, b_4, b_2)$

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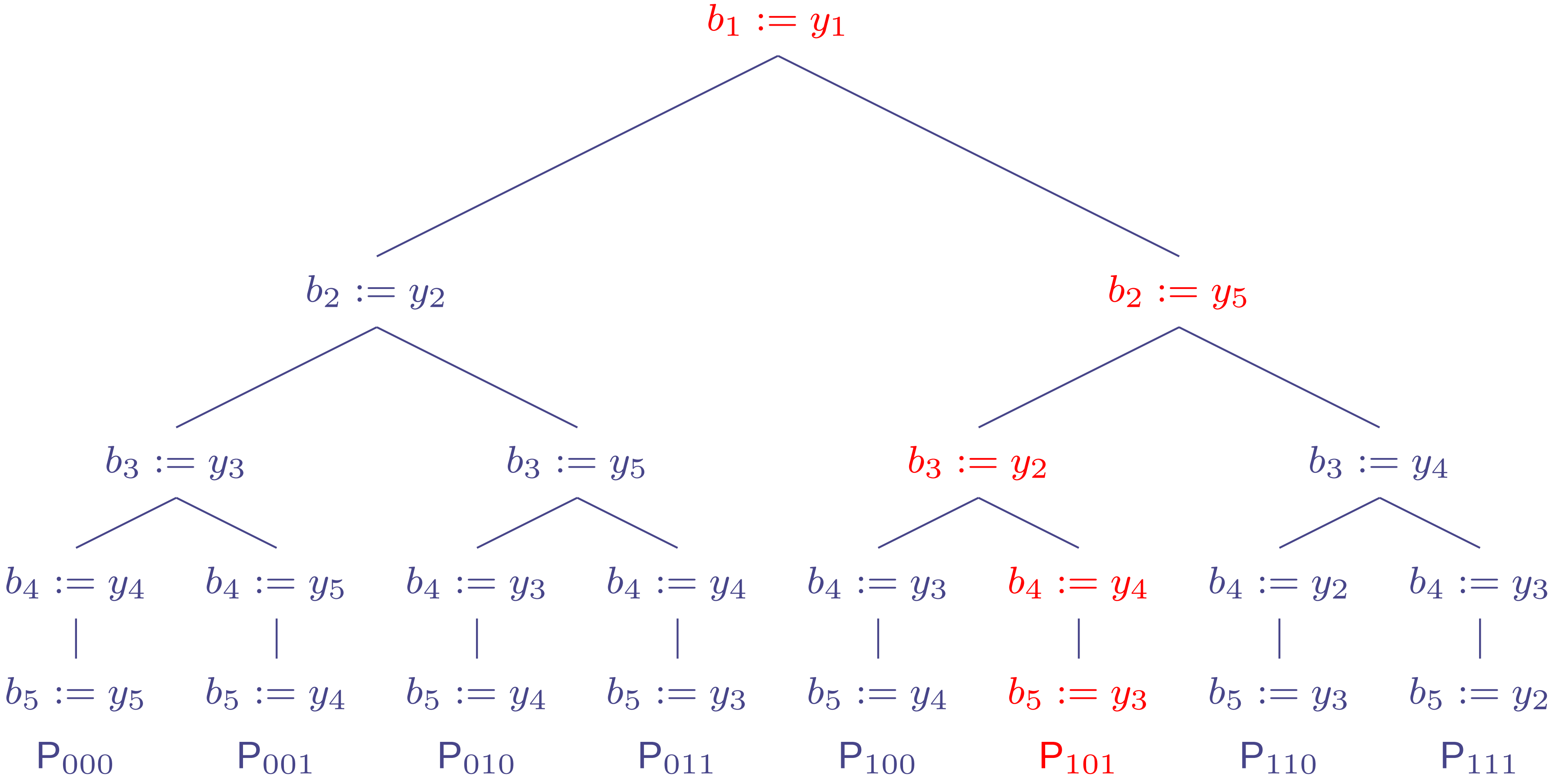

Opinion 74

Use high school algebra!

Observations

- Many candidates can be “weeded out” from consideration easily via “adjacent comparisons,” e.g.

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

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

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. . . of cardinality

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-  Thank you, Neil Sloane!

Observations

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

$$P_{11} - P_7 = 2(b_{k-4} - b_{k-3})(2b_1 + 2b_2 + \cdots + 2b_{k-5} - b_{k-2} + b_k) \geq 0.$$

Maximality Characterizations For Small k

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  - P_{110} and P_{111} tie for maximality if $b_1 - b_2 - b_3 = 0$.

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  - 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 maximiality 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 $3b_3 - 3b_4 - b_5 + b_6 = 0$.

Maximality Characterizations For Small k

For $k = 7$ there are 1312 cases.

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.

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- 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 $b_2 = y_2$?

Happy Birthday, Doron!