Counting Digraphs with Restrictions on the Strong Components

Robert W. Robinson*
Computer Science Department
415 Graduate Studies Building
The University of Georgia
Athens, GA 30602-7404, U.S.A.

Abstract

The principle of inclusion-exclusion is specialized in order to count labeled digraphs with separately specified out-components, in-components, and isolated components. Applications include counting digraphs with no in-nodes or out-nodes, digraphs with a source and a sink, and digraphs with a unique source and a unique sink.

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1 Introduction

Standard definitions and terminology for graph theoretic concepts may be found in the book [1] by Harary. Two nodes are in the same *strong component* of a digraph D if each can be reached from the other by directed paths in D. It is a standard result that the strong components of any digraph D partition the nodes.

The groundwork for counting labeled digraphs with restricted strong components is laid in [3], [4], [5], and [6]. The notation of [1] and [6] is followed herein except that *node* is now preferred to point or vertex. Strong components are henceforth referred to simply as *components*. An *out-component* is a component to which no other component is adjacent. An *out-node* is a node to which no other node is adjacent. Clearly a node is an out-node if and only if it is an out-component. *In-component* and *in-node* are the dual notions. It is well known that every nonempty digraph contains at least one out-component and at least one in-component. A component which is both an out-component and an in-component is said to be *isolated*.

A node is a *source* if every other node is reachable from it by a directed path. The dual is a *sink*. Clearly the component of a source must be an out-component, and there can be no other out-component. Conversely, if a digraph, δ, contains just one out-component γ, then every node of γ is a source of δ. Of course the dual statements serve to characterize sinks as the nodes in a unique in-component.

2 A Specialization of Inclusion-Exclusion

Let U be a finite or countable set and ω a countably additive mapping

$$\omega : U \to M$$

where M is an additive group. In our applications, U will be some set of labeled digraphs, and M will be the ring Q of rational numbers or else some ring of power series over Q, such as $Q[[x]]$.

For any $A \subseteq U$, let

$$\omega(A) = \sum_{\chi \epsilon A} \omega(\chi).$$

We call $\omega(A)$ the *enumerator* for A, since it will always be some sort of numerical count or generating function in our applications.

In this setting, we can formulate the ordinary principle of inclusion-exclusion as follows. A set of properties (subsets) of U are given, say $P_1, \ldots, P_m$. The set $E_0 = U - P_1 - \ldots - P_m$ is the focus of interest. For $I \subseteq \{1, \cdots, m\}$, let $\omega(I) = \omega\left(\bigcap_{j \epsilon I} P_j\right)$ with the understanding that if $I = \emptyset$ then the intersection is taken to be U. Then

$$\omega(E_0) = \sum (-1)^{|I|} \omega(I) \tag{1}$$

where the sum ranges over all subsets I of $\{1, \cdots, m\}$.

The proof is elementary. Because ω is additive on subsets of U, we can view each term in equation (1) as being the sum of contributions $\omega(\chi)$ for those χ in the relevant set. Suppose that χ is contained in exactly k of the sets $P_1, \cdots, P_m$ (so $0 \leq k \leq m$). The contribution of χ to $\omega(E_0)$ is just $\omega(\chi)$ if $k = 0$ and 0 if $k \geq 1$. Now consider the contribution of χ to the right side of (1). The contribution of χ to $(-1)^{|I|}\omega(I)$ will be 0 if $\chi \in P_i$ for some $i \in I$, and will be $(-1)^{|I|}\omega(\chi)$ if $\chi \in P_i$ for all $i \in I$. Since there are exactly $\begin{pmatrix} k \\ j \end{pmatrix}$ sets of j properties all of which contain χ, the sum of all these contributions is $\omega(I) \sum_{j=0}^{k} (-1)^j \begin{pmatrix} k \\ j \end{pmatrix}$. Now the sum is $(1-1)^k = 0^k$, and so is 1 if $k = 0$ and 0 if $k \geq 1$, showing that the contribution of χ to the right side of (1) is the same as its contribution to the left side. Summing this fact over all χ in U proves (1).

Now we consider a specialization of the general fact (1) to a situation in which the properties to be excluded come in dual pairs P_i and Q_i for $i = 1, \ldots, m$. Of course $\omega(E_0)$ could be expressed as a sum over the 2^{2m} subsets of the $2m$ properties using (1). One way of doing this might be as a double sum, over subsets of $\{P_1, \cdots, P_m\}$ and subsets of $\{Q_1, \cdots, Q_m\}$. However in many of our applications the evaluation of ω applied to a set of properties will depend on just what dual pairs are contained in that set. In that case, the situation can be most conveniently expressed as an ordered triple (I, J, K) of disjoint subsets of $\{1, \ldots, m\}$, the properties in the set consisting of P_i for $i \in I$, Q_j for $j \in J$, and both P_k and Q_k for $k \in K$. Let $\omega(I, J, K)$ be the enumerator for the intersection of these properties. Since there are $|I|+|J|+2|K|$ properties corresponding to (I, J, K), (1) becomes

$$\omega(E_0) = \sum(-1)^{|I|+|J|}\omega(I, J, K) \tag{2}$$

where the sum in (2) is over sequences of disjoint subsets $I, J, K \subseteq \{1, \ldots, m\}$.

3 Digraphs having no in-nodes or out-nodes

As an introductory problem, consider the number $Y[p]$ of labeled digraphs on p nodes which have no out-node. Ordinary inclusion-exclusion can be applied with U the set of all $2^{p(p-1)}$ labeled digraphs on p nodes, and property $P_i (1 \leq i \leq p)$ that the node labeled i is an out-node. Letting $\omega(\chi) = 1$ for each digraph, it is clear that for $I \subseteq \{1, \ldots, p\}$ and $|I| = m$ we have

$$\omega(I) = 2^{(p-1)(p-m)}. \tag{3}$$

This is because for each of the $p-m$ nodes not represented in I there are 2^{p-1} possible sets of arcs into it, and these choices are independent. Given these $p-m$ choices of arc sets, the digraph being counted by $\omega(I)$ is completely determined, as no arcs can be directed to any of the m nodes for which the labels lie in I. Now ordinary inclusion-exclusion (equation (1)) gives that

$$\begin{aligned} Y[p] = \omega(E_0) &= \sum_{m=0}^{p} (-1)^m \binom{p}{m} 2^{(p-1)(p-m)} \\ &= (2^{p-1} - 1)^p \end{aligned} \tag{4}$$

Of course, we could have seen this more directly by observing that the set of arcs incident to any given node must not be empty, so there are $2^{p-1} - 1$ choices for that set of arcs. A digraph on p nodes having no out-node is determined uniquely by p such choices, which are independent of each other.

Now consider the problem of counting the number of $W[p]$ of labeled digraphs having no out-node and no in-node. Our set U, enumerator ω, and properties $P_i (1 \leq i \leq p)$ can all stay the same. However in addition we need to exclude the properties $Q_i (1 \leq i \leq p)$, where Q_i holds if the node labeled i is an in-node. It is easy to see that for a set L of properties, $\omega(L)$ does not depend simply on $|L|$, or even just on the cardinalities of $L \cap \{P_1, \cdots, P_p\}$ and $L \cap \{Q_1, \cdots, Q_p\}$. This is because those i for which P_i and Q_i are both in L play a special role in determining $\omega(L)$. However equation (2) applies conveniently. Let I, J, and K be disjoint subsets of $\{1, \ldots, p\}$ with cardinalities k, m, and r, respectively. Then if $n = p - k - m - r$, we have

$$\omega(I, J, K) = 2^{n(n-1)+kn+mn+km} \tag{5}$$

This is because the arcs which may be chosen in constructing a digraph counted by $\omega(I, J, K)$ consist of the $n(n-1)$ arcs joining any node not in $I \cup J \cup K$ to any other, the kn arcs joining any node not in $I \cup J \cup K$ to any node in I, the mn arcs joining any node in J to any node not in $I \cup J \cup K$, and the km arcs joining any node in I to any in J.

In general, let $C(p; n_1, n_2, \ldots, n_q)$ denote the multinomial coefficient

$$\frac{p!}{n_1!n_2!\cdots n_q!} \tag{6}$$

when $p = n_1 + n_2 + \cdots + n_q$ and $n_1, \cdots, n_q$ are all non-negative integers, and 0 for any other set of arguments. Then $C(p; k, m, r, n)$ is precisely the number of disjoint ordered triples of subsets of $\{1, \ldots, p\}$ having cardinalities k, m, r (in order) when $n = p - k - m - r$. Since $\omega(E_0) = W[p]$ in this situation, equation (2) now gives

$$W[p] = \sum_{k,m,r} (-1)^{k+m} C(p; k, m, r, n) 2^{(k+n)(m+n)-n} \tag{7}$$

after rewriting the exponent in (5).

Note that keeping track of the number of edges in the digraphs being counted in equations (4) and (7) is straightforward. The appropriate enumerator function is then $\omega(\chi) = y^q$ where $q = q(\chi)$ is the number of edges in χ. Ordinary generating functions in y are obtained by replacing 2 with $(1 + y)$ in (4) and (7).

4 Exponential and special generating functions

The derivation of efficient recurrence relations for computing quantities such as $W[p]$ from the previous section is greatly facilitated by the use of exponential and special generating functions. Given a sequence $a = (a_0, a_1, a_2, \cdots)$ of rational numbers, the *exponential* generating function for a (in the variable x) is the infinite series

$$a(x) = \sum_{i=0}^{\infty} a_i x^i / i!$$

treated as a number of the ring $Q[[x]]$, i.e., without regard for questions of convergence. If $b(x)$ is the exponential generating function for $(b_0, b_1, b_2, \cdots)$, then the product $a(x)b(x)$ is the exponential generating function for $(c_0, c_1, c_2, \cdots)$, where

$$c_k = \sum_{i=0}^{k} \binom{k}{i} a_i b_{k-i}.$$

The reason is that $\binom{k}{i} = k!/i!(k-i)!$. This is very useful in counting labeled digraphs of various sorts, because $\binom{k}{i}$ is the number of ways to merge a linear ordering on i nodes with a linear ordering on $k-i$ disjoint nodes to produce a linear ordering on their union, all k node nodes together. This is exactly what must be done in order to construct a larger labeled digraph from the union of smaller ones. A labeling of the node set is equivalent to a linear ordering on the nodes, and the latter view is taken when digraphs are being constructed from other digraphs. An account of the uses of exponential generating function in graphical enumeration can be found in the text [2, Ch. 1].

Given a sequence $a = (a_0, a_1, a_2, \cdots)$, the special generating function for a is the infinite series

$$A(x) = \sum_{i=0}^{\infty} a_i x^i / i! 2^{i(i-1)/2}.$$

Denote by D the linear operator that transforms the exponential generating function for a to the special generating function. Then we may write $A(x) = \Delta(a(x))$ and $a(x) = \Delta^{-1}(A(x))$. If $B(x)$ is the special generating function for the sequence $b = (b_0, b_1, b_2, \ldots)$, then the product $A(x)B(x)$ is the special generating function for the sequence $d = (d_0, d_1, d_2, \ldots)$ where

$$d_k = \sum_{i=0}^{k} \binom{k}{i} 2^{i(k-i)} a_i b_{k-i}.$$

The reason is that in computing the power of 2 in the product we find

$$\binom{k}{2} - \binom{i}{2} - \binom{k-i}{2} = i(k-i).$$

Again, this is very useful in counting ways to construct digraphs, as $2^{i(k-i)}$ is the number of ways to select a set of edges directed from an i-set of nodes to a disjoint $(k-i)$-set of nodes, or *vice versa*.

If $D(x)$ is the exponential generating function for all labeled digraphs by number of nodes, then

$$D(x) = \sum_{i=0}^{\infty} 2^{i(i-1)} x^i / i! \tag{8}$$

and

$$\Delta D(x) = \sum_{i=0}^{\infty} 2^{i(i-1)/2} x^i / i! \tag{9}$$

Now, to adapt equation (2) to exponential generating functions, let $\omega(\chi) = x^p/p!$ whenever χ is a digraph on p nodes, so that the sum over all digraphs is $D(x)$. We adopt this particular enumerator for the remainder of the paper. To help keep track of the enumeration to be performed on the right side of (2) we form the mixed generating function

$$R(x,y,z,w) = \sum y^{|I|} z^{|J|} w^{|K|} \omega(I,J,K).$$

Here R is exponential in x but ordinary in y, z, and w. Then (2) can be written

$$\omega(E_0) = R(x,-1,-1,1). \tag{10}$$

In the case of digraphs without in-nodes or out-nodes, we have

$$R(x,y,z,w) = e^{wx} \Delta^{-1} \left(\Delta e^{yx} \Delta e^{zx} \Delta D(x) \right).$$

This is because

$$e^{yx} = \sum_{i=0}^{\infty} \frac{y^i x^i}{i!}$$

is the exponential generating function for sets of nodes which will be out-nodes, and which therefore have no edges between them. Likewise e^{zx} is the exponential generating function for sets of nodes which will be in-nodes, and e^{wx} for sets of nodes which will be both out-nodes and in-nodes (i.e., isolated). In the product

$$\Delta e^{yx} \Delta e^{zx} \Delta D(x)$$

we have the special generating function for labeled digraphs with specified in-nodes (counted by the power of y) and specified out-nodes (counted by the power of z), since $\Delta D(x)$ allows for all possible arcs among the unspecified nodes, while the products count in the number of ways to select edges joining unspecified nodes to in-nodes, and edges joining out-nodes to in-nodes and unspecified nodes. Applying Δ^{-1} gives the exponential generating function for these configurations, and the final product with e^{wx} counts the ways to interleave isolated nodes without adding any more edges. Thus by (10) the exponential generating function $W(x)$ for $(W[0], W[1], W[2], \cdots)$ can be expressed as

$$W(x) = e^{x} \Delta^{-1}((\Delta e^{-x})^2 \Delta D(x)). \tag{11}$$

Coefficients can be calculated from (11) in three steps. Consider

$$T(x) = \Delta^{-1}((\Delta e^{-x})^2) \tag{12}$$

to be the exponential generating function for $T[i] (i = 0, 1, 2, \cdots)$, and

$$Z(x) = \Delta^{-1}(\Delta T(x) \Delta D(x)) \tag{13}$$

to be the exponential generating function for $Z[i] (i = 0, 1, 2, \cdots)$. Then

$$W(x) = e^{x} Z(x), \tag{14}$$

and in terms of coefficients the equations (12), (13) and (14) give

$$T[n] = (-1)^n \sum_{k=0}^{n} \binom{n}{k} 2^{k(n-k)}, \tag{15}$$

$$Z[n] = \sum_{k=0}^{n} \binom{n}{k} 2^{k(n-1)} T[n-k], \tag{16}$$

$$W[n] = \sum_{k=0}^{n} \binom{n}{k} Z[k]. \tag{17}$$

In deriving (16) we have made use of (8) and the simplification $k(n-k) + k(k-1) = k(n-1)$. A table of the first few values of these coefficients is given below.

n	$T[n]$	$Z[n]$	$W[n]$
0	1	1	1
1	-2	-1	0
2	6	2	1
3	-26	14	18
4	162	1,634	1,699
5	-1,442	583,934	592,260

In terms of efficiency, note that using equation (7) directly to calculate $W[p]$ requires $O(p^3)$ arithmetic operations, and to calculate the sequence $W[0], W[1], \cdots, W[p]$ requires $O(p^4)$. On the other hand, equations (15), (16), and (17) allow the same sequence to be calculated in $O(p^2)$ arithmetic operations.

5 Digraphs with Source and Sink

Let $C(x)$ be the exponential generating function for a set of labeled strongly connected digraphs, and let $G(x)$ be the exponential generating function for the set of all labeled digraphs for which every strong component lies in the set enumerated by $C(x)$. Then we can apply (10) to derive the relation

$$\Delta(\exp(-C(x))\Delta G(x) = 1, \tag{18}$$

by which $C(x)$ can be determined from $G(x)$ or *vice versa*. The properties being excluded are that the various possible strong digraphs counted by $C(x)$ are out-components. The enumerator in which the power of y gives the number of specified out-components is

$$\Delta(\exp(yC(x)))\Delta G(x).$$

Then term $y^i C(x)^i/i!$ counts the number of ways select a set of i disjoint copies of strong digraphs counted by $C(x)$, without adding any edges between them. The product

$$\Delta(y^i C(x)^i/i!)\Delta G(x)$$

then counts the ways in which such a disjoint set of strong components can be joined by arbitrary edges to a digraph counted by $G(x)$, resulting in a digraph which again is of the type counted by $G(x)$ but now has i out-components specified. There are no dual properties (one can think of them as always false), and so no terms in z or w. So, setting $y = -1$ gives us $\omega(E_0)$. Since only the empty graph has no out-component, $\omega(E_0) = 1$, which proves (18).

Since we had just one homogeneous set of properties to exclude, the out-components, equation (18) follows from ordinary inclusion-exclusion. Indeed, (18) has been derived previously in different ways; see [2], [5], and [6].

In this section, we need (18) in order to derive equations for $\exp(-S(x))$ and $S(x)$, where $S(x)$ is the exponential generating function for labeled strongly connected digraphs. As with (18), these equations have been given previously, but we need them here for the study of digraphs with a source and a sink.

When all labeled strong digraphs are allowed as components, all labeled digraphs can be constructed from them and so (18) takes the form

$$\Delta(\exp(-S(x))\Delta D(x) = 1. \tag{19}$$

From (19) and (8) we could derive explicit and efficient recurrence relations for the coefficients of $S(x)$. This is done in [6, equations (33) and (34)], obtaining recurrences which were derived earlier by Wright [7] based on a more complicated set of recurrences due to Liskovets [3].

Now, to count digraphs with a source and a sink our strategy is to enumerate configurations in which there is a designated out-component and a separate designated in-component, and then use our specialized form of inclusion-exclusion to eliminate all other out-components and in-components. This will be correct in counting digraphs with a source and a sink, i.e., with a unique out-component and a unique in-component, except for the case of a single strong component. That has been omitted in favor of two isolated components, one designated as an out-component and the other as an in-component. Once the correction of adding $S(x) - S(x)^2$ is made, the enumeration is valid because the designated in-component and out-component are actually the only ones present and therefore are distinguished intrinsically.

To enumerate with a designated out-component and a designated in-component, we simply include a factor of $S(x)$ for each, since we are willing for any strongly connected digraphs to be the out-component, and any to be the in-component. This gives

$$\exp(wS(x))\Delta^{-1}(\Delta(S(x)\exp(yS(x))\Delta(S(x)\exp(zS(x))\Delta D(x)),$$

combining the principles applied previously to deriving equations (11) and (19). Now, following (2) we set $w = 1$ and $y = z = -1$, which along with the correction mentioned earlier leads to the expression

$$S(x) - S(x)^2 + \exp(S(x))\Delta^{-1}((\Delta(S(x)\exp(-S(x))^2\Delta D(x)) \qquad (20)$$

for the exponential generating function for all labeled digraphs having a source and a sink. It is then straightforward to derive efficient recurrence relations for those numbers based on equations (8) and (19), and expression (20).

To modify the above procedure to count labeled digraphs with a unique source and a unique sink, we simply replace $S(x)$ by x in the locations where $S(x)$ counts the possible designated out-component or in-component. For in this case we want the component to be a single node, for which x is the exponential generating function. Letting $L(x)$ denote the exponential generating function for $L[0], L[1], L[2], \cdots$ where $L(p)$ is the number of labeled digraphs with a unique source and a unique sink, we find

$$L(x) = x - x^2 + \exp(S(x))\Delta^{-1}(\Delta(x\exp(-S(x)))^2\Delta D(x)). \qquad (21)$$

Coefficients can be efficiently extracted from (21) in the usual way. We find that $L[0] = 0, L[1] = 1, L[2] = 2$, and for $n \geq 3$ that

$$L[n] = 2n(n-1)S[n-1]. \qquad (22)$$

The latter may be unexpected at first, but has an easy combinatorial proof. For $n \geq 2$, any digraph with a unique source v and a unique sink u has $v \neq u$. If u and v are identified, then the result is a strong digraph on $n-1$ nodes since every other node is reachable from the new node and *vice versa*. To see how many digraphs or order n result in a given strong digraph on $n-1$ nodes, consider the reverse process. We can choose any of $n-1$ nodes to split. The chosen node is split into an in-node and an out-node in a unique way with respect to the other nodes, but when $n \geq 3$ the edge from the new out-node to the new in-node is optional, resulting in a factor of 2 in counting the possibilities. If we consider that the new out-node inherits the label from the original node, we now have n choices for labeling the new in-node. The resulting digraph is now completely specified and labeled, and is obviously a digraph with a unique source (the new out-node) and a unique sink (the new in-node).

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