PROBABILITY MEASURES ON GRAPH TRAJECTORIES

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Abstract. The aim of this note is to construct a probability measure on the space of trajectories in a continuous time Markov chain having a finite state diagram, or more generally which admits a global bound on its degree and rates. Our approach is elementary. Our main intention is to fill a gap in the literature and to give some additional details in the proof of [1, prop. 4.8].

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1. Introduction

As is well known, Markov chains model random walks on graphs. Let $\Gamma$ be a directed graph. Its set of vertices $\Gamma_0$ represent the states of the system and its edges $\Gamma_1$ indicate transitions between states. There are two flavors of random walk: those in discrete time and those in continuous time. This note will consider the continuous time variant.

The dynamics of continuous time random walk are encoded by a master equation

$$p'(t) = \mathbb{H}(t)p(t),$$

where $\mathbb{H}(t)$ is a time dependent matrix of transition rates and $p(t)$ is a 1-parameter family of probability distributions on $\Gamma_0$. The solutions to the equation describe the time evolution of probability. For vertices $i$ and $j$, the matrix entry $\mathbb{H}(t)_{ij}$ is the instantaneous rate of change at time $t$ in jumping from state $i$ to state $j$ along the set of edges of $\Gamma$. 

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having initial vertex $i$ and terminal vertex $j$. The operator $H$ is called the master operator; its off diagonal entries are non-negative and the sum of the entries in any column add to zero.

Given a continuous time Markov chain with state diagram $\Gamma$, our goal here will be to construct a probability distribution on the space of trajectories in $\Gamma$. By a trajectory in $\Gamma$, we mean a path of contiguous edges equipped with jump times at each vertex of the path. Note that such a probability distribution amounts to a description of the stochastic process associated with the Markov chain.

Remark 1.1. We apologize to the reader in advance for our somewhat unconventional treatment: two of us are algebraic topologists and one is a chemical physicist.

2. Preliminaries

For a set $T$, let $\binom{T}{2}$ denote the set of its non-empty subsets of cardinality 2. An undirected graph consists of data

$$X := (X_0, X_1, \delta),$$

in which $X_0$ is the set of vertices, $X_1$ is the set of edges and

$$\delta: X_1 \to \binom{X_0}{2}$$

is a function. We will always assume that $X$ is locally finite in the sense that the function $\delta$ is a finite-to-one. With this definition multiple edges connecting a pair of distinct vertices are permitted, but we do not permit loop edges, i.e., edges which connect a vertex to itself.

A directed graph $\Gamma$ is defined in a similar way, but where now $\delta$ is replaced by a function $d: \Gamma_1 \to \Gamma_0(2)$, where $\Gamma_0(2) := \Gamma_0 \times \Gamma_0 \setminus \Delta$, i.e., the cartesian product with its diagonal deleted. We write $d = (d_0, d_1)$, where $d_i: \Gamma \to \Gamma_0$ is the function which assigns to a directed edge its source, respectively target. Note that the canonical map $\pi: \Gamma_0(2) \to \binom{\Gamma_0}{2}$ is a double cover, and the composition $\delta := \pi \circ d$ defines the underlying undirected graph.

Example 2.1. Given an undirected graph $X$, we may construct its double. This is the directed graph

$$DX := \Gamma = (\Gamma_0, \Gamma_1, d),$$

in which $\Gamma_0 = X_0$ and $\Gamma_1$ is the set of ordered pairs $(i, \alpha) \in X_0 \times X_1$ in which $i \in \delta(\alpha)$. The function $d: \Gamma_1 \to \Gamma_0(2)$ is given by $d(i, \alpha) = (i, j)$, where $\delta(\alpha) = \{i, j\}$. 
Remark 2.2. Let \( \mathcal{G} \) be the category of undirected graphs. An object is an undirected graph and a morphism \( f : (G_0, G_1, \delta) \to (H_0, H_1, \delta') \) consists of functions \( f_i : G_i \to H_i, \ i = 0, 1 \) such that \( \delta' f_1(\alpha) = f_0(\delta \alpha) \). Similarly, one has the category \( \mathcal{G}^+ \) of directed graphs. Then we have an adjoint functor pair
\[
U : \mathcal{G}^+ \dashv \mathcal{D} : \mathcal{G}
\]
where \( U \) is the forgetful functor and \( D \) is given by the double.

2.1. Markov chains. Let \( \Gamma \) be a directed graph. A continuous time Markov chain with state diagram \( \Gamma \) is an assignment of a continuous function
\[
k_\alpha : \mathbb{R} \to [0, \infty),
\]
to each edge \( \alpha \in \Gamma_1 \). The function \( k_\alpha \) is called the transition rate of \( \alpha \). If \( d(\alpha) = (i, j) \), then \( k_\alpha \) is to be interpreted as the instantaneous rate of change of probability in jumping from \( i \) to \( j \) along \( \alpha \).

Remark 2.3. The foundational material on Markov chains can be found in the texts of Norris [4] and Stroock [6]. When the transition rates are constant, the Markov chain is said to be time homogeneous. When the rates are not constant, the chain is said to be time inhomogeneous.\(^1\)

Remark 2.4. The canonical map \( \Gamma \to \mathcal{D} \Gamma \) is an embedding. Given a Markov chain on \( \Gamma \), one has a canonical extension to \( \mathcal{D} \Gamma \) by defining the rates to be zero on those edges which aren’t in \( \Gamma \). The Markovian dynamics of the two chains coincide. From this standpoint, there is nothing to lose by assuming that \( \Gamma = \mathcal{D}X \) for some undirected graph \( X \).

If \( \Gamma \) is infinite, we also require the following growth constraints.

Definition 2.5 (Rate Bound). For each \( t > 0 \), there exists a constant \( R \), possibly depending on \( t \), such that
\[
k_\alpha(s) \leq R
\]
for \( 0 \leq s \leq t \) and every \( \alpha \in \Gamma_1 \).

Definition 2.6 (Degree Bound). Let \( \text{deg} : \Gamma_0 \to \mathbb{N} \) be the function which assigns to a vertex its degree, i.e., the number of edges meeting it. There is a positive integer \( D \) such that
\[
\text{deg}(i) \leq D, \quad \text{for all} \quad i \in \Gamma_0.
\]

Observe that when \( \Gamma \) is a finite, both conditions hold automatically.

\(^1\)In contrast with the homogeneous case, the literature on the inhomogeneous case is scant, with the known results making strong additional assumptions. The only foundational work we are of aware of that treats the time inhomogeneous case is Stroock’s text (cf. [6, §5.5.2]).
2.2. **The master equation.** Then the rates define a time dependent square matrix $\mathbb{H} = \mathbb{H}(t)$, as follows. For $i \neq j$, set

$$h_{ij} = \sum_{d(\alpha) = (i,j)} k_\alpha,$$

where the sum is interpreted as zero when $d^{-1}(i,j)$ is the empty set. Then the matrix entries of $\mathbb{H}$ are given by

$$\mathbb{H}_{ij} = \begin{cases} h_{ij}, & i \neq j; \\ -\sum_{\ell \neq i} h_{i\ell}, & i = j, \end{cases}$$

where the indices range over $i, j \in \Gamma_0$. The time dependent matrix $\mathbb{H}$ is called the **master operator**. Associated with $\mathbb{H}$ is a linear, first order ordinary differential equation

$$(1) \quad p'(t) = \mathbb{H}p(t),$$

in which $p(t)$ is a one parameter family of (probability) distributions on the set of vertices $\Gamma_0$. Equation (1) is called the *forward* Kolmogorov *equation* or the *master equation* [6, eqn. 5.5.2]. Its solutions describe the evolution of an initial distribution $p(0)$.

**Remark 2.7.** If $\Gamma = DX$ and the transition rates are constant with value 1, then $\mathbb{H}$ is the graph Laplacian of $X$ and (1) is a combinatorial version of the heat (diffusion) equation.

**Remark 2.8.** The forward Kolmogorov equation is often written in the literature in adjoint form, i.e., as

$$q'(t) = q(t)\mathbb{W},$$

where $q(t) = p(t)^*$ and $\mathbb{W} = \mathbb{H}^*$ are the transposed matrices. The backward equation (which we will not consider here) is

$$q'(t) = \mathbb{W}q(t).$$

2.3. **Trajectories.** A path of length $n$ in $\Gamma$ consists of a sequence of edges

$$\alpha_\bullet := (\alpha_1, \ldots, \alpha_n),$$

such that $d_1(\alpha_k) = d_0(\alpha_{k+1})$ for $1 \leq k < n$. We let

$$i_k(\alpha_\bullet) := i_k$$

denote the $k$-th vertex of the path, i.e., $i_k = d_0(\alpha_k)$ if $k \leq n$ and $i_{n+1} = d_1(\alpha_n)$.

A trajectory of length $n$ and duration $t > 0$ is a pair

$$\alpha_\bullet, t_\bullet,$$
such that $\alpha_*$ is a path of length $n$ and $t_* = (t_1, \ldots, t_n)$ is a sequence of real numbers satisfying

$$0 \leq t_1 \leq \cdots \leq t_n \leq t.$$ 

In what follows, it will be convenient to set $t_0 := 0$ and $t_{n+1} =: t$.

**Remark 2.9.** For a vertex $i_k = i_k(\alpha_*)$ of the path $\alpha_*$, the number $t_k$ is called the *jump time* and the number $w_k := t_k - t_{k-1}$ is called *wait time*.

### 3. The probability of a trajectory

Let $(\Gamma, k_*)$ be as in the previous section. Given a vertex $i \in \Gamma_0$ and an interval $[a, b]$, the *escape rate* at $i$ is

$$u_i(a, b) := \exp \left( - \sum_{d_1(\alpha) = i} \int_a^b k_\alpha(s) \, ds \right) = \exp \left( \int_a^b h_{ii}(s) \, ds \right).$$

Fix an initial probability distribution $q: \Gamma_0 \to \mathbb{R}_+$. For $j \in \Gamma_0$, set $q_j := q(j)$.

Let

$$\mathcal{T}(\Gamma, n, t)$$

denote the set of trajectories of $\Gamma$ having length $n$. Define a function

$$f: \mathcal{T}(\Gamma, n, t) \to \mathbb{R}_+$$

by the formula

$$f(\alpha_*, t_*) = q_{i_1} u_{i_1}(0, t_1) k_{\alpha_1}(t_1) \cdots u_{i_n}(t_{n-1}, t_n) k_{\alpha_n}(t_n) q_{i_{n+1}}(t_n),$$

$$= q_{i_1} \prod_{m=1}^{n} u_{i_m}(t_{m-1}, t_m) \prod_{m=1}^{n} k_{\alpha_m}(t_m)$$

(compare [3, eqn. 1.112] in the constant rate case).\(^2\)

Consider the master equation

$$p'(t) = H p(t), \quad p(0) = q.$$ 

Let

$$\mathcal{P}(\Gamma, n)$$

denote the set of paths of length $n$ and let $\mathcal{P}^i(\Gamma, n) \subset \mathcal{P}(\Gamma, n)$ denote the subset of those paths which have terminus $i \in \Gamma_0$.

\(^2\)The function $f$ is a discrete analogue of the Onsager-Machlup Lagrangian [5].
Theorem 3.1. The formal solution to the master equation is the vector valued function $p(t)$ whose component at $i \in \Gamma_0$ is given by the expression

$$p_i(t) = \sum_{n=0}^{\infty} \sum_{\alpha_n \in P(t_{i_n}, n)} \int_0^{t_{i_n}} \cdots \int_0^{t_2} f(\alpha_{\bullet}, t_{\bullet}) dt_1 \cdots dt_n.$$ 

Proof. Write $H = A_0 + A_1$, where $A_0$ is the diagonal matrix with entries $h_{ii}$. For $\epsilon > 0$, set $H_\epsilon = A_0 + \epsilon A_1$. Consider the equation

$$\dot{p} = H \epsilon p, \quad p(0) = q.$$

We seek a formal solution $p = p_0 + \epsilon p_1 + \epsilon^2 p_2 + \cdots$ with $p_0(0) = q$ and $p^n(0) = 0$ for $n > 0$. Once such a solution is found, we set $\epsilon = 1$ to obtain the formal solution to the master equation.

Expanding (2) in $\epsilon$, we obtain the linear system

$$\dot{p}^n = A_0 p^n + A_1 p^{n-1}, \quad n = 0, 1, 2, \ldots$$

where by convention $p^{-1} := 0$.

For $i \in \Gamma_0$, the $i$-th equation of the system is the first order linear differential equation

$$\dot{p}_i^n = h_{ii} p_i^n + \sum_{j \neq i} h_{ij} p_j^{n-1}.$$ 

If $n = 0$, the system is uncoupled and separation of variables gives

$$p_i^0 = q_i e^{\int_0^t h_{ii}(t_1) dt_1} = q_i u_i(0, t).$$

For $n > 0$, the solution to (4) can be iteratively solved using the integrating factor. The first iteration gives

$$p_i^n(t) = \sum_{j \neq i} \int_0^t e^{\int_0^{t_n} h_{ii} dt_{i_n-1}} h_{ij}(t_n) p_j^{n-1}(t_n) dt_n$$

$$= \sum_{\alpha_n} \int_0^t u_{i_{n+1}}(t_n, t) k_{\alpha_n}(t_n) p_i^{n-1}(t_n) dt_n.$$ 

where the second sum is over all edges $\alpha_n$ with terminus $i = i_{n+1}$ and whose source is denoted in the integrand by $i_n$. We then repeat the procedure using $p_{i_{n-1}}^{n-1}$ in place of $p_i^n$, to obtain

$$p_i^n(t) = \sum_{\alpha_{\bullet}} \int_0^t \int_0^{t_n} u_{i_{n+1}}(t_n, t) k_{\alpha\bullet}(t_n) u_{i_n}(t_{n-1}, t_n) k_{\alpha\alpha}(t_{n-1}) p_{i_{n-1}}^{n-2}(t_{n-1}) dt_{n-1} dt_n,$$
where the sum is indexed over all paths of length two $\alpha = (\alpha_{n-1}, \alpha_n)$ satisfying $d(\alpha_{n-1}) = (i_{n-1}, i_n)$, $d(\alpha_n) = (i_n, i_{n+1})$, and $i_{n+1} = i$. Applying this procedure a total of $n$ times results in the desired expression for $p^n_i(t)$. □

Let $\mathcal{T}(\Gamma, t)$ denote the space of trajectories of duration $t$ of arbitrary length.

**Corollary 3.2.** Let $p(t)$ denote the formal solution to the master equation. Then $p(t)$ is a probability distribution on $\Gamma_0$ for every $t \geq 0$. In particular, the function $f$ is a probability density on $\mathcal{T}(\Gamma, t)$.

**Proof.** As the rate bound holds, there is a constant $C > 0$, independent of $n$, such $f(\alpha, t) \leq C^n$ for all trajectories of length $n$. As the degree bound holds, there is global bound $D$ on the degree function, so the number of paths of length $n$ terminating at a vertex $i$ is at most $D^n$. Consequently,

$$0 \leq \sum_{\alpha} \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} f(\alpha, t) \, dt_1 \cdots dt_n \leq \frac{(Ct)^n}{n!},$$

where the sum ranges over paths of length $n$ with terminus $i$. Here, we have used the fact that $t^n/n!$ is the volume of the $n$-simplex $0 \leq t_1 \leq \cdots t_n \leq t$. By the comparison test, $\sum_n p^n_i(t)$ converges. Therefore $p(t) = \sum_n p^n_i(t)$ also converges.

Let $1: \Gamma_0 \to \mathbb{R}$ be the row vector which is identically one at every vertex. It will suffice to show that $1 \cdot p(t) = 1$. Observe that $1 \cdot \mathbb{H} = 0$, since the entries of $\mathbb{H}$ in any column add to zero. Then for all $t$ we have

$$\frac{d}{dt}(1 \cdot p(t)) = 1 \cdot p'(t) = 1 \cdot \mathbb{H} p(t) = 0.$$

Consequently, $1 \cdot p(t)$ is a constant. But $1 \cdot p(0) = 1$, hence $1 \cdot p(t) = 1$ for all $t$. □

## 4. Fundamental solutions

Consider the master equation with initial distribution $p(0) = \delta_i$ for a fixed vertex $i$, where $\delta_i(j) = \delta_{ij}$ is the Kronecker delta function. The solution to this equation is called a fundamental solution and will be denoted by $u(i, t)$.

In this case the density $f$ is supported on the set of trajectories $(\alpha, t)$ with initial vertex $i$. Let $\mathcal{T}_i(\Gamma, t) \subset \mathcal{T}(\Gamma, t)$ denote the subspace of trajectories which start at the vertex $i$.

**Corollary 4.1.** With respect to this assumption, the function $f$ is a probability density on $\mathcal{T}_i(\Gamma, t)$. 
Remark 4.2. The general solution $p(t)$ to the master equation with initial condition $p(0) = q$ is obtained from the fundamental solutions using the identity

$$p(t) = \sum_{j \in \Gamma_0} q_j u(j, t).$$

Definition 4.3. Define the propagator $K : \Gamma_0 \times \Gamma_0 \times \mathbb{R}_+ \to \mathbb{R}_+$ by

$$K(i, j, t) = u_j(i, t),$$

i.e., the probability of the set of trajectories of duration $t$ which start at vertex $i$ and terminate at vertex $j$. Note the initial condition $K(i, j, 0) = \delta_{ij}$.

Setting $\psi(x, t) := p_x(t)$, equation (5) becomes

$$\psi(y, t) = \sum_{x \in \Gamma_0} K(x, y, t) \psi(x, 0) = \int_{x \in \Gamma_0} K(x, y, t) \psi(x, 0),$$

which is familiar to the physics literature. By Theorem 3.1, we obtain the path integral representation

$$K(x, y, t) = \sum_{n=0}^{\infty} \sum_{\alpha_\bullet \in \mathcal{P}_x^y(\Gamma, n)} \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} f(\alpha_\bullet, t_\bullet) dt_1 \cdots dt_n,$$

where $\mathcal{P}_x^y(\Gamma, n)$ is the set of paths of length $n$ which start at $x$ and terminate at $y$. Furthermore, the series converges if $\Gamma$ satisfies the rate and degree bounds.

Example 4.4. Let $X$ be an $r$-regular graph, i.e., the number of edges meeting each vertex is $r$. Assume that the rates $k_\bullet$ are constant with value one. Then the master operator $\mathbb{H}$ is the negative of the graph Laplacian. In this instance elementary to check that $f(\alpha_\bullet, t_\bullet) = \delta_0 e^{-rt}$. Let $\pi_n(i, j)$ be the number of paths of length $n$ in $\Gamma = DX$ from $i$ to $j$. Then a straightforward calculation shows

$$K(i, j, t) = e^{-rt} \sum_{n=0}^{\infty} \frac{\pi_n(i, j) t^n}{n!}.$$ 

In this case, $K$ is the combinatorial heat kernel.

As $\Gamma$ is $r$-regular, there are precisely $r^n$ paths of length $n$ which start at $i$. Set

$$\phi_n(i, j) := \frac{\pi_n(i, j)}{r^n}.$$ 

Then $\phi_n(i, j)$ is the probability of the set of paths (not trajectories), which end at $j$ after $n$-jumps, given that such paths start at $i$ (where the probability of jumping across an edge meeting any vertex is $1/r$).
Let
\[ P(n) = \frac{(rt)^ne^{-rt}}{n!}. \]
Then \( P \) is the Poisson probability mass function with parameter \( \lambda = rt \).
Consequently,
\[ K(i, j, t) = \sum_{n=0}^{\infty} \phi_n(i, j)P(n) = \mathbb{E}[\Phi_{ij}], \]
is the (Poisson) expected value of the random variable \( \Phi_{ij}(n) := \phi_n(i, j) \).
Summarizing, the continuous time random walk on an \( r \)-regular graph with uniform rate \( 1/r \) may be thought of as a discrete time random walk subordinated to a Poisson process (cf. [2, chap. X§7]).

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