

Commuting time geometry of ergodic Markov chains

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Abstract

We show how to map the states of an ergodic Markov chain to Euclidean space so that the squared distance between states is the expected commuting time, and we find a minimax characterization of commuting times. These results are familiar in the case of time-reversible chains, where techniques of classical electrical theory apply, and the minimax simplifies to a minimum principle. In presenting these results, we take the opportunity to develop Markov chain theory in a ‘conformally correct’ way.

1 Overview

In an eye-opening paper, Chandra, Raghavan, Ruzzo, Smolensky, and Tiwari [1] revealed the central importance of expected commuting times for the theory of time-reversible Markov chains. Here we extend the discussion to general, non-time-reversible chains.

We begin by showing how to embed the states in a Euclidean space so that the squared distance between states is the commuting time. In the time-reversible case, Leighton et al. have used Euclidean embeddings to great effect as a way to visualize a chain, and reveal natural clustering of states.

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Our embedding theorem shows that non-time-reversible chains should be amenable to the same treatment.

Looking beyond the Euclidean embedding, we find a natural minimax characterization of commuting times. For time-reversible chains, this simplifies to the minimum dissipation principle familiar from electrical theory.

In presenting these results, we will be taking a ‘conformally correct’ approach to Markov chains. Briefly, a conformal change to a Markov chain changes its equilibrium measure, but not its equilibrium transition rates. The opportunity to develop this conformally correct approach is at least as important to us as the particular results we’ll be discussing here.

CORRECTION

In the first version of this paper, we (Peter) claimed that the minimax characterization of commuting times implies the following monotonicity law: If all equilibrium interstate transition rates are increased, then all commuting times are diminished. For time-reversible chains, this monotonicity law is an ancient and powerful tool. As Russ Lyons and Yuval Perez have kindly pointed out, the generalization to non-reversible chains fails miserably already for a merry-go-round chain, where from $i \pmod n$ you move to $i + 1 \pmod n$ with probability $1/2$, and otherwise stay where you are. The commuting time between any two distinct states is $2n$, while for a simple random walk on the integers mod n all equilibrium transition rates are larger, but commuting times between distant states are quadratic in n .

The good news is that we had found no applications for this bogus generalization of monotonicity, and had even observed, ‘it is questionable how useful it will prove in the general case.’ Cold comfort, but comfort nonetheless.

Russ and Yuval also settled the question we had left open about whether any commuting time matrix can arise from a reversible chain: They showed that the answer is no. We’ll come back to this.

2 The problem

The *commuting time* T_{ab} between two states a, b of an ergodic Markov chain is the expected time, starting from a , to go to b and then back to a . Evidently

$$T_{ab} = T_{ba} \text{ and}$$

$$T_{ac} \leq T_{ab} + T_{bc}.$$

Thus it might seem natural to think of T_{ab} as a measure of the distance between a and b . But in fact it is most natural to think of T_{ab} as the *squared distance* between a and b . The reason is that, as we will see, there is a natural way to identify the states of the chain with points in a Euclidean space having quadratic form $\|x\|^2$ such that for any states a, b we have

$$T_{ab} = \|a - b\|^2.$$

Now that we are interpreting T_{ab} as a squared distance, the inequality $T_{ac} \leq T_{ab} + T_{bc}$ tells us that

$$\|a - c\|^2 \leq \|a - b\|^2 + \|b - c\|^2.$$

This means that all angles $\angle abc$ are acute (at least weakly: some might be right angles).

Realizing commuting times as squared distances is straight-forward for time-reversible chains. Here's a sketch, meant only for orientation: We won't rely on any of this below. Time-reversible chains correspond exactly to resistor networks, with T_{ab} corresponding to the effective resistance between a and b . This effective resistance is the energy of a unit current flow from a to b . The energy of a flow is its squared distance with respect to the energy norm on flows. If we associate to state i the unit current flow from i to some arbitrary reference vertex (the 'ground'), then the difference between the flows associated to a and b will be the unit current flow from a to b , having square norm T_{ab} .

The trick will be to extend this result to non-time-reversible chains.

Note. If it were the case that to any chain there corresponds a time-reversible chain having the same T , up to multiplication by a positive constant, this extension would be immediate. It is easy enough to compute what the transition rates of this time-reversible chain would have to be, the question is whether these are necessarily positive. Russ Lyons found by computer search that the answer is no: There are chains whose commuting-time matrix does not arise from a time-reversible chain. In fact such chains become plentiful as the number of states increases.

Before proceeding, we should observe that the triangle inequality for squared lengths is not in itself a sufficient condition for realizability of a

Euclidean simplex. It *is* sufficient for tetrahedra (four vertices in 3-space), but for five vertices we have the following counterexample. Take

$$T = \begin{pmatrix} 0 & 7 & 7 & 7 & 13 \\ 7 & 0 & 12 & 12 & 7 \\ 7 & 12 & 0 & 12 & 7 \\ 7 & 12 & 12 & 0 & 7 \\ 13 & 7 & 7 & 7 & 0 \end{pmatrix}$$

This matrix is not realizable because the associated quadratic form with matrix

$$\frac{1}{2} \begin{pmatrix} 14 & 2 & 2 & 13 \\ 2 & 14 & 2 & 13 \\ 2 & 2 & 14 & 13 \\ 13 & 13 & 13 & 26 \end{pmatrix}$$

is not positive definite: It has the eigenvalue $\frac{1}{2}(22 - \sqrt{523}) \approx -0.434597$. Since we're going to see that commuting time matrices are always realizable, this means in particular that this matrix T cannot arise as the matrix of commuting times of a Markov chain.

3 The short answer

Below we will give the honest solution to this problem, developing in a thoroughgoing way what we will call the ‘conformally correct’ approach to Markov chains. Here we just extract the answer to our embedding question, and present it in a way that should be immediately accessible to those familiar with the standard theory of Markov chains, as developed for example in Grinstead and Snell [3]. The only caveat is that we will be using tensor notation, i.e. writing some indices up rather than down. You can look at section 5 below for remarks about this, but if you prefer you can just view this as an idiosyncrasy, as long as you bear in mind that Z_i^j represents a different array of numbers from Z_{ij} .

Consider a discrete-time Markov chain with transition probabilities

$$P_i^j = \text{Prob}(\text{next at } j | \text{start at } i).$$

Assume the chain is ergodic so there is a unique equilibrium measure w^i with

$$\sum_i w^i P_i^j = w^j$$

and

$$\sum_i w^i = 1.$$

Define

$$\Delta^{ij} = w^i (I_i^j - P_i^j),$$

and note that

$$\sum_i \Delta^{ij} = \sum_j \Delta^{ij} = 0.$$

Now define

$$Z_i^j = (I_i^j - w^j) + (P_i^j - w^j) + (P^{(2)}_i^j - w^j) + \dots,$$

where $P^{(2)}_i^j = \sum_k P_i^k P_k^j$ represents the matrix square of P_i^j , and the elided terms involve higher matrix powers. Using conventional matrix notation if we define $P^{(\infty)}_i^j = w^j$ we can write

$$\begin{aligned} Z &= (I - P^{(\infty)}) + (P - P^{(\infty)}) + (P^{(2)} - P^{(\infty)}) + \dots \\ &= (I - P + P^{(\infty)})^{-1} - P^{(\infty)}. \end{aligned}$$

(Note that Grinstead and Snell [3] use the alternate definition $Z = (I - P + P^{(\infty)})^{-1}$, which is less congenial but works just as well in this context.)

Set

$$Z_{ij} = \frac{1}{w^j} Z_i^j.$$

Z_{ij} acts like an inverse to Δ^{ij} in the sense that for any u^i with $\sum_i u^i = 0$, we have

$$\sum_{jk} u^j Z_{jk} \Delta^{kl} = u^l$$

and

$$\sum_{jk} \Delta^{ij} Z_{jk} u^k = u^i.$$

Standard Markov chain theory tells us that the expected time M_{ab} to hit state b starting from state a is

$$M_{ab} = Z_{bb} - Z_{ab}.$$

So for the commuting time we have

$$T_{ab} = M_{ab} + M_{ba} = Z_{aa} - Z_{ab} - Z_{ba} - Z_{bb}.$$

For a vector $x = (x_i)_{i=1,\dots,n}$ define

$$||x||^2 = \sum_{ij} x_i \Delta^{ij} x_j.$$

Please note that this does not make Δ^{ij} the matrix of the quadratic form in the usual sense, because in general $\Delta^{ij} \neq \Delta^{ji}$. The matrix of the form in the usual sense is the symmetrized version $\frac{1}{2}(\Delta^{ij} + \Delta^{ji})$.

Because

$$\sum_i \Delta^{ij} = \sum_j \Delta^{ij} = 0$$

we have the key identity

$$||x||^2 = -\frac{1}{2} \sum_{ij} \Delta^{ij} (x_i - x_j)^2.$$

Recalling the definition of Δ^{ij} gives

$$||x||^2 = \frac{1}{2} \sum_{ij} w^i P_i^j (x_i - x_j)^2.$$

Thus the quadratic form $||x||^2$ is weakly positive definite, but not strictly so, because it vanishes for constant vectors:

$$||(c, \dots, c)||^2 = 0.$$

It becomes strictly positive definite if we identify vectors differing by a constant vector:

$$(x_i)_{i=1,\dots,n} \equiv (z_i + c)_{i=1,\dots,n}.$$

This Euclidean space (vectors mod constant vectors, with the pushed-down quadratic form) is where we will embed our chain.

To get the embedding, map state a to the vector

$$f(a) = (Z_{ai})_{i=1,\dots,n}.$$

For the difference between the images of a and b we have

$$(f(a) - f(b))_i = Z_{ai} - Z_{bi} = \sum_k (\delta_a^k - \delta_b^k) Z_{ki},$$

with δ_i^j the Kronecker delta. We want to see that $f(a) - f(b)$ has square norm T_{ab} .

From the generalized inverse relationship between Z_{ij} and Δ^{ij} and the fact that

$$\sum_k (\delta_a^k - \delta_b^k) = 0$$

we have

$$\sum_i (Z_{ai} - Z_{bi}) \Delta^{ij} = \sum_{ki} (\delta_a^k - \delta_b^k) Z_{ki} \Delta^{ij} = \delta_a^j - \delta_b^j.$$

So

$$\begin{aligned} \|f(a) - f(b)\|^2 &= \sum_{ij} (Z_{ai} - Z_{bi}) \Delta^{ij} (Z_{aj} - Z_{bj}) \\ &= \sum_j (\delta_a^j - \delta_b^j) (Z_{aj} - Z_{bj}) \\ &= Z_{aa} - Z_{ab} - Z_{ba} + Z_{bb} \\ &= T_{ab}. \end{aligned}$$

There you have it.

4 What just happened

We want to explain the proof we have just given in more conceptual terms.

Let V be a finite-dimensional real vector space, and V^* the dual space, consisting of linear functionals $\phi : V \rightarrow \mathbf{R}$. For $u \in V^*$, $x \in V$ write

$$\langle u, x \rangle_V = u(x)$$

for the natural pairing between V and V^* . Identify V with V^{**} as usual:

$$\langle x, u \rangle_{V^*} = u(x) = \langle u, x \rangle_V.$$

To a map $f : V \rightarrow W$ we associate the adjoint map $f^* : W^* \rightarrow V^*$, such that for $u \in W^*$, $x \in V$

$$\langle f^*(u), x \rangle_V = \langle u, f(x) \rangle_W = u(f(x)).$$

A bilinear form on V arises from a linear map

$$\phi : V \rightarrow V^*$$

via

$$L_\phi(x, y) = \langle \phi(x), y \rangle_V.$$

The adjoint map

$$\phi^\star : V \rightarrow V^\star$$

yields the transposed bilinear form

$$L_{\phi^\star}(x, y) = \langle \phi^\star(x), y \rangle_{V^\star} = \langle x, \phi(y) \rangle_{V^\star} = \langle \phi(y), x \rangle_V = L_\phi(y, x).$$

If ϕ is invertible the inverse

$$\phi^{-1} : V^\star \rightarrow V$$

yields the form $L_{\phi^{-1}}$ on V^\star :

$$L_{\phi^{-1}}(u, v) = \langle \phi^{-1}(u), v \rangle_{V^\star} = \langle v, \phi^{-1}(u) \rangle_V.$$

The forms L_{ϕ^\star} and $L_{\phi^{-1}}$ are conjugate, because

$$L_{\phi^{-1}}(u, v) = \langle v, \phi^{-1}(u) \rangle_V = L_\phi(\phi^{-1}(v), \phi^{-1}(u)) = L_{\phi^\star}(\phi^{-1}(u), \phi^{-1}(v)).$$

Going back the other way,

$$L_{\phi^\star}(x, y) = L_{\phi^{-1}}(\phi(x), \phi(y)).$$

From these two equations, we get two distinct ways to conjugate L_ϕ to $L_{\phi^{-1}\star}$. Plugging $\phi = (\phi^{-1})^{-1}$ into the first and putting (x, y) for (u, v) , we get

$$L_\phi(x, y) = L_{\phi^{-1}\star}(\phi(x), \phi(y)).$$

Plugging $\phi = (\phi^\star)^\star$ into the second we get

$$L_\phi(x, y) = L_{\phi^{-1}\star}(\phi^\star(x), \phi^\star(y)).$$

Now putting ϕ^\star for ϕ we see that in fact there were two ways to conjugate $L_{\phi^{-1}}$ to L_{ϕ^\star} :

$$L_{\phi^\star}(x, y) = L_{\phi^{-1}}(\phi(x), \phi(y)) = L_{\phi^{-1}}(\phi^\star(x), \phi^\star(y)).$$

Having two ways to conjugate L_ϕ to $L_{\phi^{-1}\star}$ gives us an automorphism $\phi^{-1} \circ \phi^\star$ of L_ϕ :

$$L_\phi(x, y) = L_\phi(\phi^{-1}(\phi^\star(x)), \phi^{-1}(\phi^\star(y))).$$

Along with $\phi^{-1} \circ \phi^\star$ we also have the inverse automorphism $\phi^{-1\star} \circ \phi$:

$$L_\phi(x, y) = L_\phi(\phi^{-1\star}(\phi(x)), \phi^{-1\star}(\phi(y))).$$

We could also consider powers other than -1 of our automorphism, but we don't need to, because the conjugacy between L_ϕ and L_{ϕ^\star} is canonical (in the sense of being equivariant with respect to taking duals and inverses) up to this factor of two. The difference between them, as measured by the automorphism $\phi^{-1} \circ \phi^\star$, measures the antisymmetry of L_ϕ . It is destined to play an important role in our future.

Looking now at the level of quadratic forms $Q_\phi(x) = L_\phi(x, x)$, everything in sight is conjugate:

$$Q_\phi(x) = Q_{\phi^\star}(x);$$

$$Q_{\phi^{-1}}(u) = Q_{\phi^{-1\star}}(u) = Q_\phi(\phi^{-1}(u)) = Q_\phi(\phi^{-1\star}(u)).$$

All this nonsense can be made much more concrete using matrices. Let $V = \mathbf{R}^n$ and represent $x \in V$, $u \in V^\star$ as column and row vectors respectively, so that the pairing is just multiplying a row vector by a column vector:

$$\langle u, x \rangle_V = ux.$$

Denote transposition of matrices by \star . Write

$$L_\phi(x, y) = x^\star Ay,$$

so that

$$\phi(x) = x^\star A = (A^\star x)^\star.$$

Now

$$\phi^{-1}(u) = (uA^{-1})^\star = A^{-1\star}u^\star,$$

so

$$L_{\phi^{-1}}(u, v) = \langle v, \phi^{-1}(u) \rangle_V = vA^{-1\star}u^\star = uA^{-1}v^\star.$$

Good!

Now to see the two conjugacies of L_{ϕ^\star} with $L_{\phi^{-1}}$:

$$A^\star A^{-1}A = A^\star;$$

$$AA^{-1}A^\star = A^\star.$$

These combine to give two automorphisms of L_ϕ :

$$\begin{aligned}(A^{-1}A^\star)^\star A(A^{-1}A^\star) &= AA^{-1\star}AA^{-1}A^\star = A; \\ (A^{-1\star}A)^\star A(A^{-1\star}A) &= A^\star A^{-1}A^{-1\star}A = A.\end{aligned}$$

Hmm. Why didn't we do it this way in the first place?

So, here's what happened with our Markov chain. We started with the space $V = \mathbf{R}^n/1$ with quadratic form $L_\phi(x, y) = \sum_{ij} x_i \Delta^{ij} y_j$, embedded the states in $V^\star = \mathbf{R}^n \perp 1$ with quadratic form $L_{\phi^{-1}}(u, v) = \sum_{ij} u^i Z_{ij} v^j$, and proved that $L_{\phi^{-1}}$ is positive definite by showing that it is conjugate to L_ϕ .

5 Tensor notation for Markov chains

As you will already have noticed, we are using tensor notation, rather than trying to work within the confines of matrix notation, as is usual in the theory of Markov chains. For our purposes, a tensor may be viewed as an array where some of the indices are written as superscripts rather than subscripts. Thus, for example, we write the transition rates for a Markov chain as P_i^j , and the equilibrium measure as w^i .

Where the indices of a tensor are placed makes a difference: Thus Z_i^j represents a different array from Z_{ij} . We may 'raise' and 'lower' these indices as is usual with tensors, though in this case the procedure is simpler than usual, because to raise or lower an index i we just multiply or divide by the entries of w^i . Thus we get Z_{ij} from Z_i^j by lowering the index j :

$$Z_{ij} = \frac{1}{w^i} Z_i^j.$$

We get back to Z_i^j from Z_{ij} by raising the index j :

$$Z_i^j = w^j Z_{ij}.$$

We will still be able to use matrix notation to multiply matrices (two-index tensors) and vectors (one-index tensors). The beautiful thing is that when we do this, the indices take care of themselves, as long as the indices that get summed over when multiplying matrices are paired high with low. To show by example what this means, if we write $C = AB$, it will entail (among other things) that

$$C_i^j = (AB)_i^j = \sum_k A_i^k B_k^j = \sum_k A_{ik} B^{kj},$$

and

$$C_{ij} = (AB)_{ij} = \sum_k A_i^k B_{kj} = \sum_k A_{ik} B^k_j = \sum_k A_{ik} w^k B_{kj} = \sum_k A_{ik} B^{kj} \frac{1}{w^j}.$$

Note. If you're familiar with the Einstein summation convention, be aware that we don't use it here. It wouldn't work well in this context, because we want to write $w^i Z_{ij}$ without automatically summing over i . Fortunately, for our purposes, using the notation of matrix multiplication turns out to be even more convenient than the summation convention.

6 What it means to be conformally correct

We have said that we want our approach to be 'conformally correct'. Before we go further, a word about what this means. (Skip this if you don't care.)

Conformal equivalence of Markov chains is most natural for continuous time chains. In that context two chains with transition rates A_i^j and B_i^j are conformally equivalent if

$$B_i^j = \frac{1}{a_i} A_i^j$$

where all $a_i > 0$. Generally we will also want the additional condition that $\sum_i w^i a_i = 1$ where w^i is the equilibrium probability of being at i for the A chain. With this 'volume condition' the equilibrium probability of being at i for the B chain will be $w^i a_i$ and

$$B^{ij} = w^i a_i B_i^j = w^i a_i \frac{1}{a_i} A_i^j = A^{ij}.$$

Thus while the raw transition rates A_i^j are not conformal invariants, when we raise the index i we get a new array $A^{ij} = w^i A_i^j$ whose entries are conformal invariants: They tell the rate at which transitions are made from i to j when the chain is in equilibrium.

It is possible to talk about conformal equivalence of discrete time chains, but it is not as pleasant as for continuous-time chains. This is true so often in the theory of Markov chains! And yet, for simplicity, we want to talk about discrete-time chains. So our approach will be to do everything in such a way that the discussion would be conformally invariant when translated from discrete to continuous time.

So that's what it means for chains to be conformally equivalent. As for 'conformal correctness', we mean an approach that seeks to identify and emphasize quantities that are conformally invariant. And why should we do this? Because it will pay.

7 Visualizing commuting times

One way to determine the expected commuting time T_{ab} between a and b is to run the chain for a long time T (beware of confusion!), paying attention to when the chain is at a or b and ignoring other states. If R is the number of runs of a 's (which is within 1 of the number of runs of b 's), then

$$T_{ab} \approx T/R.$$

To keep track of R we imagine painting our Markovian particle green when it reaches a and red when it reaches b . Let r_{ab} be the equilibrium rate at which red particles are being painted green. Ignoring end effects, over our long time interval T , R above is the number of times a red particle gets painted green, thus roughly Tr_{ab} , and it follows that

$$T_{ab} = \frac{1}{r_{ab}}.$$

This is an instance of the general principle from renewal theory that when events happen at rate r , the expected time between events is $1/r$.

Note. This painting business is very close to a model developed by Kingman [5] and Kelly [4]. (See exercise 1 in section 3.3 of Doyle and Snell [2].) However, I don't know that Kingman and Kelley ever made the connection to commuting times, and it is possible that their discussion concerned only time-reversible chains. Somebody should check this.

It is high time to observe that if \hat{T}_{ab} is the commuting time for the time-reversed chain (according to the general convention that time-reversed quantities wear hats), we have

$$T_{ab} = T_{ba} = \hat{T}_{ab} = \hat{T}_{ba}.$$

We claim to be able to see this from our way of approximating T_{ab} by observing the chain over a long time. If we reverse a record of the chain moving forward for a long time, we see roughly a record of the time-reversed chain

starting in equilibrium. In fact if we started the original chain in equilibrium we're golden. If we started the chain not in equilibrium (e.g. by starting at a , as we might well be tempted to do), there will be problems toward the end of the time-reversed record, as the time-reversed chain gets drawn to end where the forward chain began. But this effect is negligible when T is large.

8 The Laplacian and the cross-potential

Consider a discrete-time Markov chain with transition probabilities

$$P_i^j = \text{Prob}(\text{next at } j | \text{start at } i).$$

Assume the chain is ergodic, so that there is a unique equilibrium measure w^i with

$$\begin{aligned} \sum_i w^i P_i^j &= w^j, \\ \sum_i w^i &= 1. \end{aligned}$$

Define the *Laplacian*

$$\Delta^{ij} = w^i (I_i^j - P_i^j).$$

For $i \neq j$, $-\Delta^{ij}$ tells the equilibrium rate of transitions from i to j ; Δ^{ii} tells the total rate of transitions to and from states other than i . The time-reversed Markov chain has Laplacian $\hat{\Delta}^{ij} = \Delta^{ji}$. A time-reversible chain has $\Delta^{ij} = \Delta^{ji}$.

We have

$$\sum_i \Delta^{ij} = \sum_j \Delta^{ij} = 0.$$

So considered as a matrix, Δ^{ij} is not invertible. However, it has a generalized inverse Z_{ij} with the property that for any measure of total mass 0, which is to say for any u^i with $\sum_i u^i = 0$, we have

$$\sum_{jk} u^j Z_{jk} \Delta^{kl} = u^l$$

and

$$\sum_{jk} \Delta^{ij} Z_{jk} u^k = u^i.$$

An equivalent way to write this is

$$\sum_{jk} \Delta^{ij} Z_{jk} \Delta^{kl} = \Delta^{il},$$

because if we think of Δ^{ij} as a matrix, its rows and columns both span the space of measures with total mass 0.

A sensible choice for the generalized inverse Z_{ij} is

$$Z_{ij} = \frac{1}{w^j} Z_i^j$$

where

$$Z_i^j = (I_i^j - w^j) + (P_i^j - w^j) + (P^{(2)}_i^j - w^j) + \dots,$$

where $P^{(2)}_i^j = \sum_k P_i^k P_k^j$ represents the matrix square of P_i^j , and the elided terms involve higher matrix powers. Define $P^{(\infty)}_i^j = w^j$, to suggest that the ‘infiniteth power’ of P_i^j has all rows equal to the vector w^i . We can write

$$\begin{aligned} Z &= (I - P^{(\infty)}) + (P - P^{(\infty)}) + (P^{(2)} - P^{(\infty)}) + \dots \\ &= (I - P + P^{(\infty)})^{-1} - P^{(\infty)}. \end{aligned}$$

This naturally translates into the formula we’ve given for Z_i^j , and from there, by ‘lowering the index j ’, we get Z_{ij} .

For this choice of Z we have the natural interpretation that Z_i^j is the expected excess number of visits to j for a chain starting at i compared to a chain starting in equilibrium. For the time-reversed chain we get

$$\hat{Z}_{ij} = Z_{ji},$$

and so in particular if the chain is time-reversible we have $Z_{ij} = Z_{ji}$.

This is all very well, but we still do not want to prescribe this particular choice of Z because it is not conformally invariant: It depends on the equilibrium measure w^i , and not just on the Laplacian ‘matrix’ Δ^{ij} . This makes it insufficiently canonical for us.

What *is* canonical is the bilinear form

$$B(u, v) = \sum_{ij} u^i Z_{ij} v^j$$

when u and v are restricted to the subspace S of measures of total mass 0:

$$S = \{u^i : \sum_i u^i = 0\}$$

Fixing a, b, c, d and setting

$$u = \delta_a^i - \delta_b^i; \quad v = \delta_c^i - \delta_d^i$$

gives us the *cross-potential*

$$N_{abcd} = B(\delta_a^i - \delta_b^i, \delta_c^i - \delta_d^i) = Z_{ac} - Z_{ad} - Z_{bc} + Z_{bd}.$$

N satisfies

$$N_{bacd} = N_{abdc} = -N_{abcd}.$$

For the time-reversed process

$$\hat{N}_{abcd} = N_{cdab}.$$

Clearly, knowing N is the same as knowing B , or Δ . If we know w as well as N we can recover our sensible-but-not-canonical Z :

$$Z_{ij} = \sum_{kl} N_{ikjl} w^k w^l.$$

Different choices of w in this formula lead to different Z 's, but they all determine the same bilinear form B . From Z and w we can recover P .

In general, it is useful to think of an ergodic Markov chain as specified by the cross-potential N , which determines its conformally invariant properties, together with the equilibrium measure w . Expressing formulas in these terms allows us to see the extent to which quantities are conformally invariant (like N , B , and Δ) or not (like w , Z , P).

Complaint. N and w together don't quite determine the original transition rates for a continuous-time Markov chain, or rather, they wouldn't do so if we had some way to distinguish between remaining at i and moving from i to i . Such a distinction is not possible for discrete-time chains represented by matrices, but we could handle it in the continuous case by allowing for non-zero transition rates on the diagonal. Better yet, we could reformulate Markov chain theory in the context of queuing networks based on 1-complexes (graphs where loops and multiple edges are allowed). This would give us a way to distinguish different ways of stepping from i to j . A further step would be to allow a general distribution for the time it takes to make a transition for i to j . This would be very helpful when watching the chain only when it is in a subset of its states, as in the case above where we contemplated watching the chain only when it is at a or b . We didn't say just what we meant by this, because it doesn't conveniently fit into the usual formulation of Markov chain theory.

9 Probabilistic and electrical interpretation

We may interpret N_{abcd} probabilistically as the equilibrium concentration difference between c and d due to a unit flow of particles entering at a and leaving at b . Here's what this means. Introduce Markovian particles at a at a unit rate, and remove them when they reach b . Write the 'dynamic equilibrium' measure of particles at i as $w^i\phi_i$, so that ϕ_i tells the concentration of particles relative to the 'static equilibrium' measure w^i . Conservation of particles implies that

$$w^i\phi_i \sum_j P_i^j - \sum_j w^j\phi_j P_j^i = \delta_a^i - \delta_b^i.$$

We hasten to rewrite this in the conformally correct form

$$\sum_j \phi_j \Delta^{ji} = \delta_a^i - \delta_b^i.$$

Since also

$$\sum_j (Z_{aj} - Z_{bj}) \Delta^{ji} = \delta_a^i - \delta_b^i$$

and since the Laplacian Δ kills only constants, it follows that

$$\phi_j = Z_{aj} - Z_{bj} + C,$$

and thus

$$\phi_c - \phi_d = Z_{ac} - Z_{bc} - Z_{ad} + Z_{bd} = N_{abcd}.$$

From this probabilistic interpretation of N we can see that $N_{abab} = C_{ab}$, the commuting time between a and b . Indeed, in the particle-painting scenario introduced earlier, C_{ab} is the reciprocal of the rate at which red particles are turning green at a . Paying attention only to green particles, we see green particles appearing at a at rate $1/C_{ab}$, and disappearing at b . The equilibrium concentration of green particles at i is the probability p_i of hitting a before b for the time-reversed chain, and in particular $p_a = 1$ and $p_b = 0$, so the concentration difference between a and b is 1. Multiplying the green flow by C_{ab} normalizes it to a unit flow with concentration difference C_{ab} between a and b . So

$$C_{ab} = N_{abab}.$$

If we embellish this probabilistic scenario by imagining that our particles carry a positive charge, we may identify the net flow of particles with

electrical current; the concentration of particles (relative to the equilibrium measure) with electrical potential; and differences of concentration with voltage drop. With this terminology, N_{abcd} tells the voltage drop between c and d due to a unit current from a to b . Traditionally this way of talking is reserved for time-reversible Markov chains, which are precisely those for which we have the ‘reciprocity law’ $N_{abcd} = N_{cdab}$. For such chains, if we build a resistor network where nodes $i \neq j$ are joined by a resistor of conductance (i.e., reciprocal resistance) $-\Delta^{ij}$, then N_{abcd} will indeed be the voltage drop between c and d due to a unit current from a to b . We propose to extend this way of talking to non-time-reversible chains.

In electrical terms, the voltage drop N_{abab} between a and b due to a unit current between a and b is the *effective resistance*. This is the same as the reciprocal of the current that flows when a 1-volt battery is connected up between a and b —which is what we get in effect when we measure commuting times using green and red paint. So the commuting time $C_{ab} = N_{abab}$ is the same as the effective resistance between a and b .

The connection of commuting time to effective resistance, and the general recognition that commuting times play a key role in understanding Markov chains, is due to Chandra et al. [1].

Note. Now we are in a position to understand the significance of the name ‘cross-potential’. This name is meant to indicate the connection of N_{abcd} to the cross-ratio of complex function theory. If we extend our notions about Markov chains to cover Brownian motion on the Riemann sphere, we get

$$\begin{aligned} N_{abcd} &= -\frac{1}{2\pi}(\log|a-c| - \log|a-d| - \log|b-c| + \log|b-d|) \\ &= -\frac{1}{2\pi} \log \left| \frac{a-c}{a-d} \frac{b-d}{b-c} \right| \\ &= -\frac{1}{2\pi} \Re \log \frac{a-c}{a-d} \frac{b-d}{b-c}. \end{aligned}$$

We don’t have to specify a metric on the sphere here, because the Laplacian is a conformal invariant in two dimensions. Thinking of the sphere as being an electrical conductor with constant conductivity (say, 1 mho ‘per square’), the electrical interpretation becomes exact. The advantage of having N to take four ‘arguments’ now becomes apparent, because $N_{abcb} = \infty$. That’s why engineers using look for cracks in nuclear reactor cooling pipes with a *4-point probe*. To get a sensible generalization of C_{ab} we will need to do some kind of

renormalization, which will introduce a dependence on the metric. We should not be sorry about this, because it brings curvature into the picture—and you know that can't be bad.

10 Realization

Now, finally, to realize commuting times as squared distances. From the bilinear form B we get the quadratic form

$$Q(u) = ||u||^2 = B(u, u) = \sum_{ij} u^i Z_{ij} u^j.$$

$$C_{ab} = N_{abab} = Q(\delta_a^i - \delta_b) = ||\delta_a - \delta_b||^2.$$

So if we map i to δ_i then the commuting time C_{ab} becomes the squared distance between the images in the Q -norm.

That is, if what we're calling the Q -norm is indeed a norm. Is Q really positive definite?

To understand better what is going on here, it is useful to look at the bilinear form

$$L(\phi, \psi) = \sum_{ij} \phi_i \Delta^{ij} \psi_j,$$

where we think of ϕ and ψ as being defined only modulo additive constants. If we think of ϕ_i as the potential of the measure

$$\sum_i \phi_i \Delta^{ik},$$

then this is the same bilinear form as before, except that now instead of measures of total mass 0 it takes as its arguments the corresponding potentials, the first with respect to the original chain, and the second with respect to the time-reversed chain:

$$L(\phi, \psi) = B(\sum_i \phi_i \Delta^{ik}, \sum_i \psi_i \Delta^{ki}) = B(\sum_i \phi_i \Delta^{ik}, \sum_i \hat{\Delta}^{ik} \psi_i).$$

This follows from the formula $\Delta Z \Delta = \Delta$ above.

Now to get the equivalent of Q in this context we restrict to the subspace

$$V = \{(\phi, \psi) : \sum_i \phi_i \Delta^{ik} = \sum_j \Delta^{kj} \psi_j\}$$

and take as our quadratic form

$$R((\phi, \psi)) = L(\phi, \psi).$$

In the case of a time-reversible chain, V is just the diagonal $\phi = \psi$, and

$$Q(\phi\Delta) = R((\phi, \phi)) = L(\phi, \phi) = \sum_{ij} \phi_i \Delta^{ij} \phi_j = \frac{1}{2} \sum_{ij} (-\Delta^{ij})(\phi_i - \phi_j)^2.$$

This is evidently positive-definite. Indeed, if we associate to (ϕ, ϕ) the vector with $\binom{n}{2}$ coordinates $\sqrt{-\Delta^{ij}}(\phi_i - \phi_j)$, $i < j$, then we will have embedded the normed space (V, R) , and along with it our Markov chain, in Euclidean $\binom{n}{2}$ -space.

Electrically, what we have done here is to account for the energy being dissipated in the network by adding up the energy dissipated by individual resistors. And there should be some kind of probabilistic interpretation as well.

That's how it works for time-reversible chains, for which $\Delta^{ij} = \Delta^{ji}$. However, the argument extends to the general case by what amounts to a trick. The key is the observation that for $(\phi, \psi) \in V$ we have

$$L(\phi, \psi) = L(\phi, \phi) = L(\psi, \psi).$$

(But please note that in general $L(\phi, \psi) \neq L(\psi, \phi)$!) So

$$Q(\phi\Delta) = R((\phi, \psi)) = L(\phi, \psi) = L(\phi, \phi) = \sum_{ij} \phi_i \Delta^{ij} \phi_j = \frac{1}{2} \sum_{ij} (-\Delta^{ij})(\phi_i - \phi_j)^2.$$

So there is the positive-definiteness we need.

Now, though, we don't see any natural way to interpret the terms of the sum electrically or probabilistically. (Which is not to say that there isn't one!) In putting ϕ in both slots of L we leave the subspace V , and thereby commit what appears to be an unnatural act. But it seems to have paid off.

11 Minimax characterization of commuting times and hitting probabilities

Fix states $a \neq b$, and let

$$S_{a,b} = \{\phi | \phi_a = 1, \phi_b = 0\}$$

Here we really should be thinking of ϕ as being defined only up to an additive constant, which means we should write $\phi_a - \phi_b = 1$, but we're going to be sloppy about this, because we want to focus attention on two distinguished elements of $S_{a,b}$ which are naturally 1 and a and 0 at b . These are

$$\bar{\phi}_i = \text{Prob}(\text{hit } a \text{ before } b \text{ starting at } i \text{ going backward in time})$$

and

$$\bar{\psi}_i = \text{Prob}(\text{hit } a \text{ before } b \text{ starting at } i \text{ going forward in time}).$$

We've met $\bar{\phi}$ before: It's proportional to the equilibrium concentration of green particles in our painting scenario. $\bar{\psi}$ is the analogous quantity for the reversed chain. The pair $(\bar{\phi}, \bar{\psi})$ belongs to our subset V , because

$$(\bar{\phi}\Delta)^i = (\Delta\bar{\psi})^i = r_{ab}(\delta_a^i - \delta_b^i).$$

Here we once again are writing $r_{ab} = \frac{1}{T_{ab}}$ for the equilibrium rate of commuting between a and b . Observe that any f we have

$$L(\bar{\phi}, f) = L(f, \bar{\psi}) = r_{ab}(f_a - f_b).$$

So whenever f is in $S_{a,b}$ we have

$$L(\bar{\phi}, f) = L(f, \bar{\psi}) = r_{ab},$$

and in particular

$$L(\bar{\phi}, \bar{\psi}) = r_{ab}.$$

Theorem.

$$r_{ab} = \frac{1}{T_{ab}} = \min_{\alpha} \max_{\phi+\psi=2\alpha} L(\phi, \psi).$$

Here and below, α , ϕ , and ψ are restricted to lie in $S_{a,b}$, i.e. to take value 1 at a and 0 at b .

Proof. Whatever α is, we may take $\phi = \bar{\phi}$ (and thus $\psi = 2\alpha - \bar{\phi}$), and have

$$L(\phi, \psi) = L(\bar{\phi}, \psi) = r_{ab}$$

as above. So

$$\min_{\alpha} \max_{\phi+\psi=2\alpha} L(\phi, \psi) \geq r_{ab}.$$

To prove the inequality in the other direction, and in the process identify where the minimax is achieved, take

$$\alpha = \frac{1}{2}(\bar{\phi} + \bar{\psi}).$$

If $\phi + \psi = 2\alpha$ then we can write

$$\phi = \bar{\phi} + f$$

and

$$\psi = \bar{\psi} - f,$$

where $f_a = f_b = 0$.

Now

$$L(\bar{\phi}, f) = L(f, \bar{\psi}) = r_{ab}(f_a - f_b) = 0,$$

so

$$L(\phi, \psi) = L(\bar{\phi} + f, \bar{\psi} - f) = L(\bar{\phi}, \bar{\psi}) - L(f, f) = r_{ab} - L(f, f).$$

And even though we claim it is a travesty to put the same f into both slots of L , we still have

$$L(f, f) \geq 0 :$$

That was the upshot of our embedding investigation. So

$$L(\phi, \psi) \leq r_{ab},$$

still assuming $\alpha = \frac{1}{2}(\bar{\phi} + \bar{\psi})$ and $\phi + \psi = 2\alpha$. Hence

$$\min_{\alpha} \max_{\phi+\psi=2\alpha} L(\phi, \psi) \geq r_{ab}. \quad \blacksquare$$

In the time-reversible case, where $\Delta^{ij} = \Delta^{ji}$, this minimax can be reduced to a straight minimum. That's because in this case for any g, f we have $L(f, g) = L(g, f)$, and hence

$$L(g + f, g - f) = L(g, g) - L(f, f).$$

So to maximize $L(\phi, \psi)$ while fixing the sum $\phi + \psi = 2\alpha$ we take $\phi = \psi = \alpha$.

Corollary. When Δ^{ij} is symmetric

$$r_{ab} = \min_{\phi(a)=1, \phi(b)=0} L(\phi, \phi). \quad \blacksquare$$

This minimum principle for resistances was known already to 19th century physicists, specifically Thomson (a.k.a. Kelvin), Maxwell, and Rayleigh: For more about this, see Doyle and Snell [2].

Having a straight minimum is a lot better than having a minimax, because now we can plug in any ϕ with $\phi(a) = 1, \phi(b) = 0$ and get an upper bound for r_{ab} , corresponding to a lower bound for T_{ab} . This method is a staple of electrical theory—the part of electrical theory that doesn't extend to non-time-reversible chains because it depends on the relation $L(f, g) = L(g, f)$.

For time-reversible chains there are also complementary methods for finding lower bounds for r_{ab} , and thus upper bounds for T_{ab} . These emerge from the minimum principle through the mystery of convex duality.

12 The obstruction to time-reversibility

We close with an application to characterizing time-reversible chains.

Let M_{ij} be the expected time to reach j starting from i . Coppersmith, Tetali, and Winkler showed that a Markov chain is time-reversible just if for all a, b, c

$$M_{ab} + M_{bc} + M_{ca} = M_{ac} + M_{cb} + M_{ba}.$$

And in this case the expected time to traverse a cycle of any length will be the same in either direction. Note that the M_{ij} s themselves are not conformally invariant, these cycle sums are. For a cycle of length 2, the cycle sum is our best friend the commuting time.

We always have

$$M_{ab} + M_{bc} + M_{ca} = \hat{M}_{ac} + \hat{M}_{cb} + \hat{M}_{ba}$$

(look at a long record of the chain backwards), so an equivalent condition is that for all a, b, c

$$M_{ab} + M_{bc} + M_{ca} = \hat{M}_{ab} + \hat{M}_{bc} + \hat{M}_{ca}.$$

This is true despite the fact that in general

$$\hat{M}_{ab} \neq M_{ba}.$$

So, why is this true? It comes down to the fact that a conformal class of chains is reversible just if our bilinear form $L(\phi, \psi)$ on $V = \{x^i \mid \sum_i x_i = 0\}$

is symmetric. To any bilinear form $\sum_{ij} u^i Z_{ij} v^j$ on V there corresponds a natural cohomology class

$$Z_{ij} - Z_{ji},$$

which is to say, an antisymmetric matrix defined up to addition of a matrix of the form $B_{ij} = a_i - a_j$. This class represents the obstruction to symmetrizing the matrix of the form within its ab -equivalence class. This class vanishes just if it integrates to 0 around any cycle, and cycles of length 3 span the space of cycles. Indeed, they span it in a very redundant way. To verify reversibility, it would suffice to check any basis for the space of cycles, e.g. only cycles of length 3 involving the fixed state n (the ‘ground’).

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