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PATTERNS IN TREES*

Nachum DERSHOWITZ
Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

Shmuel ZAKS
Department of Computer Science, Technion, Haifa 32000, Israel

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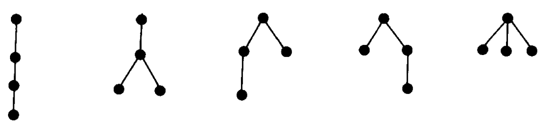
We give a general formula for the number of occurrences of a pattern, or set of patterns, in the class of ordered (plane-planted) trees with a given number of edges. The proof is combinatorial. Many known enumerations of ordered and binary trees are special cases of this formula.

1. Introduction

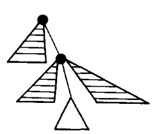
An *ordered* (or "plane-planted") tree is a tree in which the order of the outgoing edges of each node is significant. The *degree* of a node is the number of outgoing edges it has. By T_n we denote the class of ordered trees with n edges; the number of trees in T_n is the well-known Catalan number

$$C_n = |T_n| = \frac{1}{n+1}\binom{2n}{n} \approx \frac{4^n}{(n+1)\sqrt{\pi n}}.$$

We draw trees with the root at the top and with outgoing edges pointing downwards. For example, the five trees in T_3 are



A "pattern" is like an ordered tree except that it also contains "open" and "closed" slots. For example, the pattern



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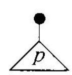
occurs wherever a node has a grandchild through its youngest child. The slots in the pattern are depicted as triangles and match any subtree, including the trivial (single-node) tree. An open slot is depicted as an unshaded triangle hanging off an edge (where a node would otherwise be); a closed slot, as a shaded triangle hanging off a node (like an edge). Slots may not be adjacent in a pattern.

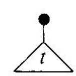
We are interested in enumerating occurrences of patterns in classes of ordered trees. For example, the above pattern occurs five times in the above class T_3, twice in the first tree (once at the root and once at its only child), twice in the second (once for each of the root's two grandchildren), and once in the fourth. Formally, we have four cases:

(1) The pattern ● occurs at any leaf (that is, end vertex of degree 0).

(2) An open slot $\triangle$ or closed slot $\blacktriangle$ occurs at any nonempty subtree (of at least one node).

(3) If a pattern p occurs at a tree t,

then the pattern 

occurs at the tree 

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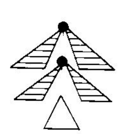
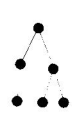
(4) If p occurs at t and p' occurs at t', and $p \vdots p'$ is a legal pattern (i.e. has no adjacent slots), then $p \vdots p'$ occurs at $t \vdots t'$.

The composite pattern $p \vdots p'$ is obtained by merging the roots of two patterns, with p to the left and p' to the right; similarly, $t \vdots t'$ is the result of merging the roots of two trees t and t'. Thus, $p \vdots p'$ appears at $t \vdots t'$, if the latter can be decomposed into two subtrees, with p occurring at the left part t and p' occurring at the right part t'.

Each occurrence of a pattern p in a tree t defines a one-to-one correspondence from the nodes in p (including nodes at the top of closed slots) into the nodes of t (cases (1) and (3)) and from edges in p (including those from which an open slot hangs) into those in t (case (3)), which preserves the edge-incidence relation. The number of occurrences of p in t is the number of distinct correspondences. For example, the pattern

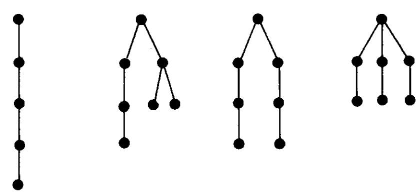


occurs four times in the tree



once for each grandparent-grandchild relationship (three times at the root and once at its oldest child).

Closed slots act like a variable number (including zero) of open slots. The distinction between open and closed slots becomes important when considering occurrences of more than one pattern. To denote a multiset of patterns, we write $\{n_1 * p_1, n_2 * p_2, \ldots, n_k * p_k\}$, where n_i is the number of instances of the pattern p_i in the multiset. A multiset of patterns occurs in a tree if each of its individual patterns occurs and the nodes of their occurrences are disjoint. An occurrence of such a multiset of patterns in a tree t defines a one-to-many correspondence from each node in a pattern p_i to n_i nodes of t and from each edge in p_i to n_i edges in t, such that the incidence relation is preserved. The number of occurrences is the number of such correspondences. Note that one pattern may occur at the same subterm as that matched by an open slot of another, but that a tree node corresponding to the root of a closed slot cannot match any other node in the patterns (since that would make one node of the tree correspond to more than one pattern node). For example, the multiset of two of the above grandparent-grandchild patterns occurs six times among the four trees



once in the first tree, twice in the second, and three times in the third. It does not occur in the fourth tree at all, since any two such relations share the grandparent node.

2. Enumeration formula

Our main result is the following:

Theorem 2.1. *The total number of occurrences of a multiset*

$$\{n_1 * p_1, n_2 * p_2, \ldots, n_k * p_k\}$$

of patterns among all ordered trees with n edges is

$$\frac{1}{n-e+d+1}\binom{n-e+d+1}{n+1-\upsilon, n_1, n_2, \ldots, n_k}\binom{2n-\upsilon+c-e}{n-e},$$

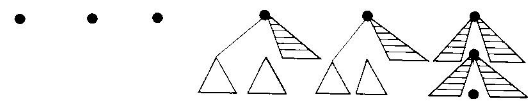
where e is the total number of edges in the patterns, υ is the total number of nodes in the patterns, c is the total number of closed slots, and d is the total number of open slots.

The second factor is the multinomial coefficient

$$\frac{(n-e+d+1)!}{(n+1-v)! \cdot n_1! \cdot n_2! \cdots n_k!}$$

and is taken to be 0 when $n+1<v$. Note that $v+d=e+n_1+\cdots+n_k$.

For example, the number of occurrences of the multiset



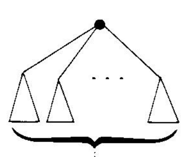
of patterns (three leaves, two nodes of degree at least two, and one leaf at level two or below) in the class T_8 of 1430 ordered trees with eight edges ($n=8$, $k=3$, $n_1=3$, $n_2=2$, $n_3=1$, $e=6$, $v=8$, $c=6$, and $d=4$) is

$$\frac{1}{7}\binom{7}{1,3,2,1}\binom{8}{2}=1680.$$

Proof of Theorem 2.1. The patterns leave $n+1-v$ of the nodes in a tree unrestricted, for each of which a single closed slot pattern $\triangle$ is added. The $\sum n_i+n+1-v=n-e+d+1$ patterns can be arranged in sequence in

$$\binom{n-e+d+1}{n+1-v, n_1, n_2, \ldots, n_k}$$

ways. The $c+n+1-v$ closed slots now present can each be replaced with an open slot pattern of the form



for some i, $i\geq 0$, in

$$\binom{(c+n+1-v)+(n-e)-1}{n-e}=\binom{2n-v+c-e}{n-e}$$

ways, such that among themselves the new patterns contain the $n-e$ edges unaccounted for in the given patterns.

Each of the

$$\binom{n-e+d+1}{n+1-v, n_1, n_2, \ldots, n_k}\binom{2n-v+c-e}{n-e}$$

such sequences is placed on a cycle; each such cycle of patterns can be put together in a unique way to form a tree. To see this, we adapt the Cycle Lemma in [9] (see

[7]). There are $n-e+d$ open slots among the $n-e+d+1$ patterns. If $n-e+d>0$, then there must be at least one slotless pattern p that is followed by a pattern q with slots. Removing p from the cycle and grafting it into the leftmost slot of q leaves a cycle with one less pattern and one less slot. Continuing to graft in this manner until no slots remain, one ends up with a single (slotless) tree. Since the order of grafting does not change the outcome, and filling one slot does not affect the filling of another, the resultant tree is unique.

Thus, of every $n-e+d+1$ sequences of patterns that give the same cycle, exactly one can be coalesced, by grafting adjacent patterns, to yield a tree. Our formula follows. Since each distribution of edges into the closed slots corresponds to a different occurrence, the formula enumerates occurrences, not trees. Since only open slots are filled, the patterns do not share nodes. □

Alternatively, this theorem can be proved using generating functions [30], with Lagrange inversion playing a role analogous to that of the Cycle Lemma (see, e.g., [11]).

The above formula counts trees whenever there can be at most one occurrence of the multiset of patterns in a tree. It generalizes the following known enumerations:

- (Harary, Prins, and Tutte [15]) the Catalan number

$$\frac{1}{n+1}\binom{2n}{n}$$

for unrestricted ordered trees with n edges ($k=0$, $e=\upsilon=c=d=0$);

- (Cayley [3]) the Catalan number

$$\frac{1}{2r+1}\binom{2r+1}{r}$$

for unrestricted binary (degree-2) trees with r binary nodes and $2r$ leaves ($n=2r$, $k=2$, $n_1=r$, $n_2=2r$, $e=d=2r$, $\upsilon=3r$, $c=0$);

- (Tutte [31]) the multinomial formula

$$\frac{1}{n+1}\binom{n+1}{n_0, n_1, \ldots, n_n}$$

for enumerating trees with n_i nodes of degree i and a total of n edges ($k=n$, $e=d=n$, $\upsilon=n+1$, $c=0$);

- (Flajolet and Steyaert [10]) the binomial formula

$$\binom{2n-2e+d-1}{n-e}$$

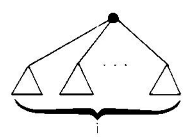
for occurrences of a single pattern with no closed slots (and no leaves), containing d open slots and e edges, among all ordered trees with n edges ($k=1$, $n_1=1$, $\upsilon=e-d+1$, $c=0$) and the binomial formula

$$\binom{2r-u+1}{r+1}$$

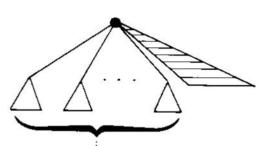
for occurrences of a single pattern, containing u binary nodes and no leaves, among all binary trees with r binary nodes ($n=e=2r$, $k=2$, $n_1=1$, $n_2=r-u$, $v=r$, $c=0$, $d=2r-u+1$).

3. Applications

The pattern enumeration formula of the previous section has wide applicability. We give here some corollaries and representative illustrations, using the following notations: T_n for the class of ordered trees with n edges; B_r^t for the subclass of T_{tr} in which all r internal (nonleaf) nodes are of degree t; $B_r = B_r^2$ is the class of binary trees. In the following, all trees in T_n, B_r^t, or B_r are assumed equiprobable. We let Δ_i denote the pattern for a node of degree i:



and $\Delta_{\geq i}$ the pattern:



See [12] for a survey of tree enumerations. We make free use of identities in [18, 23] for evaluating combinatorial expressions in what follows.

3.1. Tree enumeration

When there can be at most one occurrence of a multiset of patterns per tree, our formula counts trees. This is the case, in particular, when the patterns cover all the nodes in the tree (i.e. $v=n+1$), there is at most one closed slot at any pattern node, and no two different patterns can occur at the same node (i.e. they do not "overlap" each other). Then, we have

$$\frac{1}{m}\binom{m}{n_1,\ldots,n_k}\binom{2n-m-2e+s}{n-e}$$

trees in T_n composed of m patterns $\{n_1 * p_1, \ldots, n_k * p_k\}$, $m=\sum n_i$, containing a total of s slots of either kind ($s=c+d$) and e edges. (If there are no closed slots, the last factor is 0 or 1.) More generally, inclusion/exclusion arguments can often be used to enumerate trees.

3.1.1. According to Theorem 2.1, the total number of occurrences of the patterns $\{i*\Delta_{\ge b}\}$ in T_n is

$$\frac{1}{n+1}\binom{n+1}{i}\binom{2n-ib}{n}$$

($n_1=v=c=i$, $e=d=ib$). Thus, the number of trees in T_n, all of whose nodes have degree less than b, is given by inclusion/exclusion:

$$\frac{1}{n+1}\sum_{i=1}^{\lfloor n/b\rfloor}(-1)^i\binom{n+1}{i}\binom{2n-ib}{n}$$

(cf. [17]). For $b=3$, this gives the number of "unary-binary" trees containing only leaves, unary (degree-1) nodes, and binary (degree-2) nodes:

$$\frac{1}{n+1}\sum_{i=1}^{\lfloor n/3\rfloor}(-1)^i\binom{n+1}{i}\binom{2n-3i}{n}=\sum_{k=0}^{\lfloor n/2\rfloor}\binom{n}{2k}C_k.$$

These are the same as the numbers for polygon partitions appearing in [20] (see [8]).

3.1.2. The number of trees in T_n with exactly l leaves is equal to the number of occurrences of $\{l*\Delta_0,(n+1-l)*\Delta_{\ge 1}\}$. Since the patterns cover all the nodes, we can let $n_1=l$, $n_2=e=n+1-l$, $m=n+1$, and $s=2e$ in the above formula, and obtain

$$\frac{1}{n+1}\binom{n+1}{l}\binom{n-1}{l-1}.$$

This enumeration appears in [21] in the context of ballots, in [23] in reference to a communication problem, and in [5,24] for trees.

3.1.3. The number of "reduced" ordered trees in T_n with l leaves, having no unary nodes, is equal to the number of occurrences of $\{l*\Delta_0,(n+1-l)*\Delta_{\ge 2}\}$. By letting $n_1=l$, $n_2=n+1-l$, $e=2(n+1-l)$, and $s=3(n+1-l)$, one obtains

$$\frac{1}{n+1}\binom{n+1}{l}\binom{l-2}{n-l}.$$

Summing this for all possible n, one gets a total of

$$\frac{1}{l}\sum_{n=l}^{2l-2}\binom{n}{l-1}\binom{l-2}{n-l}=\frac{1}{l}\sum_{k=0}^{l-2}\binom{k+l}{l-1}\binom{l-2}{k}=\frac{1}{2}\sum_{k=0}^{l-1}\binom{l+k-1}{2k}C_k$$

l-leaf reduced ordered trees. These numbers were investigated by Schröder [29]; their relation to trees appears in [18, p. 587]. For given n, the total number of reduced trees is

$$\frac{1}{n+1}\sum_{l=\lceil n/2\rceil-1}^{n}\binom{n+1}{l}\binom{l-2}{n-l}=\frac{1}{n+1}\sum_{k=1}^{\lfloor n/2\rfloor}\binom{n+1}{k}\binom{n-k-1}{k-1}.$$

Alternatively, one can count each occurrence of m unary nodes Δ_1 $(0\le m\le n)$ in a tree $(e=s=d=n_1=m)$ and use inclusion/exclusion. That gives

$$\frac{1}{n+1}\sum_{m=0}^{n}(-1)^m\binom{n+1}{m}\binom{2n-2m}{n-m}=\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}C_k$$

reduced trees with n edges, which is equal to the previous expression. These enumerations are also related to the Motzkin numbers (see [8,25]).

3.1.4. The total number of trees in B_r^t is [17] equal to the number of occurrences of $\{r*\Delta_t,(t-1)r*\Delta_0\}$ in T_{tr}:

$$\frac{1}{tr+1}\binom{tr+1}{r}=\frac{1}{r}\binom{tr}{r-1}$$

(letting $n=e=tr$, $n_1=r$, $n_2=(t-1)r$, and $s=d=tr$). Grunert [14] gives the analogous result for polygons.

3.2. *Single pattern*

The enumeration formula is substantially simpler when there is exactly one pattern p. Setting k and n_1 to 1, we get

$$\frac{1}{n-e+d+1}\binom{n-e+d+1}{n+1-v,1}\binom{2n-v+c-e}{n-e}=\binom{2n-2e+s-1}{n-e}$$

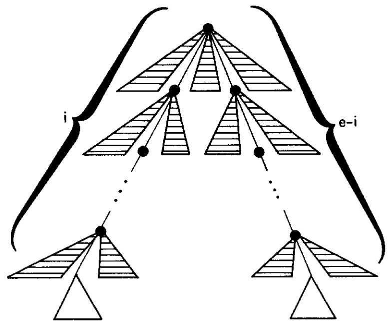
for the number of occurrences of e-edge pattern containing s slots (of any kind) in T_n (cf. [10]).

3.2.1. The expected number of nodes of degree d in a tree in T_n is

$$\frac{\binom{2n-d-1}{n-1}}{\frac{1}{n+1}\binom{2n}{n}}.$$

(Let $p=\Delta_d$, $e=s=d$.) This enumeration appears in [5]. Considering the degree-zero case, the expected number of leaves (or internal nodes, for that matter) is $\frac{1}{2}(n+1)$. The latter result appears also in [4].

3.2.2. The expected distance between nodes in a tree in T_n can be found using the pattern

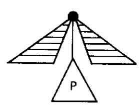


$(s=2e+1)$. There are $\binom{2n}{n-e}$ occurrences of such a pattern and e such patterns for given distance e; hence, the expected distance is [26]

$$\frac{\sum_e e^2\binom{2n}{n-e}}{\binom{n+1}{2}C_n}=\frac{2^{2n-1}}{\binom{2n}{n}}=\tfrac{1}{4}\pi\binom{n}{\frac{1}{2}}\approx\tfrac{1}{2}\sqrt{\pi n}.$$

3.3. Root pattern

A pattern p can be constrained to appear at the root of a tree by enumerating its occurrences and then subtracting the number of occurrences of the pattern



for nonroot occurrences. Using the above formula for a single pattern, we get

$$\binom{2n-2e+s-1}{n-e}-\binom{2n-2e-2+s+2-1}{n-e-1}=\frac{s}{2n-2e+s}\binom{2n-2e+s}{n-e}$$
$$=\frac{s}{n-e}\binom{2n-2e+s-1}{n-e-1}$$

for the number of occurrences of an s-slot, e-edge rooted pattern in T_n. This formula counts trees whenever the pattern can occur only once at the root, i.e. when it has at most one closed slot at each of its nodes.

3.3.1. The number of ordered trees in T_n with root degree r is the number of root occurrences of Δ_r $(e=r)$, viz.

$$\frac{r}{n}\binom{2n-r-1}{n-1}.$$

It follows that the expected root degree of a tree in T_n is

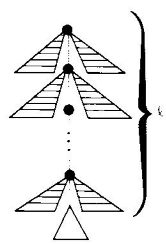
$$\frac{\sum_r r^2 \binom{2n-r-1}{n-1}}{n\,C_n} = \frac{3n}{n+2}.$$

This enumeration appears in [33]; alternative proofs are given in [6, 28] (see also [1]). Higher moments can also be calculated; for example, the variance of the root degree is

$$\frac{\sum_r r^3 \binom{2n-r-1}{n-1}}{n\,C_n} - \left[\frac{3n}{n+2}\right]^2$$

$$= \frac{2\binom{2n}{n+3} + 3\binom{2n+1}{n+3} + \binom{2n+2}{n+3}}{\dfrac{n}{n+1}\binom{2n}{n}} - \left[\frac{3n}{n+2}\right]^2 \approx 1\tfrac{1}{4}.$$

3.3.2. Using the root pattern



($e = l$, $s = 2l + 1$), we can determine the expected number of nodes on level l of a tree in T_n:

$$\frac{\dfrac{2l+1}{2n+1}\binom{2n+1}{n-l}}{C_n}.$$

Thus, the expected level of a node in T_n is

$$\frac{\sum_l l \dfrac{2l+1}{2n+1}\binom{2n+1}{n-l}}{\binom{2n}{n}} = \tfrac{1}{4}\pi\binom{n}{\frac{1}{2}} - \tfrac{1}{2} \approx \tfrac{1}{2}\sqrt{\pi n} - \tfrac{1}{2}.$$

Generating function derivations of this result have been given by Volosin [32], Meir and Moon [19], and Dasarathy and Yang [4].

3.3.3. With a similar pattern, the expected number of leaves on level l of a tree in T_n is found to be

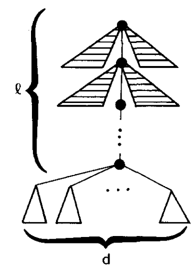
$$\frac{\frac{l}{n}\binom{2n}{n+l}}{C_n} = \frac{l\binom{2n}{n-l}}{\binom{2n}{n-1}}.$$

It also follows that the expected level of a leaf in T_n is

$$\tfrac{1}{4}\pi\binom{n}{\frac{1}{2}} \approx \tfrac{1}{2}\sqrt{\pi n}.$$

The "external path length" of a tree (as defined in [18]) is the sum of the levels of its leaves. Thus, the expected external path length is approximately $\frac{1}{4}(n+1)\sqrt{\pi n}$. In a similar manner, the expected level of an internal node and expected "internal path length" (sum of the levels of its nonleaf nodes) can be computed (see [6]).

3.3.4. The pattern



$(e=l+d,\ s=2l+d)$ counts the total number of nodes in T_n of degree d on level l:

$$\frac{2l+d}{2n-d}\binom{2n-d}{n+l}.$$

This result was first proved by Dershowitz and Zaks [5]; alternative proofs were given by Dershowitz and Zaks [6], Ruskey [26], and Kemp [16]. Thus, the expected degree of a node on level l of a tree in T_n is [5]

$$\frac{\sum_d \frac{2l+d}{2n-d}\binom{2n-d}{n+l}}{\binom{2n}{n}} = \frac{2l+3}{2l+1}\,\frac{n-l}{n+l+2} \approx 1+\frac{2}{2l+1}.$$

3.4. Fixed-arity trees

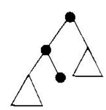
Frequently, one wishes to enumerate patterns in the subclass B_r^t of t-ary trees in T_{tr}. This can be done by adding an appropriate number of patterns Δ_0 and Δ_t, constraining all nonpattern nodes to be of degree zero or t. In particular, for a single

t-ary pattern p, setting $n=e=tr$, and letting u and w denote the number of internal nodes and open slots in p (respectively), one obtains the formula

$$\frac{1}{t(r-u)+w+1}\binom{t(r-u)+w+1}{1,r-u,(t-1)(r-u)+w}\binom{-1}{0}=\binom{t(r-u)+w}{r-u}$$

for the number of occurrences of p in B_r^t. Note that, in the fixed-arity case, there is no point in using closed slots (cf. [10]).

3.4.1. The number of left children having right leaves among the binary trees in B_r is equal to the number of occurrences of the pattern



By letting $t=2$ and $u=w=2$ in the formula, one obtains

$$\binom{2r-2}{r-2}=\binom{2r-2}{r}.$$

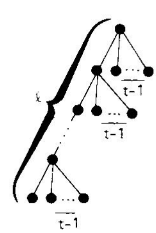
This formula is derived in [2] using generating functions (see also [13]).

3.5. Rooted fixed-arity patterns

The same technique as for ordered trees may be used to restrict a pattern in a t-ary tree to appear at the root. This gives us the following enumeration of t-ary trees containing a pattern with u internal nodes and w open slots:

$$\binom{t(r-u)+w}{r-u}-t\binom{t(r-u-1)+w+t-1}{r-u-1}=\frac{w}{r-u}\binom{t(r-u)+w-1}{r-u-1}.$$

3.5.1. The number of leaves in B_r^t on level l is t^l times the number of occurrences of the rooted pattern



($u=l$, $w=tl-l$). Thus, the expected external path length of a tree in B_r^t is

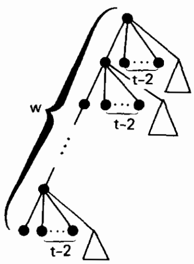
$$\frac{(t-1)\sum_l \frac{t^l l^2}{r-l}\binom{tr-l-1}{r-l-1}}{\frac{1}{r}\binom{tr}{r-1}}.$$

In particular, for binary trees ($t=2$), this simplifies to

$$\frac{4^r+2r}{\frac{1}{r+1}\binom{2r}{r}}-3r+1\approx(r+1)\sqrt{\pi r}-3r+1$$

(see [18, Section 2.3.4.5]).

3.5.2. The number of ordered forests containing w t-ary trees with a total of n internal nodes (of degree t) may be determined by counting the number of occurrences of the rooted pattern



in B^t_{n+w}. It is

$$\frac{w}{tn+w}\binom{tn+w}{n}.$$

4. Conclusion

We have presented general-purpose formulae for the enumeration of occurrences of patterns in ordered, binary, and t-ary trees, and demonstrated their flexibility. It is perhaps instructive to note some of the counting problems for which the formulae are not well-suited. We cannot, for example, express extremum conditions, such as "lowest" node. Nor can we, in general, demand symmetry, i.e. that different slots be filled by identical subtrees.

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