Principle of Inclusion and Exclusion

1 A Formula

Let $A_1, \ldots, A_n$ be n subsets of a universe U of objects; often we will use $A_0 := U$. We say an element x has i properties if it belongs to exactly i of the sets chosen from $A_1, \ldots, A_n$. Often we want to find out how many elements have *exactly* i properties. However, sometimes it is easier to answer how many elements have "at least i properties". The principle of inclusion and exclusion[1] is based upon the simple observation that the number of elements that satisfy exactly i properties is the number of elements that satisfy at least $(i+1)$ properties subtracted from the number of elements that satisfy at least i properties.

Given two sets A, B, the answer to the question, if we want to know how many elements satisfy no property then the answer is $|A_0| - |A \cup B| = |A_0| - |A| - |B| + |A \cap B|$. What is the answer in general? The answer is $|A_0| - |\cup_{i=1}^n A_i|$, since $|\cup_{i=1}^n A_i|$ is the number of elements that have at least one property. What is the formula corresponding to $|A \cup B|$? Before we give the formula, we need some convenient notation: Let $I \subseteq [n]$, the define $A_I := \cap_{j \in I} A_j$.

Claim: The number of elements with *at least one property* is

$$|\cup_{i=1}^n A_i| = \sum_{I \subseteq [n] \setminus \emptyset} (-1)^{|I|-1} |A_I|. \tag{1}$$

We give two proofs: one by induction and another combinatorial.

¶1. Induction: From the formula for two sets we get

$$|\cup_{i=1}^n A_i| = |\cup_{i=1}^{n-1} A_i| + |A_n| - |\cup_{i=1}^{n-1} A_i \cap A_n|.$$

By induction hypothesis $|\cup_{i=1}^{n-1} A_i| = \sum_{I \subseteq [n-1]} |A_I|$. Clearly, none of the terms A_I contain A_n. To get those terms we have to apply the induction hypothesis to the $\cup_{i=1}^{n-1} A_i \cap A_n = \cup_{i=1}^{n-1} B_i$, where $B_i := A_i \cap A_n$:

$$\begin{aligned}
|\cup_{i=1}^{n-1} B_i| &= \sum_{I \subseteq [n-1] \setminus \emptyset} (-1)^{|I|-1} |B_I| \\
&= \sum_{I \subseteq [n-1] \setminus \emptyset} (-1)^{|I|-1} |\cap_{i \in I} A_i \cap A_n| \\
&= \sum_{I \subseteq [n-1] \setminus \emptyset} (-1)^{|I|-1} |\cap_{i \in I \cup \{n\}} A_i| \\
&= \sum_{I' \subseteq [n] \setminus \emptyset : \{n\} \subset I'} (-1)^{|I|'-2} |\cap_{i \in I'} A_i|
\end{aligned}$$

Thus

$$|\cup_{i=1}^n A_i| = \sum_{I \subseteq [n-1] \setminus \emptyset} (-1)^{|I|-1} |\cap_{i \in I} A_i| + |A_n| + \sum_{I' \subseteq [n] \setminus \emptyset : \{n\} \subset I'} (-1)^{|I|} |\cap_{i \in I'} A_i|,$$

which proves the desired claim.

[1] It is also called the sieve method, principle of cross-classification, the symbolic method.

¶2. Combinatorial: The LHS of (1) counts every $x \in \cup A_i$. We have to show that the RHS does the same. Let $J \subseteq [n]$ be the set of properties that x satisfies, i.e., $x \in A_i$, for all $i \in J$. Then on the RHS of (1) x is counted exactly once in $|A_I|$ for all subsets $I \subseteq J$. Thus the count of x is

$$\sum_{I \subseteq J \setminus \emptyset} (-1)^{|I|-1} = \sum_{k=1}^{|J|} \binom{|J|}{k} (-1)^{k-1} = (-1)[(1-1)^{|J|} - 1] = 1.$$

The emptyset in the summation is annoying feature of the description. A much better way to write (1) is to count the *number of elements that do not have any property*

$$\sum_{I \subseteq [n]} (-1)^{|I|} A_I. \tag{2}$$

The art of applying the princinple is to define A_I appropriately. If we want to count the number of elements that do not have a property, then we generally choose A_i's to be sets of elements that have the property, and carefully sieve out these sets.

¶3. *Problem des rencontres* or Derangements: [2] We first consider the number of permutations D_n that do not have any fixed points. Earlier we had derived a formula by way of generating functions; here we give a direct approach. Let A_i be the number of permutations that fix i; the universe A_0 is the set of all permutations. Then what is $\cup_{i=1}^n A_i$? It is the set of permutations that fix at least one element. Thus $D_n = n! - |\cup_{i=1}^n A_i|$. To figure out an explicit from for $|\cup_{i=1}^n A_i|$ using (1), we need to understand what the terms $|A_I|$, $I \subseteq [n]$ mean. Well $|A_I|$ is the set of permutations that fix all $j \in I$; they may fix other elements as well, but they certainly fix the elements in I. How many such permutations can we have? Clearly, $(n - |I|)!$ Thus

$$\sum_{I \subseteq [n] \setminus \emptyset} (-1)^{|I|-1} |A_I| = \sum_{k=1}^{n} (-1)^{k-1} \binom{n}{k} (n-k)! = \sum_{k=1}^{n} (-1)^{k-1} \frac{n!}{k!}.$$

Thus

$$D_n = n! + \sum_{k=1}^{n} (-1)^k \frac{n!}{k!} = n!(1 - 1 + \frac{1}{2!} - \frac{1}{3!} + \cdots)$$

the formula we had derived earlier. But as $n \to \infty$, how many derangements do we have? The answer is roughly $n!/e$.

¶4. Euler's Totient Function: Let $\phi(n)$ be number of numbers $m < n$ relatively prime to n, i.e., their gcd is one. Can we derive a formula for $\phi(n)$ using the principle? Let's start with easy cases. For a prime p, clearly $\phi(p) = p - 1$. What is $\phi(p^k)$? Let us find the numbers not relatively prime to p^k. These are the numbers of the form $p, 2p, 3p, \dots, (p-1)p, \dots, p^2, 2p^2, \dots, p^{k-1}p$, i.e., p^{k-1} such numbers. Thus $\phi(p^k) = p^k(1 - 1/p)$. Suppose $n = p_1^{e_1} p_2^{e_2} \dots p_k^{e_k}$ is the prime factorization of n. How should we define our sets A_i? Let it be the number of numbers divisible by p_i. Then for an index set $I \subseteq [k]$, $|A_I|$ is the number of numbers at most n that are divisible by $p_I := \prod_{j \in I} p_j$. What is the cardinality of A_I? How many numbers $\leq n$ are divisible by p_I? It is easy to see that there are n/p_I of them. Thus

$$\phi(n) = \sum_{I \subseteq [k]} (-1)^{|I|} \frac{n}{p_I},$$

where $p_\emptyset = 1$. However, a better way to express the above relation is

$$\phi(n) = n \left(1 - \frac{1}{p_1}\right) \left(1 - \frac{1}{p_2}\right) \cdots \left(1 - \frac{1}{p_k}\right).$$

[2] First posed by Pierre de Montmort in 1708, and solved by him in 1713. Nicholas Bernoulli also solved it roughly at the same time using PIE.

2 A Generating Function Approach to PIE

The formula in (2) gives us the number of elements that have no property. What if we want to know the number of elements that have exactly one property, or t properties? We can still apply (2) recursively; e.g., to get the number of elements with exactly one property we count the number of elements with at least two properties and subtract it from the cardinality of the union. Let E_t be the number of elements in the universe that have exactly t properties. Then (2) gives the formula for E_0, and in general we want to find the formula for E_t. How do we generalize (2)? We had remarked earlier that PIE helps us answer these questions, by transforming the answers to the easier question, How many elements have *at least a certain set of properties*?

Given $S \subseteq [n]$, let N_S be the number of elements that have at least the properties in S. In other words, for an element a, if $P(a) \subseteq [n]$ is the set of properties that a has then N_S is the number of elements a such that $S \subseteq P(a)$. For $r \geq 0$, further define

$$N_r := \sum_{|S|=r} N_S.$$

What is N_0? It is $N_\emptyset$, which by definition is the number of elements a that have $\emptyset \subseteq P(a)$, i.e., the size of the universe U. What is N_1? By definition

$$N_1 = \sum_{|S|=1} N_S = N_{\{1\}} + N_{\{2\}} + \cdots + N_{\{n\}} = |A_1| + |A_2| + \cdots + |A_n|$$

since all the elements in the set A_i have i in their property set. Similarly, we can see that

$$N_2 = \sum_{i,j:i\neq j} N_{A_i \cap A_j} = \sum_{i,j:i\neq j} |A_i \cap A_j|.$$

Thus the N_i's capture the elements that appear on the RHS of (2).

Another way to express N_r is as follows:

$$\begin{aligned} N_r &= \sum_{|S|=r} N_S \\ &= \sum_{|S|=r} \sum_{a\in U: S\subseteq P(a)} 1 \\ &= \sum_{a\in U} \sum_{|S|=r: S\subseteq P(a)} 1. \end{aligned}$$

But the second sum counts the number of subsets of $P(a)$ of size r. Thus

$$N_r = \sum_{a\in U} \binom{P(a)}{r}.$$

Each element that has t properties contributes $\binom{t}{r}$ to the summation, and there are E_t many such elements. Thus we have

$$N_r = \sum_{t\geq 0} \binom{t}{r} E_t. \tag{3}$$

Recall that we wanted to express E_t's in terms of N_r's, but here we have the other way round. Nevertheless, using this expression we can recover what we want. Let

$$N(x) := \sum_{r\geq 0} N_r x^r \text{ and } E(x) := \sum_{t\geq 0} E_t x^t.$$

Then multiplying (3) by x^r and summing for $r \geq 0$ we get

$$N(x) = \sum_{r\geq 0} \sum_{t\geq 0} \binom{t}{r} E_t x^r = \sum_{t\geq 0} E_t (1+x)^t = E(1+x).$$

Thus to express E_t's in terms of N_r's we observe that

$$E(x) = N(x-1). \tag{4}$$

This simple expression helps us answer the question, how many numbers have exactly t properties

$$E_t = \sum_{r \geq t} (-1)^{r-t} \binom{r}{t} N_r. \tag{5}$$

In particular,

$$E_0 = \sum_{r \geq 0} (-1)^r N_r = N_0 - N_1 + N_2 - N_3 + \cdots$$

the formula in (2). Let's apply this result to our earlier examples. For derangements, the property A_i is the same, namely, that i is a fixed point of the permutation. Given a subset of properties $S \subseteq [n]$, N_S is the number of permutations that keep the elements in S fixed. There are $(n - |S|)!$ such permutations, as the remaining elements can permute in all possible ways. Thus

$$N_r = \sum_{|S|=r} N_S = \sum_{|S|=r} (n - |S|)! = \binom{n}{r}(n-r)! = \frac{n!}{r!}$$

from which we can obtain the desired formula for D_n. Similarly, the properties defined for Euler's totient function carry over in this framework as well.

There is an interesting question we can ask: Suppose we pick a permutation uniformly at random. What is the expected number of fixed points it has? In general, suppose we pick an element uniformly at random from U. What is the expected number of properties it has? The answer is $\sum_t tE_t/N_0 = N_1/N_0$. Thus N_1 plays a especial role. For the case of permutations, our answer is $N_1/N_0 = 1$.

3 Permutations with Restrictions

The *problem des rencontres* and *des ménages* can be viewed as special cases of a more general setting of counting permutations with restrictions. The graph of a permutation $\pi : [n] \to [n]$ can be drawn on an $n \times n$ grid, where we plot the pairs $(i, \pi(i))$. Restrictions are a subset R of the $n \times n$ grid. We are interested in counting the number of permutations that avoid R. For instance, in the case of derangements, the restriction-set is $\{(i,i) : i = 1, \ldots, n\}$; for the *problem des ménages* the restriction-set is $\{(i, i+1 \mod n) : i = 1, \ldots, n\}$. A nice way to answer these counting questions is by couting the number of ways to place non-attacking rooks on a subset of the board. The next section develops this theory.

3.1 Rook Polynomials

In how many ways can we place n non-attacking rooks on an $n \times n$ chess board? Two rooks are non-attacking iff they do not share either the x or y-coordinate. Let us label the columns by the n rooks. Let π be the map that assigns the ith rook to the $\pi(i)$-th row. Since the rooks are non-attacking, it means that for two different rooks $i, j \in [n]$, $\pi(i) \neq \pi(j)$. Thus the map π is infact a permutation. Vice versa, the graph $G(\pi)$ of a permutation π gives us a non-attacking placement of n rooks. Thus there are $n!$ ways to place n non-attacking roots on an $n \times n$ chess board.

What has placing non-attacking rooks to do with counting the number of permutations that avoid a restriction-set R, i.e., those permutations for which $G(\pi) \cap R = \emptyset$? Let E_t be the number of permutations such that have exactly t restrictions from R, i.e., $|G(\pi) \cap R| = t$; we want to count E_0. From (4) we know that $E(x) = N(x-1)$, where N_j is defined as follows:

$$N_j = \# \{\pi : \text{ for all } S \subseteq R, \text{ where } |S| = j,\ S \subseteq G(\pi) \cap R\}.$$

If we can count N_j, then we can derive a formula for E_t, as we had done earlier. The placement of non-attacking rooks helps us derive the fomula. Let r_j be the number of ways to place j non-attacking rooks on the board covered by R. Given $S \subseteq R$, $|S| = j$, any permutation π that satisfies the constraints in S has to place j non-attacking rooks on S. The number r_j precisely counts these choices over all permutations; the remaining $n - j$ rooks then have to just form a permutation. Thus

$$N_j = r_j(n-j)!.$$

This implies that

$$E(x) = \sum_t E_t x^t = \sum_{j \geq 0} r_j (n-j)!(x-1)^j. \tag{6}$$

Define $\Delta^{-j}(n) := (n-j)!$, then the equation above can be succintly represented as

$$E(x) = R((x-1)\Delta^{-1}),$$

where we implicitly assume that Δ^{-1} is applied to n. In particular, substituting $x = 0$ we obtain

$$E_0 = E(0) = \sum_{j \geq 0} r_j (n-j)!(-1)^j.$$

Let's apply this to the problems of derangements and ménages. For derangements, the restriction-set is the set of diagonal elements. The number of ways to put j non attacking rooks on the diagonal is $\binom{n}{j}$. Thus

$$D_n = \sum_{j \geq 0} \binom{n}{j} (n-j)!(-1)^j = n! \sum_{j \geq 0} \frac{(-1)^j}{j!}.$$

For the ménage problem the number of ways to place j non-attacking rooks is

$$g(2n, j) = \frac{2n}{2n-j} \binom{2n-j}{k},$$

since the crosses in the restriction-set can be arranged around a circle such that placing j non-attacking rooks is equal to picking j non-adjacent positions around the circle.

Corresponding to a restriction-set B, the **Rook polynomial** $R_B(x)$ is the generating function for the sequence $r_j(B)$, i.e., $R_B(x) = \sum_j r_j(B)x^j$. The corresponding polynomial $E_B(x) := R_B((x-1)\Delta^{-1})$ is called the **hit polynomial**. Let $M_n(x)$ be the rook polynomial corresponding to the $n \times n$ menage board, i.e,

$$M_n(x) := \sum_{j=0}^{n} g(2n, j) x^j \tag{7}$$

and

$$E_n(x) = \sum_{j=0}^{n} g(2n, j)(x-1)^j (n-j)! \tag{8}$$

the corresponding hit polynomial. The nth **menage number** $e_n := E_n(0)$.

Rook polynomials can be constructed recursively, much like determinant computation. For instance, if B_1, B_2 is a partition of B such that no cell of one is on the same row or column of the other, then $R_B(x) = R_{B_1}(x)R_{B_2}(x)$; inductively, if we have an r-partition $B_1, \ldots, B_r$ of B such that any two B_i, B_j have a cell on the same row or column, then

$$R_B(x) = \prod_{i=1}^{r} R_{B_i}(x). \tag{9}$$

The number $r_k(B)$ can be computed recursively by expanding along the cells in B as follows in two ways: fix a cell c

1. $r_k(B)$ is either obtained by placing a rook at c in B; in which case, the remaining $k-1$ roots are placed on the board B_i obtained from removing the corresponding row and column from B.

2. no rook is placed on c; in this case, the k rooks are placed on the board B_e obtained by exluding c from B.

Thus

$$r_k(B) = r_{k-1}(B_i) + r_k(B_e).$$

This gives rise to the following recursion of the corresponding generating functions:

$$R_B(x) = xR_{B_i}(x) + R_{B_e}(x).$$

Let's see how to apply these observations to construct the rook polynomial corresponding to derangements and ménages. For the derangements, let $L_n(x)$ be the rook polynomial. Then by the rule above, we get $L_n(x) = (1+x)L_{n-1}(x)$, and since $L_1(x) = 1$, we get $L_n(x) = (1+x)^n$ as expected. For the ménage problem, it helps to first get the rook polynomial of the relaxed ménage problem. That polynomial satisfies the recurrence $L_k(x) = L_{k-1}(x) + xL_{k-2}(x)$, where $L_k(x)$ is the rook polynomial for the first k cells of the restriction-set for the relaxed ménage problem.

4 PIE Viewed as Matrix Inversion

We can describe PIE in a slightly more general setting. Let S be a set of size n; we can take S to be $[n]$, which would correspond to the property index-set in the standard description of PIE. Consider the set $\mathcal{F}$ of all functions $f : 2^S \to \mathbb{R}$; in general, $\mathbb{R}$ can be replaced with any field (this is basically to guarantee that $\mathcal{F}$ is a vector space). Define the functional $\phi : \mathcal{F} \to \mathcal{F}$ as follows: for all $T \subset S$

$$\phi f(T) = \sum_{Y \supseteq T} f(Y).$$

Clearly, ϕ is a linear transformation over $\mathcal{F}$. The PIE in this setting basically states that ϕ^{-1} exists and is given as

$$\phi^{-1} f(T) = \sum_{Y \supseteq T} (-1)^{|Y \setminus T|} f(Y). \tag{10}$$

Thus PIE is a very simple result from linear algebra, but with profound applications. Let's see why the formula for the inverse is true. To prove correctness, we've to show that the composition of ϕ and ϕ^{-1} yields back f:

$$\begin{aligned}
\phi(\phi^{-1} f)(T) &= \sum_{Y \supseteq T} \phi^{-1} f(Y) \\
&= \sum_{Y \supseteq T} \sum_{Y' \supseteq Y} (-1)^{|Y' \setminus Y|} f(Y') \\
&= \sum_{Y' \supseteq Y \supseteq T} \left(\sum_{Y' \supseteq Y \supseteq T} (-1)^{|Y' \setminus Y|} \right) f(Y') \\
&= \sum_{Y' \supseteq Y \supseteq T} (1-1)^{|Y' \setminus T|} f(Y') \\
&= f(T).
\end{aligned}$$

We now apply the result to obtain PIE. Let S be a set of properties that elements of a universe set U satisfy. Given a set $T \subseteq S$, let $f_=(T)$ be the number of elements in U with exactly the properties in T. Given this function it is easy to count the number of elements that have at least the properties in T, namely

$$f_{\geq}(T) = \sum_{Y \supseteq T} f_=(Y).$$

This is the easier part, expressing the "at least" in terms of the "exact". What (16) does is gives us the converse:

$$f_=(T) = \sum_{Y \supseteq T} (-1)^{|Y \setminus T|} f_{\geq}(Y).$$