Note: a conjectured compactification of some finite reversible MCs

There are two established theories which concern different aspects of the behavior of finite state Markov chains as the size of the state space increases. One is weak convergence. Here prototype results concern convergence of birth-and-death processes to one-dimensional diffusions, and the d-dimensional analogs [9]. More generally, for any continuous time and space Markov process which seems mathematically natural, one could seek necessary and sufficient conditions for a sequence of discrete chains to converge to that limit. The second theory concerns mixing times [7, 1]. At one level this concerns definitions of various "mixing times" and estimation of their orders of magnitude in general examples. At another level, for more specific examples there has been extensive study of the "cutoff" phenomenon for distance to stationarity, mostly in the context of variation distance [4] but also for L^2 distance [3] which will be more relevant to this note.

This note describes a conjecture which says, roughly, that these are the only two possibilities, at least for reversible chains. In a little more detail, the conjecture is

> Given a sequence of n-state reversible chains which does not have the L^2 cutoff property, there is a subsequence in which, after relabeling states, the transition densities converge to those of some limit general-state-space reversible Markov process.

We emphasize that the n-state chains are arbitrary in the sense that we do not assume any connection between the chains as n varies. The conjectured behavior is a compactness assertion, in the spirit of recent work on dense graph limits [8, 5].

The rest of this note states the conjecture more precisely and outlines how one might try to start a proof. For simplicity we work with uniform stationary distributions, but we anticipate that the general reversible case will be similar.

0.1 Setup

Consider an n-state irreducible continuous-time Markov chain with symmetric transition rate matrix – in other words, reversible with uniform stationary distribution. Write $p(i,j;t)$ for the transition probabilities $\mathbb{P}(X(t) = j|X(0) = i)$. Consider the function

$$G(t) := \sum_i p(i,i;t).$$

The basic convergence theorem implies $G(t) \to 1$ as $t \to \infty$, and the spectral representation gives the more detailed result

$$G(t) = 1 + \sum_{u=2}^{n} e^{-\lambda_u t} \tag{1}$$

where $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$ are the eigenvalues associated with the transition rate matrix. Note the probabilistic interpretation

$$G(t) = \frac{\mathbb{P}(X(t) = X(0))}{\frac{1}{n}} \quad \text{where } X(0) \text{ has uniform dist.}$$

One can regard the time τ at which $G(\tau) = 2$ as one of many possible notions of "mixing time". Rescaling time by this τ, we can standardize according to the convention

$$G(1) = 2.$$

The notion of L^2 cutoff studied in detail in [3] is, in our context, the property that a sequence of time-standarized chains has

$$G^{(n)}(t) \to \infty,\ t < 1; \quad G^{(n)}(t) \to 1,\ t > 1. \tag{2}$$

Now imagine a continuous-space analog. That is, a probability measure π on a space S and an S-valued Markov process $X^*(t)$ such that for $t > 0$ there exist transition densities

$$p^*(x,\cdot;t) = \text{density of } \mathbb{P}(X^*(t) \in \cdot|X^*(0) = x) \text{ w.r.t. } \pi$$

which are symmetric: $p^*(x,y;t) = p^*(y,x;t)$. The analog of $G(t)$ is

$$G^*(t) := \int_S p^*(x,x;t)\ \pi(dx).$$

Assume $G^*(t) < \infty$ for $t > 0$. Then we expect (see remark below) the analog of (1)

$$G^*(t) = 1 + \sum_{u=2}^{\infty} e^{-\lambda_u^* t} \tag{3}$$

where $0 = \lambda_1^* < \lambda_2^* \leq \lambda_3^* \leq \ldots$ are the eigenvalues associated with the appropriate generator. And we can standardize to make $G^*(2) = 1$.

Now consider a sequence of chains with $n \to \infty$, where n is the number of states, but without assuming any relation between the chains as n varies, except for the assumption

$$\sup_n G^n(t) < \infty \ \forall 0 < t < 1. \tag{4}$$

As a standard analytic fact, because each $G^{(n)}$ is of form (1) there is a subsequence in which $G^n(\cdot) \to G^*(\cdot)$ for some limit function of form (3). This starts to hint at what is going on; the conjectured limit continuous-space process will be one with this function $G^*(\cdot)$.

Remark. Perhaps the simplest example is continuous-time random walk on the n-cycle, which has eigenvalues

$$\lambda_u^{(n)} = 1 - \cos(2\pi(u-1)/n), \ u = 1, \ldots, n$$

and mixing time $\sim cn^2$. After time-standardizing, the $n \to \infty$ limit is (for some constant c)

$$G^*(t) = 1 + \sum_{u \geq 1} \exp(-2\pi^2 c(u-1)^2 t)$$

which is (as it should be) the density $p(0,0;t)$ for time-standardized Brownian motion on the unit circle. This illustrates why we anticipate limits $G^*\cdot)$ having the form (3) rather than a general spectral measure $\int_0^\infty e^{-\lambda t} \ \Psi(d\lambda)$.

0.2 An analogy

Here is an analogy for what we shall do in the next section.

Question: Can we characterize a "metric space with probability measure" up to measure-preserving isometry? That is, can we tell whether two such spaces (S_1, d_1, μ_1) and (S_1, d_1, μ_1) have a MPI?

Answer: Yes. Given (S, d, μ), take i.i.d.(μ) random elements $(\xi_i, 1 \leq i < \infty)$ of S, form the array

$$X_{i,j} = d(\xi_i, \xi_j);\ \ i,j \geq 1$$

and let Ψ be the distribution of this infinite random array. It is obvious that, for two isometric "metric spaces with probability measure", we get the same Ψ. The converse – that Ψ determines the space up to MPI – is not obvious but is true; it was first stated explicitly by Vershik (2004) but in fact is a simple albeit technical consequence of the "structure theory for partially exchangeable arrays" developed by Hoover-Aldous-Kallenberg (1978-1985) and treated in detail in [6]. See [2] for my own recent account of its uses in the broad field of representing continuous limits of discrete random structures. The conjectures we state in this note are a novel instance of this methodology.

0.3 Isomorphic processes

Consider a Markov process on a measurable space S with stationary distribution π, which we will view naively as a family of symmetric densities $p^*(\cdot, \cdot; t)$ satisfying the Chapman-Kolmogorov relations, with a UTC[1] on the $t \downarrow 0$ behavior. Analogous to the previous section, define an infinite partially exchangeable random array whose entries are functions of t by

$$\text{take i.i.d.}(\pi) \text{ random elements } (\xi_i, 1 \leq i < \infty) \text{ of } S$$

$$\text{set } X^*_{ij} = p^*(\xi_i, \xi_j; t),\ \ i,j \geq 1. \tag{5}$$

As in the previous section, this array has some distribution Ψ. There is a natural notion of "isomorphism" between two stationary Markov processes X^1 and X^2 on different spaces S_1 and S_2 – a bijection ϕ that preserves joint distributions

$$(\phi(X^1_0), \phi(X^1_t)) =_d (X^2_0, X^2_t)$$

[1] unspecified technical condition

and hence transition densities. And as before it is obvious that, for two isomorphic processes, we get the same Ψ.

Conjecture 1. *If two symmetric Markov processes have the same Ψ then they are isomorphic.*

See discussion later.

0.4 Convergence of processes

We can do exactly the same array construction for chains on finite sets S^n:
take i.i.d. uniform random elements $(\xi_i, 1 \leq i < \infty)$ of S^n
set $X^n_{ij} = p_n(\xi_i, \xi_j; t),\ i, j \geq 1$.
Time-standardize, and consider the property discussed earlier:

$$G^n(t) \to G^*(t) \text{ as } n \to \infty \tag{6}$$

for some limit function with $1 < G^*(t) < \infty$ for $0 < t < \infty$. This is just saying that $\mathbb{E}X^n_{11} \to G^*(\cdot)$. Now an easy argument gives $\mathbb{E}X_{12} \leq \mathbb{E}X_{11}$, and so we can take a subsequence in which

$$(X^n_{ij}, i, j \geq 1) \to_d (X^*_{ij}, i, j \geq 1) \text{ as } n \to \infty \tag{7}$$

(in the usual sense of convergence of finite sub-arrays) for some limit random function-valued array.

Conjecture 2. *For any array $(X^*_{ij}, i, j \geq 1)$ that arises as a limit (7) from finite chains, there exists a general-space chain with some transition densities p^* such that the representation (5) holds.*

0.5 Summary

We can now fill in some details of our original conjecture, as follows.

> Given a sequence of n-state reversible chains which does not have the L^2 cutoff property, we can pass to a subsequence satisfying (4) and then to a further subsequence satisfying (7); Conjecture 2 (if true) will identify the limit with some general-space process, which Conjecture 1 (if true) says is unique up to isomorphism.

We presented Conjecture 2 in “convergence” format, but there is a more “intrinsic” way to look at what’s going on, analogous to the basic representation theorem for partially exchangeable arrays [6, 2]. We want to abstract a list of properties that an array (X^*_{ij}) arising as (5) must “obviously” have:
(i) partial exchangeability
(ii) Chapman-Kolmogorov
(iii) The UTC from section 0.3
(iv) ......

The more definitive underlying Conjecture is that an array with a certain list of such properties has a representation in form (5). Such a result, with properties preserved under convergence in distribution, would of course imply Conjecture 2.

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