Appendix C

Recursion and the Möbius Inversion Formula

> The belief that pure mathematics is only fortuitously useful is widely shared, even by mathematicians.
>
> – John Maddux [96]

The Möbius inversion formula from number theory [94, 95] has gained attention in the current physics literature through the work of Chen, who has proved a generalization of the theorem to continuous variables [93]. Although its practical utility remains to be seen, the Chen-Möbius theorem provides an elegant formal method to solve nonlinear inversion problems. As described in Chapter 4.1, an important application in theory of solid cohesion is the problem of inverting a crystal energy versus volume curve to obtain the interatomic forces (assumed to act radially between pairs of atoms) [97]. In that case, the Chen-Möbius theorem is a more compact but equivalent statement of an inversion formula originally derived by Carlsson, Gelatt and Ehrenreich (CGE) [90]. In Chapter 4.1.4, a simple, recursive proof of the CGE formula is given that provides insight into the physical meaning of the inversion process and generalizes it to more complicated situations (nonradial forces and nonuniform deformations). In this Appendix, we shall see that the idea of recursion can also be used to derive a discrete analog of the CGE inversion formula. By comparing with the Möbius inversion formula, an interesting expression for the number-theoretic Möbius function can also be derived in terms of combinatorial quantities that generalize the Stirling numbers of the second kind [157].

C.1 A Recursive Approach to Möbius Inversion

We begin by stating the Möbius inversion formula.

Theorem: Given $f : N \to N$, define $F : N \to N$ by

$$F(n) = \sum_{d|n} f(d). \tag{C.1}$$

Then $\forall n \in N$,

$$f(n) = \sum_{d|n} \mu(d) F(n/d), \tag{C.2}$$

where $\mu : N \to \{0, 1, -1\}$ is the Möbius function,

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1 \\ (-1)^\ell & \text{if n = product of } \ell \text{ distinct primes} \\ 0 & \text{otherwise} \end{cases} . \tag{C.3}$$

Proof: Substitute Eq. (C.1) in the right side of Eq. (C.2) and simplify:

$$\sum_{d|n} \mu(d) F(n/d) = \sum_{d|n} \mu(d) \sum_{c|(n/d)} f(c) = \sum_{c|n} f(c) \sum_{d|(n/c)} \mu(d) = f(n) \tag{C.4}$$

using $\sum_{d|n} \mu(d) = \delta_{n1}$ in the last step [95].

Following the arguments of Section 4.1.4, we can easily derive another, albeit more complicated, inversion formula.

Lemma: Let s be the number of factors (not necessarily distinct) in the prime decomposition of n. Then, given the assumptions of the theorem, $\forall n \in N$,

$$\begin{aligned} f(n) \;=\; F(n) \;-\; \sum_{d_1|n}{}' F(n/d_1) \;+\; \sum_{d_1|n}{}' \sum_{d_2|n}{}' F(n/d_1 d_2) \\ -\; \sum_{d_1|n}{}' \sum_{d_2|n}{}' \sum_{d_3|n}{}' F(n/d_1 d_2 d_3) \;+\; \ldots\; (-1)^s F(1), \end{aligned} \tag{C.5}$$

where the kth multiple sum is restricted so that $(d_1 d_2 \ldots d_k)|n$ and $\sum_d'$ denotes summation with $d = 1$ excluded.

Proof: Rewrite Eq. (C.1) as,

$$F(n) = \sum_{d|n} f(n/d), \tag{C.6}$$

and solve for the $d = 1$ term of the sum,

$$f(n) = F(n) - \sum_{d|n}{}' f(n/d). \tag{C.7}$$

The result follows by recursive substitution.

In spite of the complexity of the explicit formula, recursion clearly reveals how the process of Möbius inversion takes place, in analogy with the contraction of a greatly expanded crystal down to condensed volumes in the case of solid cohesion. Let us order the divisors of n in decreasing order, $n = d^{(1)} > d^{(2)} > \ldots > d^{(s)} = 1$. The procedure starts with $F(n)$ as an initial guess for the unknown $f(n)$. The error is corrected by subtracting $f(d^{(i)})$ for all *smaller* divisors, $i \geq 2$. After one iteration, we have

$$f(n) = F(n) - \sum_{d_1|n}{}' F(n/d_1) + \sum_{d_1|n}{}' \sum_{d_2|n}{}' f(n/d_1 d_2). \tag{C.8}$$

Now the same initial guess, $f(d^{(i)}) = F(d^{(i)})$, has been applied to get the first correction from the $i \geq 2$ divisors. The error at this stage is removed by adding $f(d^{(i)})$ for smaller divisors, $i \geq 3$, and $F(n)$ and $F(d^{(2)})$ have already made their full contributions. As the process continues, new corrections come from successively smaller divisors until the last step, when the entire error is concentrated in $F(1)$. Note that the convergence of the (finite) series in Eq. (C.5) is quite slow, as pointed out by Chen and Ren in the case of the CGE formula [97], because the terms are oscillatory and often quite large, as described in the next section.

C.2 A Combinatorial Expression for the Möbius Function

By combining like terms, Eq. (C.5) can be written in the form,

$$f(n) = \sum_{d|n} c(d) F(n/d). \tag{C.9}$$

where, of course, $c(d) = \mu(d)$ by linear independence. In this way, the Lemma can be used to prove the following result.

Theorem: Let d have prime decomposition $d = \prod_{i=1}^{\ell} p_i^{\alpha_i}$, with $m = \sum_{i=1}^{\ell} \alpha_i$. Then,

$$\mu(d) = \sum_{k=1}^{m} (-1)^k \, \mathcal{B}(d,k), \tag{C.10}$$

where $\mathcal{B}(d,k)$ is the number of distinct decompositions of d into k nontrivial factors.

Equivalently, $\mathcal{B}(d,k) = \mathcal{B}(\{\alpha_i\}_{i=1}^{\ell}, k)$ is the solution to the following counting problem[1]:

Exercise: Suppose we have a set of m colored balls with α_i identical balls of the ith color, $i = 1, \ldots, \ell$. How many ways are there to distribute the balls among k distinct containers, placing at least one ball in each?

The general solution of the exercise is quite difficult, perhaps even intractable, so we pose it as a challenge to the reader. Whatever the solution, however, it must satisfy the sum rule of Eq. (C.10), indicating a subtle cancelation of these complex quantities during recursive inversion. There are two limiting cases in which the exercise reduces to well-known (but nontrivial) counting problems:

[1] Analysis of the counting exercise was done in close collaboration with Adam Lupu-Sax.

1. In the case of indistinguishable balls of a single color ($\ell = 1$ and $m = \alpha_1$), which corresponds to $d = p^m$ for some prime p, a binomial coefficient, $\mathcal{B}(d,k) = \binom{m-1}{k-1}$, solves the exercise [157][2]. In this case, the sum rule implied by Eq. (C.10) is,

$$\sum_{k=1}^{m}(-1)^k \mathcal{B}(p^m,k) \;=\; \begin{cases} 1 & \text{if } m = 1 \\ -(1-1)^{m-1} = 0 & \text{if } m > 1 \end{cases} \;=\; \mu(p^m), \tag{C.11}$$

which is easily verified with the binomial formula.

2. In the case of distinguishable balls, ($\alpha_i = 1, \forall i = 1, \ldots, \ell$), which corresponds to d being a product of ℓ distinct primes, the solution to the exercise is $\mathcal{B}(d,k) = k!\,\mathcal{S}_\ell^{(k)}$, where $\mathcal{S}_\ell^{(k)}$ is a Stirling number of the second kind [157]. In this case, as a simple consequence of our lemma, we have the sum rule for Stirling numbers of the second kind [156], which we state as a corollary.

Corollary:

$$\sum_{k=1}^{\ell}(-1)^k k!\,\mathcal{S}_\ell^{(k)} = (-1)^\ell. \tag{C.12}$$

This same fact can also be derived using standard combinatorial formulae. Substituting the expression for Stirling numbers of the second kind [156, 157], we have

$$c(d) = \sum_{k=1}^{\ell}\sum_{j=0}^{k}(-1)^j\binom{k}{j}j^\ell. \tag{C.13}$$

By exchanging the order of summation and performing the inner sum using Eq. (0.151.1) of Ref. [159], we obtain,

$$c(d) = \sum_{j=1}^{\ell}(-1)^j\binom{\ell+1}{j+1}j^\ell. \tag{C.14}$$

[2]This formula is easily proved with the following insight [158]: Represent the balls by a sequence of m dots and the container walls by $k-1$ vertical lines. The number of ways to distribute the balls into the containers is equal to the number of ways to distribute the lines among the $m-1$ spaces between the dots, one per space and without regard to order, which is simply $\binom{m-1}{k-1}$. For example, $B(p^4, 3) = 3$: •|•|••, •|••|•, ••|•|•.

Next we separate the $j = \ell$ term and break the sum into two parts using Eq. (24.1.1.II.A) of Ref. [156],

$$c(d) = (-1)^\ell \ell^\ell + \sum_{j=1}^{\ell-1} (-1)^j \binom{\ell}{j} j^\ell - \sum_{j=1}^{\ell} (-1)^j \binom{\ell}{j} (-1+j)^\ell. \tag{C.15}$$

Finally, evaluating the sums with Eqs. (0.154.4) and (0.154.6) of Ref. [159], we arrive at the desired result, $c(d) = (-1)^\ell$.

The general case of m balls of an arbitrary number of distinct colors is much more complicated, but the answer must be related to the Möbius function through Eq. (C.10).

In conclusion, we use recent developments in the theory of solid cohesion to provide a fresh perspective on the process of Möbius inversion. We prove a variant of the Möbius inversion formula and from it derive a representation of the Möbius function in terms of the combinatorial quantities $\mathcal{B}(d, k)$, which reduce to the Stirling numbers of the second kind in a special case. In this way, we arrive at a unified view of a wide class of counting problems related to the Möbius function.