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Enum of acyclic digraphs

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ENUMERATION OF ACYCLIC DIGRAPHS

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For basic notation we follow Harary [3]. A digraph is <u>acyclic</u> just if it contains no directed cycle of length >1. We will be concerned only with digraphs on a finite number of points, and the empty digraph. Contrary to [3] we say that a point is a <u>source</u> of a digraph just if it has in-degree 0. Any point of a digraph which is not a source is called a <u>non-source</u>. A digraph d' is said to be an <u>extension</u> of d just if d is the subgraph of d' which is induced by the non-sources of d'. A <u>labeling</u> of a digraph is a linear ordering of the points. A subgraph of a labeled digraph is labeled by the inherited ordering. Thus we can use the notion of extension for labeled graphs as well as unlabeled.

It is easy to see that every non-empty acyclic digraph has at least one source. Also, any digraph is acyclic just if it is an extension of an acyclic digraph. These facts lead to enumerations of acyclic digraphs, labeled and unlabeled.

§1. <u>Labeled acyclic digraphs</u>. Let $a_{j,k}$ be the number of non-isomorphic labeled acyclic digraphs with exactly j sources and k non-sources. It will be conveniant to frame our results in terms of the generating function

$$a(x,y) = \sum_{j,k=0}^{\infty} a_{j,k} x^j y^k .$$

Let d be a labeled digraph with exactly j sources and k non-sources, and consider how d may be extended to a labeled digraph with exactly i sources. There are $\binom{i+j+k}{i}$ ways that the new sources can be ordered among the points of d . The i new sources are incident only to arcs which are directed to points in d . Each source of d must be incident to at least one of these new arcs. Thus for the extension there are 2^i-1 ways of drawing new arcs to each source of d , and 2^i ways of drawing new arcs to each non-source of d . These possibilities are independent, so that in all there are $(2^i-1)^j 2^{ik} \binom{i+j+k}{i}$ non-isomorphic extensions of d with i sources.

Now for all i,j,k let

$$x^i * x^j y^k = (2^i-1)^j 2^{ik} \binom{i+j+k}{i} x^i y^{j+k} ,$$

and extend * to be bilinear on generating functions. Then our argument shows that

$$a(x,y) = 1 + \sum_{i=1}^{\infty} x^i * a(x,y) ,$$

since an acyclic digraph is either empty or else a proper extension of another acyclic digraph. By solving this relation recursively, terms of a(x,y) of successively higher order are found. The first few terms are

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$$a(x,y) = 1 + x + x^2 + 2xy + x^3 + 9x^2y + 15xy^2 + x^4 + 28x^3y + 198x^2y^2 + 316xy^3 + x^5 + 75x^4y + 1{,}610x^3y^2 + 10{,}710x^2y^3 + 16{,}885xy^4 + \dots .$$

In Figure 1 are pictured the two non-isomorphic acyclic digraphs with 2 sources and 1 non-source.

Figure 1

There are 6 non-isomorphic labeled versions of 1(a) and 3 non-isomorphic labeled versions of 1(b), which correspond to the term $9x^2y$ from $a(x,y)$.

§2. Unlabeled acyclic digraphs. The generating function approach of §1 does not lend itself to enumerating unlabeled acyclic digraphs. To illustrate the difficulty, consider the two digraphs of Figure 1. Any labeled version of either graph has 360 non-isomorphic extensions to labeled digraphs with 2 sources. However, 1(a) has 5 non-isomorphic extensions to unlabeled digraphs with two sources, pictured in the top row of Figure 2, while 1(b) has only 4 such extensions, pictured in the bottom row of Figure 2.

The difficulty arises from a symmetry of 1(b) which 1(a) does not exhibit.

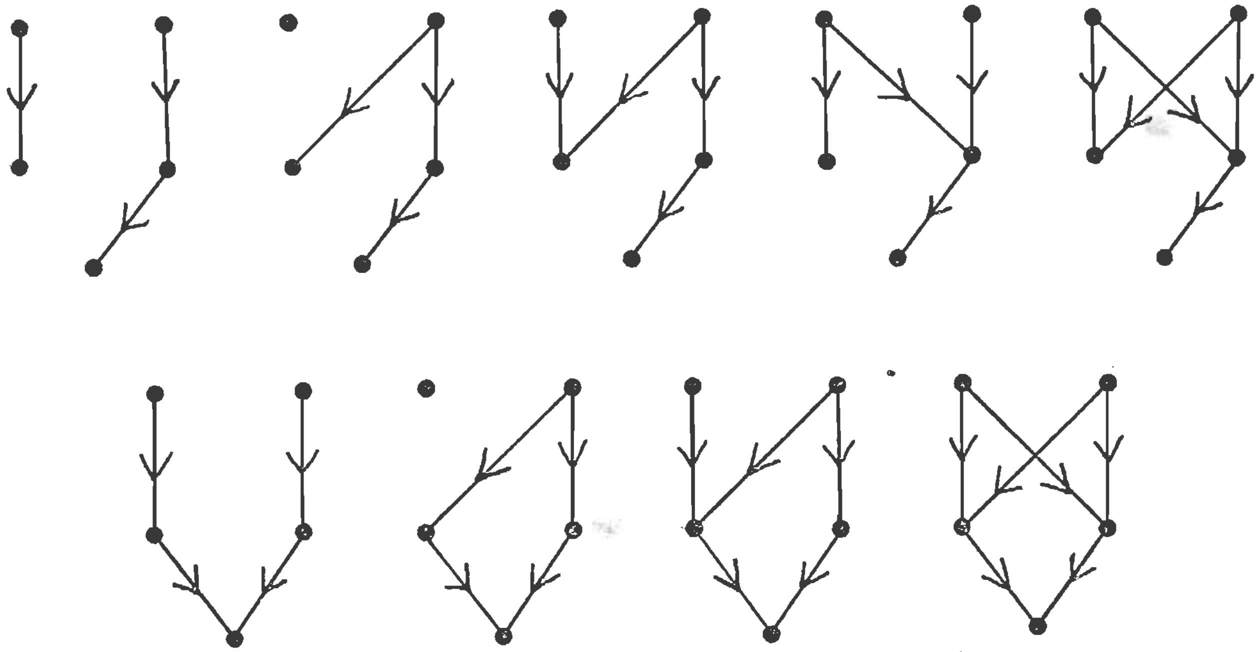

Figure 2

The necessary information on symmetry is carried by the cycle index of the automorphism group of a digraph. Now, instead of dealing in two variable generating functions we will consider generating functions in infinitely many variables a_1, b_1, a_2, b_2, ... If G is a permutation group and L and M are unions of orbits of G, then the <u>cycle index</u> $Z_{L,M}(G)$ <u>of</u> G <u>over</u> L,M is the polynomial

$$Z_{L,M}(G) = \frac{1}{|G|} \sum_{g \in G} \prod_i a_i^{\lambda(g,i)} b_i^{\mu(g,i)}$$

where $|G|$ is the order of G, $\lambda(g,i)$ is the number of cycles in the disjoint cycle decomposition of g which have length i and lie in L, and $\mu(g,i)$ is the number of similar cycles in M. We write $Z(G)$ for the special case of $Z_{L,\phi}(G)$ where L is is the object set of G. For any natural number n we denote the symmetric group on $1,2,\ldots,n$ by S_n. It is well known (see [2] or [4]) that

$$Z(S_n) = \sum \prod_i \frac{a_i^{\sigma_i}}{i^{\sigma_i}\sigma_i!}$$

where the sum is over all sequences $(\sigma_1,\sigma_2,\ldots,\sigma_n)$ of non-negative integers such that $\sum_{i=1}^{n} i\sigma_i = n$.

If d is any digraph then $\mathrm{aut}(d)$ denotes the automorphism group of d, and $Z_{S,N}(\mathrm{aut}(d))$ denotes the cycle index of $\mathrm{aut}(d)$ over the sources and non-sources of d. If we let d' range over extensions of d which have n sources so as to include just one from each isomorphism class, then

$$\sum Z_{S,N}(\mathrm{aut}(d')) = \frac{1}{n!\,|\mathrm{aut}(d)|}\sum \#(p,q)\prod_i a_i^{\lambda(p,i)} b_i^{\lambda(q,i)+\mu(q,i)} . \tag{1}$$

The second sum is over all $p \in S_n$ and all $q \in \mathrm{aut}(d)$. The factor $\#(p,q)$ is the number of extensions of d to a digraph with sources $1,2,\ldots,n$ which contain the permutation (p,q) in their automorphism groups. Fact (1) is essentially a variation on Burnside's lemma. It can be proved in much the same way as Redfield's decomposition theorem [4, p. 445], or it can be viewed as an application of a more general theorem of the author [7, equation (2)].

Now $\#(p,q)$ may be calculated explicitly. In order for an extension of d to be fixed by (p,q) for $p \in S_n$ and $q \in \mathrm{aut}(d)$ it is necessary and sufficient that all the new arcs be permuted among themselves by (p,q). The ij possible arcs from the points of a cycle of length i induced by p to the points of a cycle of length j induced by q fall into $\mathrm{g.c.d.}(i,j)$ cycles each of length $\mathrm{l.c.m.}(i,j)$ in the disjoint cycle decomposition of (p,q) viewed as a permutation on arcs. Thus there are $2^{\mathrm{g.c.d.}(i,j)}$ ways of drawing these new arcs so as to be invariant under (p,q). For a cycle of length j induced by q among the non-sources of d, there are a total of $2^{\sum_i \mathrm{g.c.d.}(i,j)\lambda(p,i)}$ ways of drawing new arcs to this cycle which are invariant under (p,q). If the cycle of length j is induced among the sources of d by q then we must subtract 1 because at least one new arc must be drawn to every source of d in an extension of d. Thus

$$\#(p,q) = \left[\prod_j \left(2^{\sum_i \mathrm{g.c.d.}(i,j)\lambda(p,i)} - 1\right)^{\lambda(q,j)}\right] 2^{\sum_{i,j} \mathrm{g.c.d.}(i,j)\lambda(p,i)\mu(q,j)} . \tag{2}$$

To deal entirely with cycle indices let $A = \sum Z_{S,N}(\mathrm{aut}(d))$ (one d from each isomorphism class of acyclic digraphs). For any sequences $\{\rho_i\},\{\sigma_i\},\{\tau_i\}$ let

$$\left(\prod_i a_i^{\rho_i}\right) \otimes \left(\prod_j a_j^{\sigma_j} b_j^{\tau_j}\right) = \prod_j \left(2^{\sum_i \mathrm{g.c.d.}(i,j)\rho_i} - 1\right)^{\sigma_j}$$

$$\times 2^{\sum_{i,j} \mathrm{g.c.d.}(i,j)\rho_i\tau_j} \prod_i a_i^{\rho_i} b_i^{\sigma_i+\tau_i}$$

and extend $\circledast$ to be bilinear. Then statements (1) and (2) may be combined into

$$Z_{S,N}(aut(d')) = Z(S_n) \circledast Z_{S,N}(aut(d))$$

where the sum is over representatives of all the isomorphism classes of extensions of d which have n sources. Summing this over all n and one d from each isomorphism class of acyclic digraphs we have

$$A = 1 + \sum_{n=1}^{\infty} Z(S_n) \circledast A . \tag{3}$$

This is justified by the fact that every acyclic digraph which is non-empty is a proper extension of some other acyclic digraph.

Relation (3) may be solved in a recursive fashion for terms of A of successively higher order. For the first few terms it is found that

$$A = 1 + a_1 + \frac{1}{2}a_1^2 + \frac{1}{2}a_2 + a_1b_1 + \frac{1}{6}a_1^3 + \frac{1}{2}a_1a_2$$
$$+ \frac{1}{3}a_3 + \frac{3}{2}a_1^2b_1 + \frac{1}{2}a_2b_1 + \frac{5}{2}a_1b_1^2 + \frac{1}{2}a_1b_2 + \ldots .$$

In Figure 3 are pictured the 6 non-isomorphic digraphs on 3 points. The first digraph of Figure 3 accounts for the terms $\frac{1}{6}a_1^3+\frac{1}{2}a_1a_2+\frac{1}{3}a_3$, the next two account for the terms $\frac{3}{2}a_1^2b_1+\frac{1}{2}a_2b_1$, and the remaining three account for $\frac{5}{2}a_1b_1^2 + \frac{1}{2}a_1b_2$.

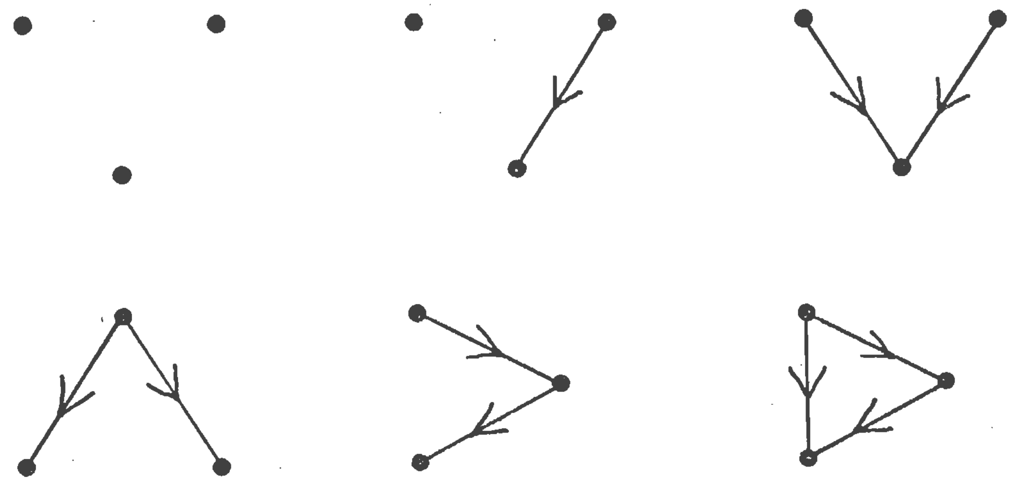

Figure 3

We denote by $A[a_i \to x^i;\ b_i \to y^i]$ the result of substituting x^i for each occurrence of a_i and y^i for each occurrence of b_i for all $i \geqslant 1$. Then $A[a_i \to x^i;\ b_i \to y^i]$ is the counting function for acyclic digraphs in terms of the number of sources and the number of non-sources. This is because a_i always represents i sources of a digraph and b_i represents i non-sources, and because the sum of the coefficients of the cycle index of any group is 1. To terms of order 6,

$$\begin{aligned} A[a_i \to x^i;\ b_i \to y^i] = {} & 1 + x + x^2 + xy + x^3 + 2x^2y + 3xy^2 \\ & + x^4 + 3x^3y + 11x^2y^2 + 16xy^3 \\ & + x^5 + 4x^4y + 25x^3y^2 + 108x^2y^3 \\ & + 164xy^4 + x^6 + 5x^5y + 47x^4y^2 \\ & + 422x^3y^3 + 2{,}168x^2y^4 + 3{,}341xy^5 + \dots . \end{aligned}$$

Of course $A[a_i, b_i \to x^i]$ is the counting function for acyclic digraphs in terms of just the total number of points, which to order 6 is

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$$A[a_i, b_i \to x^i] = 1+x+2x^2+6x^3+31x^4+302x^5+5{,}984x^6 + \ldots .$$

§3. Additional results. Standard methods apply to enumerating connected acyclic digraphs given the solution for all digraphs. Also standard is the introduction of the total number of arcs as an additional enumeration parameter. The relevant methods are at least implicit in [1] for the labeled problems and [2] for the unlabeled problems. Also, self-converse acyclic digraphs can be enumerated by an extension of the methods of §2.

On the other hand the enumeration of transitive digraphs seems immune to the techniques of this paper and remains, to the best of the author's knowledge, unsolved.

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