Minimum-Dimension Trace Maps for Substitution Sequences

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We construct trace maps for products of 2×2 matrices generated by arbitrary substitution sequences. The dimension of the underlying space of our trace map is the minimal possible, namely $3r-3$ for an alphabet of size $r\geq 2$.

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The discovery of quasicrystals [1] and their one-dimensional modeling [2] have led to a deep mathematical study of Schrödinger operators with arbitrary deterministic potential sequences. This instance should be thought of as lying in between the case of random potentials and that of periodic potential. The study of quasicrystals leads to the Fibonacci chain [3], which arises from a certain substitution (see below) on a two-letter alphabet. Other sequences obtained by substitutions on such alphabets were studied, in particular generalizations of the Fibonacci chain [4] and the Thue-Morse sequence [5]. Systems originating from substitutions on larger alphabets were considered as well; the Circle [6] sequence and the ternary quasiperiodic sequences [7] arise from three-letter alphabets, the Rudin-Shapiro sequence [8] studied in [9] and quarternary quasiperiodic sequences [10]—from four-letter alphabets, and the N-ternary Fibonacci lattice [11]—from alphabets of arbitrary size.

An efficient method in the analysis of such systems is that of transfer matrices, first introduced by Brillouin [12]. The next step is obtaining trace maps, which was first carried out by Kohmoto, Kadanoff, and Tang and Ostlund *et al.* [3]; see also Kohmoto and Oono [13]. Allouche and Peyrière [14] proved, more generally, that for any substitution on a two-letter alphabet, one can effectively construct a trace map acting (in the case of unimodular matrices) on three-dimensional space. Kolář and Nori [15] have shown that trace maps of higher dimensions do exist for substitution sequences containing more than two letters. The dimension in their construction increases, however, faster than exponentially as a function of the alphabet size r. The dimension was later [16] reduced to 2^r-1, and Iguchi [17] reduced it further to $r(r+1)/2$. (It is worth mentioning here that there are other approaches which are not based on trace maps of transfer matrices [18].)

In this paper we get the best possible result in this sense by reducing the dimension of the trace map to $3r-3$. (In the trivial case $r=1$ the dimension is 1. We shall avoid this case.) In the general case, the dimension cannot be made smaller.

It has recently been demonstrated that a crystal with the structure of a Thue-Morse chain can be grown. Therefore, fabrication of one-dimensional quasicrystals with other substitution rules might be experimentally accessible. Hence, the trace map we suggest here may serve as an important theoretical tool for the investigation of new artificial structures.

Definitions and notation. Let Σ be a finite alphabet, say $\Sigma=\{1,2,\ldots,r\}$, and let σ be a substitution on Σ, namely σ is a function from Σ to Σ^*, the set of all (finite) words over Σ:

$$\sigma(k)=\sigma_{k1}\sigma_{k2}\cdots\sigma_{kq_k},\quad k=1,2,\ldots,r \qquad (\sigma_{ki}\in\Sigma,\ 1\leq i\leq q_k)\,. \tag{1}$$

We extend σ to a mapping from Σ^* to Σ^* by

$$\sigma(x_1x_2\cdots x_s)=\sigma(x_1)\sigma(x_2)\cdots\sigma(x_s)\,,\qquad x_1,x_2,\ldots,x_s\in\Sigma\,. \tag{2}$$

For example, the Fibonacci chain mentioned earlier is obtained from the two-letter substitution defined by $r=2$, $\sigma(1)=12$, $\sigma(2)=1$. For an extensive treatment of substitutions, especially from the point of view of dynamical systems, see Queffélec's book [19].

Substitutions may serve as a means of defining sequences of matrices. Given r initial square matrices $A_{10},A_{20},\ldots,A_{r0}$ of the same size and a substitution σ on $\{1,2,\ldots,r\}$, we define the sequences of matrices $\{A_{kn}\}_{n=0}^{\infty}$, $1\leq k\leq r$ by

$$A_{k,n+1}=A_{\sigma_{kq_k}n}\cdots A_{\sigma_{k2}n}A_{\sigma_{k1}n}\,,\qquad 1\leq k\leq r,\quad n=0,1,2\ldots \tag{3}$$

For the Fibonacci substitution, for instance, we have two sequences of matrices $\{A_n\}_{n=0}^{\infty}$ and $\{B_n\}_{n=0}^{\infty}$ satisfying $A_{n+1}=A_nB_n$, $B_{n+1}=A_n$.

The matrices in the applications we have in mind are usually unimodular. They belong to SL(2,**R**) or some conjugate subgroup of SL(2,**C**). We shall henceforward usually assume that our matrices are such, although it will be evident that, using information on the determinants of the matrices in question, analogous results can be obtained for arbitrary matrices with complex entries (or, indeed, over any ground field). Thus, we pass from the r matrices A_{kn}, $1\leq k\leq r$ of the nth stage to the r matrices $A_{k,n+1}$, $1\leq k\leq r$ of the $(n+1)$st stage by means of a certain "monomial" transformation of $SL(2,\mathbf{R})^r$.

Unfortuantely, the dynamics of this kind of transformation turns out to be quite complicated already for very simple substitutions. A possible approach to attack this problem is to restrict ourselves to part of the information only, i.e., to consider only the traces of the matrices in question, and not the matrices themselves. Whereas $SL(2,\mathbf{R})^4$ is $3r$ dimensional, we can keep track of all trace information in a space of smaller dimension. Of course, the trace of a product of matrices is not determined by the traces of the individual matrices in the product, so we cannot work in an r-dimensional space. However, since conjugating all matrices by some fixed matrix has no effect on the trace of any monomial in the given matrices, we can expect to reduce the dimension by 3, from $3r$ to $3r-3$. A *trace map* is a mapping which, given the traces of several monomials in the matrices of the nth stage, enables us to calculate the traces of the same monomials for the next stage. The trace map constructed by Allouche and Peyrière [14] in the case $r=2$ acts on a space of the right dimension $3\times 2-3=3$. For example, in the case of the Fibonacci substitution, if A_n and B_n are 2×2 matrices of determinant 1, and we set $a_n=t_{A_n}$, $b_n=t_{B_n}$, then $a_{n+3}=a_{n+1}a_{n+2}-a_n$ (and of course $b_{n+1}=a_n$). (Here and later t_M denotes the trace of the matrix M.) All trace maps constructed hitherto for $r>2$ act on higher-dimensional spaces, and as r gets large these dimensions are much larger than the $3r$ needed to keep all matrix information (except that the trace map given by Iguichi [17] acts on a space of dimension $3\times 3-3=6$ in the case $r=3$).

The main result of this paper is obtaining a trace map of dimension $3r-3$ for any r.

The trace map. In this section we derive formulas connecting various monomials in several matrices, and matrices of these monomials. The formulas for traces appearing up to and including Lemma 4 are known [20], but our approach enables us to obtain more results for the matrices themselves, and not merely for the traces.

Denote by I the identity matrix. The following was proved in Ref. [16].

Lemma 1. Let A and B be 2×2 matrices. Then

$$BA=(t_{AB}-t_At_B)I+t_AB+t_BA-AB\,. \quad (4)$$

Corollary 1. Let $A_1,A_2,\ldots,A_r$ be 2×2 matrices. Define the following 2^r matrices:

$$B_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}=A_1^{\varepsilon_1}A_2^{\varepsilon_2}\cdots A_r^{\varepsilon_r}\quad(\varepsilon_j=0,1,\ 1\le j\le r)\,. \quad (5)$$

Then any monomial $A_{j_1}A_{j_2}\cdots A_{j_s}$ ($1\le j_i\le r$ for $1\le i\le s$) can be effectively written as a linear combination of the matrices $B_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}$, namely,

$$A_{j_1}A_{j_2}\cdots A_{j_s}=\sum_{\varepsilon_1=0}^{1}\sum_{\varepsilon_2=0}^{1}\cdots\sum_{\varepsilon_r=0}^{1}c_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}B_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}\,, \quad (6)$$

where each coefficient $c_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}$ is a polynomial in the traces t_{A_j}, $1\le j\le r$, the traces $t_{A_jA_k}$, $1\le j<k\le r$, and the determinants $\det A_j$, $1\le j\le r$.

The corollary is almost the same as Theorem 1 of Ref. [16], except for the additional observation that the coefficients $c_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}$ may be expressed as polynomials in the traces of single matrices A_j and products of pairs of such matrices, but traces of products of three or more matrices are not required. This fact will play a crucial role in the proof of Lemma 4 in the sequel.

Corollary 2. Let $A_1,A_2,\ldots,A_r$ be 2×2 matrices. Then the trace $t_{A_{j_1}A_{j_2}\cdots A_{j_s}}$ of any monomial $A_{j_1}A_{j_2}\cdots A_{j_s}$ can be effectively written as a polynomial in the traces $t_{B_{\varepsilon_1\varepsilon_2\cdots\varepsilon_r}}$ and the determinants $\det A_j$, $1\le j\le r$, which is linear in the traces of all products of three or more of the basic matrices.

Lemma 2. Let A,B,C be 2×2 matrices. Then

$$\begin{aligned}ABC=\tfrac{1}{2}[&(t_{ABC}-t_{AB}t_C-t_At_{BC}+t_At_Bt_C)I\\&+(t_{BC}-t_Bt_C)A-t_{AC}B+(t_{AB}-t_At_B)C\\&+t_CAB+t_BAC+t_ABC]\,.\end{aligned} \quad (7)$$

The simplest proof for Lemma 2, as well as for Lemmas 3 and 4 later, goes via Lemma 1. As one can, however, check both lemmas directly we shall not provide proofs.

Remark 1. Taking the traces of both sides in (7), we are led to a trivial identity. The reason is the appearance of t_{ABC} on the right hand side. It is natural to ask for a formula expressing ABC as a linear combination of I,A,B,C,AB,AC,BC with coefficients depending only on the traces of these matrices. However, such a representation would prove in particular that t_{ABC} is determined by these traces, which turns out to be false (see Remark 2 below).

Lemma 3. Let A,B,C,D be 2×2 matrices. Then,

$$\begin{aligned}ABCD=\tfrac{1}{2}[&(t_{ABC}-t_{AB}t_C-t_At_{BC}+t_At_Bt_C)D+(t_{BC}-t_Bt_C)AD-t_{AC}BD\\&+(t_{AB}-t_At_B)CD+t_CABD+t_BACD+t_ABCD]\,.\end{aligned} \quad (8)$$

In particular,

$$\begin{aligned}t_{ABCD}=\tfrac{1}{2}(&t_{ABC}t_D+t_{ABD}t_C+t_{ACD}t_B+t_{BCD}t_A+t_{AB}t_{CD}-t_{AC}t_{BD}+t_{AD}t_{BC}\\&-t_{AB}t_Ct_D-t_{AD}t_Bt_C-t_{BC}t_At_D-t_{CD}t_At_B+t_At_Bt_Ct_D)\,.\end{aligned} \quad (9)$$

Employing Corollary 1, we immediately obtain from Lemma 3:

Corollary 3. Let $A_1,A_2,\ldots,A_r$ be 2×2 matrices. Then any monomial $A_{j_1}A_{j_2}\cdots A_{j_s}$ can be effectively written as a linear combination of the individual matrices A_j, the biproducts A_jA_k and the triproducts $A_jA_kA_l$, the coefficients being polynomials in the traces of these matrices and the determinants $\det A_j$. In particular, each trace $t_{A_{j_1}A_{j_2}\cdots A_{j_s}}$ can be effectively written as a polynomial in these traces and determinants.

Lemma 4. Let A,B,C be unimodular 2×2 matrices. Then,

$$t_{ABC}^2+(t_At_Bt_C-t_At_{BC}-t_Bt_{AC}-t_Ct_{AB})t_{ABC}+(t_{AB}^2+t_{AC}^2+t_{BC}^2+t_A^2+t_B^2+t_C^2 -t_At_Bt_{AB}-t_At_Ct_{AC}-t_Bt_Ct_{BC}+t_{AB}t_{AC}t_{BC}-4)=0\,. \tag{10}$$

The last identity is known as the Fricke identity [20].

Remark 2. The lemma means that, given the traces of the matrices A,B,C and products of pairs thereof, t_{ABC} is determined (generically) up to one of two possible values. This indeterminacy is unavoidable. In fact, as the coefficients in the quadratic equation (10) are invariant (for unimodular matrices) under inverting all three matrices A,B,C, the trace $t_{A^{-1}B^{-1}C^{-1}}$ satisfies the same equation. Now one verifies easily that usually $t_{ABC}\neq t_{A^{-1}B^{-1}C^{-1}}$. Thus, we cannot expect an improvement of (10) in this sense.

Lemma 5. Let A,B,C,D be unimodular 2×2 matrices. Then,

$$\begin{vmatrix} t_A^2-2 & t_{AB} & t_{AC} & t_{AD} & t_A \\ t_{AB} & t_B^2-2 & t_{BC} & t_{BD} & t_B \\ t_{AC} & t_{BC} & t_C^2-2 & t_{CD} & t_C \\ t_{AD} & t_{BD} & t_{CD} & t_D^2-2 & t_D \\ t_A & t_B & t_C & t_D & 2 \end{vmatrix}=0\,. \tag{11}$$

Proof. We shall obtain (11) as a special case of a more general formula. Let M_1,M_2,M_3,M_4,M_5 be any 2×2 matrices. Since the space of all 2×2 matrices, considered as a linear space over the base field, is four dimensional, there exist scalars $\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5$, not all 0, such that

$$\alpha_1M_1+\alpha_2M_2+\alpha_3M_3+\alpha_4M_4+\alpha_5M_5=0\,. \tag{12}$$

Multiplying (12) consecutively by each of the matrices M_i, $1\le i\le 5$, and taking traces we arrive at

$$(t_{M_iM_j})\boldsymbol{\alpha}=0\,, \tag{13}$$

where $\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5)$. Thus, the matrix $(t_{M_iM_j})_{i,j=1}^5$ is singular, whence its determinant is 0. The special case $M_1=A$, $M_2=B$, $M_3=C$, $M_4=D$, $M_5=I$ leads to (12).

In view of the lemma, t_{CD} is generically determined, up to one of two possible values, by the nine traces $t_A,t_B,t_C,t_D,t_{AB},t_{AC},t_{AD},t_{BC},t_{BD}$. Indeed, (11) yields a quadratic equation in t_{AD}, the coefficient of t_{AD}^2 being

$$-\begin{vmatrix} t_A^2-2 & t_{AB} & t_A \\ t_{AB} & t_B^2-2 & t_B \\ t_A & t_B & 2 \end{vmatrix}=2(t_A^2+t_B^2+t_{AB}^2-t_At_Bt_{AB}-4) =2(t_{A^{-1}B^{-1}AB}-2)\,, \tag{14}$$

which is usually nonzero.

Remark 3. One should not expect the abovementioned nine traces to always determine t_{CD} to within finitely many possibilities. For example, if $A=B=I$ then we only know t_C and t_D, which can be seen to say little regarding t_{CD}.

The last lemma provides the key for our trace map. Given r unimodular matrices $A_1,A_2,\ldots,A_r$, suppose we know the r individual traces t_{A_j}, $1\le j\le r$, the $r-1$ traces of products of pairs of matrices containing A_1, namely t_{A_1,A_j}, $2\le j\le r$, and the $r-2$ traces of products of pairs of matrices containing A_2, namely $t_{A_2A_j}$, $3\le j\le r$. Employing (11), with A_1,A_2,A_i,A_k in place of A,B,C,D, respectively, we get quadratic equations determining generically (up to finitely many possible values) all traces of the form $t_{A_jA_k}$, then all traces of the form $t_{A_jA_{j+4}}$, etc. Then, employing (10) we can find (again, up to finitely many possibilities) all traces of triproducts, $t_{A_jA_kA_l}$. By Corollary 3, we can then calculate the trace of any monomial. These considerations lead one to expect the following results to hold.

Theorem 1. Given a substitution on an alphabet of size r, one can effectively construct a corresponding trace map acting on a $(3r-3)$-dimensional variety in $\mathbf{R}^{r+\binom{r}{2}+\binom{r}{3}}$. The dimension of the variety cannot in general be reduced.

The discussion preceding the theorem does not constitute a full proof, as the traces singled out there determine all the other traces (up to finitely many possibilities) only in the generic case. To complete the proof we need the following two lemmas.

Lemma 6. The algebraic variety defined in $\mathbf{R}^{r+\binom{r}{2}}$ by means of the polynomials

$$P_{ijkl}=\begin{vmatrix} X_i^2-2 & Y_{ij} & Y_{ik} & Y_{il} & X_i \\ Y_{ij} & X_j^2-2 & Y_{jk} & Y_{jl} & X_j \\ Y_{ik} & Y_{jk} & X_k^2-2 & Y_{kl} & X_k \\ Y_{il} & Y_{jl} & Y_{kl} & X_l^2-2 & X_l \\ X_i & X_j & X_k & X_l & 2 \end{vmatrix} \tag{15}$$

$$1\le i<j<k<l\le r$$

is $(3r-3)$ dimensional.

Lemma 7. The image of the mapping T: $\mathrm{SL}(2,\mathbf{R})^r\to\mathbf{R}^{r+\binom{r}{2}}$, defined by

$$T(A_1,\ldots,A_r)=[(t_{A_j})_{1\le j\le r},(t_{A_jA_k})_{1\le j<k\le r}]\,, \tag{16}$$

$$A_1,\ldots,A_r\in\mathrm{SL}(2,\mathbf{R})$$

is $(3r-3)$ dimensional.

In view of the preceding results it suffices to show that the variety in Lemma 6 is at most $(3r-3)$ dimensional and the image in Lemma 7 is at least $(3r-3)$ dimensional.

Proof of Lemma 6. For distinct integers $i,j,k,l \in \{1,2,\ldots,r\}$ denote by $P_{\{ijkl\}}$ the polynomial P_{abcd} defined in (15), where a,b,c,d are defined by $\{a,b,c,d\}=\{i,j,k,l\}$ and $a<b<c<d$. Define also the polynomials

$$Q_{ij}=X_i^2+X_j^2+Y_{ij}^2-X_iX_jY_{ij}-4, \quad 1\le i<j\le r. \tag{17}$$

Let $\mathcal{P}$ be the ideal generated by the polynomials P_{ijkl}, $\mathcal{Q}$ be the ideal generated by the polynomials Q_{ij}, and $\mathcal{V}(\mathcal{P})$ and $\mathcal{V}(\mathcal{Q})$ the varieties of these ideals. Denoting $\mathbf{x}=(x_i)_{1\le i\le r}$ and $\mathbf{y}=(y_{ij})_{1\le i<j\le r}$ we have

$$\mathcal{V}(\mathcal{P})=\cup_{1\le i<j\le r}[\mathcal{V}(\mathcal{P})\cap\{(\mathbf{x},\mathbf{y}):Q_{ij}(\mathbf{x},\mathbf{y})\ne 0\}]\cup\mathcal{V}(\mathcal{Q}). \tag{18}$$

In view of the discussion preceding Remark 3 each of the sets $\mathcal{V}(\mathcal{P})\cap\{(\mathbf{x},\mathbf{y}):Q_{ij}(\mathbf{x},\mathbf{y})\ne 0\}$ is $(3r-3)$ dimensional, while $\mathcal{V}(\mathcal{Q})$ is clearly r dimensional. This proves the lemma.

Proof of Lemma 7. It clearly suffices to show the conclusion of the lemma holds if the mapping T is replaced by

$$S(A_1,\ldots,A_r)=[(t_{A_j})_{j=1}^r,(t_{A_1A_j})_{j=2}^r,(t_{A_2A_j})_{j=3}^r], \quad A_1,\ldots,A_r\in SL(2,\mathbf{R}). \tag{19}$$

Taking a "random" point, it suffices to verify that the Jacobian matrix of S at this point (with respect to appropriately chosen local coordinates) is of rank $3r-3$. This can be accomplished by induction. We omit the details.

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