4.7 The Transfer-matrix Method

4.7.1 Basic Principles

The transfer-matrix method, like the Principle of Inclusion-Exclusion and the Möbius inversion formula, has simple theoretical underpinnings but a very wide range of applicability. The theoretical background can be divided into two parts—combinatorial and algebraic. First we discuss the combinatorial part. A (finite) *directed graph* or *digraph* D is a triple (V, E, ϕ), where $V = \{v_1, \dots, v_p\}$ is a set of *vertices*, E is a finite set of (directed) *edges* or *arcs*, and ϕ is a map from E to $V \times V$. If $\phi(e) = (u, v)$, then e is called an edge *from u to v*, with *initial vertex u* and *final vertex v*. This is denoted $u = \operatorname{init} e$ and $v = \operatorname{fin} e$. If $u = v$ then e is called a *loop*. A *walk* Γ in D of *length* n from u to v is a sequence $e_1 e_2 \cdots e_n$ of n edges such that $\operatorname{init} e_1 = u$, $\operatorname{fin} e_n = v$, and $\operatorname{fin} e_i = \operatorname{init} e_{i+1}$ for $1 \le i < n$. If also $u = v$, then Γ is called a *closed walk based at u*. (Note that if Γ is a closed walk, then $e_i e_{i+1} \cdots e_n e_1 \cdots e_{i-1}$ is in general a different closed walk. In some graph-theoretical contexts this distinction would not be made.)

Now let $w \colon E \to R$ be a *weight function* with values in some commutative ring R. (For our purposes here we can take $R = \mathbb{C}$ or a polynomial ring over $\mathbb{C}$.) If $\Gamma = e_1 e_2 \cdots e_n$ is a walk, then the *weight* of Γ is defined by $w(\Gamma) = w(e_1) w(e_2) \cdots w(e_n)$. Let $i, j \in [p]$ and $n \in \mathbb{N}$. Since D is finite we can define

$$A_{ij}(n) = \sum_{\Gamma} w(\Gamma),$$

where the sum is over all walks Γ in D of length n from v_i to v_j. In particular, $A_{ij}(0) = \delta_{ij}$. If all $w(e) = 1$, then we are just counting the *number* of walks of length n from u to v. The fundamental problem treated by the transfer matrix method is the evaluation of $A_{ij}(n)$. The first step is to interpret $A_{ij}(n)$ as an entry in a certain matrix. Define a $p \times p$ matrix $A = (A_{ij})$ by

$$A_{ij} = \sum_{e} w(e),$$

where the sum ranges over all edges e satisfying $\operatorname{init} e = v_i$ and $\operatorname{fin} e = v_j$. In other words, $A_{ij} = A_{ij}(1)$. The matrix A is called the *adjacency matrix* of D, with respect to the weight function w. The eigenvalues of the adjacency matrix A play a key role in the enumeration of walks. These eigenvalues are also called the *eigenvalues of D* (as a weighted digraph).

4.7.1 Theorem. *Let $n \in \mathbb{N}$. Then the (i, j)-entry of A^n is equal to $A_{ij}(n)$. (Here we define $A^0 = I$ even if A is not invertible.)*

Proof. The proof is immediate from the definition of matrix multiplication. Specifically, we have

$$(A^n)_{ij} = \sum A_{ii_1} A_{i_1 i_2} \cdots A_{i_{n-1} j},$$

where the sum is over all sequences $(i_1, \dots, i_{n-1}) \in [p]^{n-1}$. The summand is 0 unless there is a walk $e_1 e_2 \cdots e_n$ from v_i to v_j with $\operatorname{fin} e_k = v_{i_k}$ $(1 \le k < n)$ and $\operatorname{init} e_k = v_{i_{k-1}}$ $(1 < k \le n)$.

If such a walk exists, then the summand is equal to the sum of the weights of all such walks, and the proof follows. □

The second step of the transfer-matrix method is the use of linear algebra to analyze the behavior of the function $A_{ij}(n)$. Define the generating function

$$F_{ij}(D,\lambda) = \sum_{n\geq 0} A_{ij}(n)\lambda^n.$$

4.7.2 Theorem. *The generating function $F_{ij}(D,\lambda)$ is given by*

$$F_{ij}(D,\lambda) = \frac{(-1)^{i+j}\det(I-\lambda A : j,i)}{\det(I-\lambda A)}, \tag{4.34}$$

where $(B : j,i)$ denotes the matrix obtained by removing the jth row and ith column of B. Thus in particular $F_{ij}(D,\lambda)$ is a rational function of λ whose degree is strictly less than the multiplicity n_0 of 0 as an eigenvalue of A.

Proof. $F_{ij}(D,\lambda)$ is the (i,j)-entry of the matrix $\sum_{n\geq 0}\lambda^n A^n = (I-\lambda A)^{-1}$. If B is any invertible matrix, then it is well-known from linear algebra that $(B^{-1})_{ij} = (-1)^{i+j}\det(B : j,i)/\det(B)$, so equation (4.34) follows.

Suppose now that A is a $p\times p$ matrix. Then

$$\det(I-\lambda A) = 1+\alpha_1\lambda+\cdots+\alpha_{p-n_0}\lambda^{p-n_0},$$

where

$$(-1)^p\left(\alpha_{p-n_0}\lambda^{n_0}+\cdots+\alpha_1\lambda^{p-1}+\lambda^p\right)$$

is the characteristic polynomial $\det(A-\lambda I)$ of A. Thus as polynomials in λ, we have $\deg\det(I-\lambda A) = p-n_0$ and $\deg\det(I-\lambda A : j,i)\leq p-1$. Hence

$$\deg F_{ij}\leq p-1-(p-n_0) < n_0. \quad \square$$

One special case of Theorem 4.7.2 is particularly elegant. Let

$$C_D(n) = \sum_{\Gamma} w(\Gamma),$$

where the sum is over all closed walks Γ in D of length n. For instance, $C_D(1) = \operatorname{tr} A$, where tr denotes trace.

4.7.3 Corollary. *Let $Q(\lambda) = \det(I-\lambda A)$. Then*

$$\sum_{n\geq 1} C_D(n)\lambda^n = -\frac{\lambda Q'(\lambda)}{Q(\lambda)}.$$