A detailed derivation of the transfer matrix method formula

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For an $n \times n$ matrix $A = (a_{i,j})$, we refer to the entry $a_{i,j}$ also as $A_{i,j}$ and by A^k we denote the k-th power of A; the $n \times n$ matrix A^k has entries

$$(A^k)_{i,j} = \sum_{i_1,i_2,\ldots,i_{k-1}} a_{i,i_1}a_{i_1,i_2}\ldots a_{i_{k-1},j} = \sum_{i_1,i_2,\ldots,i_{k-1}} A_{i,i_1}A_{i_1,i_2}\ldots A_{i_{k-1},j}.$$

By $A(i,j)$ we denote the $(n-1)\times(n-1)$ submatrix obtained from A by deleting the i-th row and j-th column. I denotes the unit matrix, $I_{i,j} = \delta_{i,j}$ where $\delta_{i,j}$ is Kronecker's symbol ($= 1$ if $i = j$ and $= 0$ else).

The transfer matrix method formula. *For every matrix $A \in \mathbb{C}^{n\times n}$, in the ring of power series $\mathbb{C}[[x]]$ we have for every $1 \le i,j \le n$ the identity*

$$\sum_{k\ge 0}(A^k)_{i,j}x^k = \frac{(-1)^{i+j}\det((I-xA)(j,i))}{\det(I-xA)}.$$

The $n\times n$ matrix $I - xA$ has entries $(I - xA)_{i,j} = \delta_{i,j} - a_{i,j}x$.

Note that the numerator and denominator lie in the ring of polynomials $\mathbb{C}[x]$ (which we embed naturally in $\mathbb{C}[[x]]$) and that $\det(I - xA)$ has nonzero constant term 1. Thus the power series $\det(I - xA)$ is invertible in $\mathbb{C}[[x]]$ and the right side of the formula is well defined.

The aim of this note is to discuss in detail algebraic steps in derivation of the TMM formula. For more condensed treatment and many applications in combinatorial enumeration see Stanley [3, section 4.7] or Flajolet and Sedgewick [1, section V.5].

The derivation of the TMM formula. *Since*

$$\begin{aligned}\left(\sum_{k\ge 0}(A^k)_{i,j}x^k\right)_{i,j=1}^{n} &= \sum_{k\ge 0}A^k x^k \\ &= (Ix^0 - Ax)^{-1} \\ &= (I-xA)^{-1} \\ &= \left(\frac{(-1)^{i+j}\det((I-xA)(j,i))}{\det(I-xA)}\right)_{i,j=1}^{n},\end{aligned}$$

comparison of entries in the initial and final $n \times n$ matrices yields the TMM formula.

Let us discuss and explain this calculation. The first and third $=$ signs are not really equalities—they "equate" matrices with power series—and are to be understood in the sense of isomorphism. The second and fourth $=$ signs are acceptable as equalities since they have on both sides structures of the same type, power series in the former case and $n \times n$ matrices in the latter.

We are working here with two distinct (but isomorphic) rings

$$R = \mathbb{C}[[x]]^{n\times n} \ \text{ and } \ S = \mathbb{C}^{n\times n}[[x]],$$

the ring R of $n \times n$ matrices whose entries are power series from $\mathbb{C}[[x]]$ and the ring S of power series whose coefficients are $n \times n$ matrices from $\mathbb{C}^{n\times n}$. In the derivation, we start in R, switch to S, go to S, switch to R and finish in R:

$$R \to S \to S \to R \to R.$$

Rings R and S both have 1 but are noncommutative and have zero divisors. They are isomorphic via the mappings ($[x^k]F$ denotes the coefficient of x^k in the power series F)

$$\kappa:\ R \to S,\ \kappa:\ M \mapsto \sum_{k\geq 0} \left([x^k]M_{i,j}\right)_{i,j=1}^n x^k$$

and

$$\lambda:\ S \to R,\ \lambda:\ \sum_{k\geq 0} M(k)x^k \mapsto \left(\sum_{k\geq 0} M(k)_{i,j}x^k\right)_{i,j=1}^n.$$

It is clear that κ and λ send 1 to 1 and preserve addition. To check that they preserve multiplication is a little notational challenge, which we postpone for a while. Also, $\kappa \circ \lambda$ and $\lambda \circ \kappa$ are identical mappings. Thus they provide an isomorphism of R and S.

Let $M \in R$ be the initial matrix, $M_{i,j} := \sum_{k\geq 0}(A^k)_{i,j}x^k$. We will discuss in turn the four $=$ signs in the derivation. The first one is just the application of κ: we go from M to $\kappa(M)$. The second $=$ sign is the formula for sum of a formal geometric series. This is the easily verifiable identity

$$1 = (1 - ax)(1 + ax + a^2x^2 + \cdots)$$

holding in every ring of power series $U[[x]]$ over a (not necessarily commutative) ring U with 1 (here $U = \mathbb{C}^{n\times n}$). Thus

$$\kappa(M) = f^{-1} \quad \text{where} \quad f := Ix^0 - Ax \in S.$$

The third $=$ sign is the heart of the matter. It is an assertion that for $f = Ix^0 - Ax$ we have in the ring R the identity

$$\lambda(f^{-1}) = \lambda(f)^{-1}.$$

It suffices if we convince ourselves that multiplicative inverses in any (not necessarily commutative) ring U with 1 are unique. Indeed, if $a, b, c \in U$ are such that $ab = ba = 1$ and $ca = 1$ or $ac = 1$, then multiplication by b from right or left gives that $c = b$. Now, in $U = R$, $1 = \lambda(1) = \lambda(ff^{-1}) = \lambda(f)\lambda(f^{-1})$, hence $\lambda(f^{-1}) = \lambda(f)^{-1}$.

The fourth and last $=$ sign is Cramer's formula from linear algebra for the entries of the matrix inverse in $U^{n\times n}$, where U is a commutative ring with 1 (here $U = \mathbb{C}[[x]]$).

Summarizing the calculation,

$$\kappa(M) = f^{-1} \quad \text{thus} \quad M = \lambda(\kappa(M)) = \lambda(f^{-1}) = \lambda(f)^{-1} = (I - xA)^{-1}$$

which is the TMM formula. No fake $=$ sign now!

We check that λ is multiplicative homomorphism, which suffices. Let $F, G \in S$, $F = \sum_{k\geq 0} M(k)x^k$ and $G = \sum_{k\geq 0} N(k)x^k$ with $M(k), N(k) \in \mathbb{C}^{n\times n}$. Then

$$\lambda(FG) = \lambda\Big(\sum_{k\geq 0}\Big(\sum_{l=0}^{k} M(l)N(k-l)\Big)x^k\Big) = \lambda\Big(\sum_{k\geq 0} P(k)x^k\Big)$$

where

$$P(k)_{i,j} = \sum_{l=0}^{k}\sum_{i_1=1}^{n} M(l)_{i,i_1}N(k-l)_{i_1,j}.$$

So

$$\lambda(FG) = \left(\sum_{k\geq 0} P(k)_{i,j}x^k\right)_{i,j=1}^{n} = \left(\sum_{k\geq 0}\Big(\sum_{l=0}^{k}\sum_{i_1=1}^{n} M(l)_{i,i_1}N(k-l)_{i_1,j}\Big)x^k\right)_{i,j=1}^{n}.$$

On the other hand,

$$\begin{aligned}
\lambda(F)\lambda(G) &= \left(\sum_{k\geq 0} M(k)_{i,j}x^k\right)_{i,j=1}^n \left(\sum_{k\geq 0} N(k)_{i,j}x^k\right)_{i,j=1}^n \\
&= \left(\sum_{i_1=1}^n \Big(\sum_{k\geq 0} M(k)_{i,i_1}x^k\Big)\Big(\sum_{k\geq 0} N(k)_{i_1,j}x^k\Big)\right)_{i,j=1}^n \\
&= \left(\sum_{i_1=1}^n \sum_{k\geq 0} \Big(\sum_{l=0}^k M(l)_{i,i_1} N(k-l)_{i_1,j}\Big)x^k\right)_{i,j=1}^n .
\end{aligned}$$

Changing the order of summation and moving the outer sum $\sum_{i_1=1}^n$ inside, we see that indeed

$$\lambda(F)\lambda(G) = \lambda(FG).$$

Final remarks and acknowledgments. The isomorphism of the rings R and S follows naturally from their construction as tensor products, in the two possible orders, of the algebras $\mathbb{C}^{n\times n}$ and $\mathbb{C}[[x]]$. Also, the additive structure of R and S is in fact irrelevant for the derivation and we could have worked with them just as multiplicative monoids. The field $\mathbb{C}$ can be replaced by any commutative ring with 1.

Derivations of the TMM formula in the literature often do not properly distinguish between R and S (but see Goulden and Jackson [2, section 1.1.10] for an exception), if they give details at all. This is a bit unfortunate because neither the summation of formal geometric series nor Cramer's formula but the switching between R and S is the main device propelling the derivation.

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References

[1] P. Flajolet and R. Sedgewick, *Analytic Combinatorics*, Cambridge University Press, to appear.

[2] I. P. Goulden and D. M. Jackson, *Combinatorial Enumeration*, John Wiley & Sons, 1983.

[3] R. P. Stanley, *Combinatorial Enumeration. Volume I*, Wadsworth & Brooks/Cole, 1986.