

Various proofs of the Fundamental Theorem of Markov Chains

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Abstract

This paper is a survey of various proofs of the so called *fundamental theorem of Markov chains*: every ergodic Markov chain has a unique positive stationary distribution and the chain attains this distribution in the limit independent of the initial distribution the chain started with. As Markov chains are stochastic processes, it is natural to use probability based arguments for proofs. At the same time, the dynamics of a Markov chain is completely captured by its initial distribution, which is a vector, and its transition probability matrix. Therefore, arguments based on matrix analysis and linear algebra can also be used. The proofs discussed below use one or the other of these two types of arguments, except in one case where the argument is graph theoretic. Appropriate credits to the various proofs are given in the main text.

Our first proof is entirely elementary, and yet the proof is also quite simple. The proof also suggests a mixing time bound, which we prove, but this bound in many cases will not be the best bound. One approach in proving the fundamental theorem breaks the proof in two parts:

- (i) show the existence of a unique positive stationary distribution for irreducible Markov chains, and
- (ii) assuming that an ergodic chain does have a stationary distribution, show that the chain will converge in the limit to that distribution irrespective of the initial distribution.

For (i), we survey two proofs, one uses probability arguments, and the other uses graph theoretic arguments. For (ii), first we give a coupling based proof (coupling is a probability based technique), the other uses matrix analysis. Finally, we give a proof of the fundamental theorem using only linear algebra concepts.

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1 Introduction

Every ergodic, that is, both irreducible and aperiodic, finite Markov chain has a unique positive stationary distribution and this distribution is attained by the chain in the limit, starting with any initial probability distribution. This fact, known as the fundamental theorem of Markov chains, is mainly responsible for the wide variety of applications that Markov chains find in diverse fields. Let us briefly mention one application: the page rank algorithm. Without doubt, the phenomenal success of Google started with the discovery

of this algorithm. When a user makes a search in the Internet, the underlying database identifies a set of web pages relevant to the search query. The number of such pages usually will be very large, possibly in hundreds of thousands. The challenge is to present to the user a certain number of pages in the decreasing order of their relevance. The page rank algorithm solves this challenge by viewing the set of discovered pages as a directed graph, where the edges are the hyperlinks, going from web pages to web pages. The algorithm considers this digraph to be defining a random walk Markov chain, the state space of which is the set of web pages discovered by the database relevant to the search query, and the transition probability of going from the page p_i to the page p_j is k/d , where d is the total number of hyperlinks occurring in the page p_i , out of which k are to the page p_j . By adding some extra hyperlinks, if necessary, the page rank algorithm first makes the random walk Markov chain ergodic, and then for some n , identifies the n webpages which have the n highest probabilities in an appropriate approximation of the stationary distribution of the random walk Markov chain. These web pages are displayed with decreasing order of their stationary probabilities. Thus, the ranking algorithm tries to capture the intuitive notion of ordering of relevance of web pages by their stationary probabilities in a random walk, which appears reasonable. That there exists a unique stationary distribution of the random walk Markov chain and we can come closer and closer to the stationary distribution, by doing a random walk independent of where we start the walk, is a consequence of the fundamental theorem which the page rank algorithm makes use of.

Like most fundamental results, this theorem too can be proved in various ways, this paper is a survey of a number of proofs of the fundamental theorem. It is natural to use reasoning based on probability for proving properties of Markov chains, as they are stochastic processes. At the same time, the dynamics of Markov chains of concern here are entirely captured by their initial distributions, which are vectors, and their transition probability matrices. Therefore, matrix analysis and linear algebra can also be used for dealing with Markov chains. Proofs discussed here use one or the other of these two types of reasoning, except in one case, in which the heart of the argument is, surprisingly, graph theoretic.

The next section deals with the basic definitions and notations. Section 3 details a very simple and an elementary proof of the fundamental theorem. Some proofs of the theorem splits the proof in two parts, they first establish that a stationary distribution, in which each component is positive, exists for irreducible. The second part proves, assuming a stationary distribution does exist, that every initial distribution converges to that stationary distribution, thereby proving simultaneously, the uniqueness of the stationary probability. Section 4 deals with this approach. Section 5 provides a proof entirely based on linear algebra.

2 Preliminaries

The notations used here and some basic definitions are as follows, for greater details, we refer to [Ha02], [No97], [LPW09]. The Markov chains considered here have finite state spaces, are discrete time, and time-homogeneous. The symbol Ω has been generally used to denote a state space. A Markov chain with a finite state space is called a *finite* Markov chain. A sequence $(X_i)_{i \geq 0}$ of rvs taking their values from a finite set Ω is a Markov chain over the state space Ω if

$$\Pr(X_{n+1} = i_{n+1} | X_0 = i_0, X_1 = i_1, \dots, X_n = i_n) = \Pr(X_{n+1} = i_{n+1} | X_n = i_n)$$

for all $i_0, \dots, i_{n+1} \in \Omega, n \geq 0$. As we deal with only time homogeneous chains, $(X_i)_{i \geq 0}$ further satisfies: for all $i, j \in \Omega$, and for all $n \geq 0$, $\Pr(X_{n+1} = j | X_n = i)$ is independent of n , and therefore, there is an $\Omega \times \Omega$ matrix P , called the *transition probability matrix*, or simply the *transition matrix*, such that $\Pr(X_{n+1} = j | X_n = i) = P(i, j)$, for all $i, j \in \Omega$ and for all $n \geq 0$. For any matrix A , we denote its ij th entry as $A(i, j)$ or as a_{ij} , or, as well as A_{ij} . We use the notation $A(x, \cdot)$ for the x th row of A . Clearly, for a transition matrix P , $P(x, \cdot)$ is the next state probability distribution when the present state is x . It is easy to see (say, by induction) that P^k is the k step transition probability matrix, that is, its ij th entry, P_{ij}^k , is the probability of the chain moving to state j at time $t + k$, given that it is in state i at time t . A probability distribution π on the state space is a *stationary distribution* of the chain if $\pi P = \pi$. A matrix such as a transition matrix P , which has every entry $P_{ij} \in [0, 1]$, and with each row entries summing to 1, is called a *stochastic* matrix. If every entry of a matrix A is positive, i.e., $A_{ij} > 0$ for all i, j , then A is called *positive*, often denoted as $A > 0$.

Let $G(P)$ denote the *underlying transition graph*: it is a directed graph that has a vertex for every state and has an edge from the vertex labeled i , representing the state i , to the vertex labeled j , for all $i, j \in \Omega$ iff $P_{ij} > 0$. If $G(P)$ is strongly connected then the corresponding Markov chain is called *irreducible*. The term *aperiodicity* means that for every state s , the gcd of the lengths of all walks in $G(P)$, each of which starts at vertex s and ends back in s is 1. A Markov chain is *ergodic* if it is both irreducible and aperiodic.

The fundamental theorem of Markov chains states

Theorem 1 (Fundamental Theorem of Markov chains) *If a discrete time, finite, and time-homogeneous Markov chain is ergodic then it will have a unique stationary distribution that assigns positive probability to every state and the chain, starting with any initial distribution, will attain the stationary distribution in the limit.*¹

It is easy to see that both irreducibility and aperiodicity are necessary for the fundamental theorem to hold: if the chain has, say, two connected components, and if the initial starting

¹The result extends also for chains with denumerable state spaces.

state is one of these components, then all future states will be from the same component. Therefore, the limiting distribution cannot be independent of the initial distribution on states. On the other hand, if the transition graph is, say, bipartite, violating the aperiodicity condition, then again there will not exist a stationary distribution which the chain reaches in the limit because, if the initial state at $t = 0$ is in one of the components, then the state at every even t will be from this component, and for every odd t the state will be from the other component. It is truly remarkable that these two easy-to-see necessary conditions are also sufficient conditions for the fundamental theorem to hold, which is a strong result also in the following sense: whereas the existence of a unique stationary distribution for a stochastic matrix that is irreducible does follow from Perron-Frobenius Theorem, the stationary distribution may not ever be attained,² the fundamental theorem guarantees that for ergodic chains not only a unique stationary distribution exists, but also convergence to it, *no matter what might be the initial distribution*.

In some of the proofs we shall need the following:

Claim 2 *If a finite state space, discrete time, and time homogeneous Markov chain with transition probability matrix P is **ergodic**, that is, both aperiodic and irreducible, then there exists a finite k such that for all $l \geq k$, P^l is positive, that is, for all i, j , $P_{ij}^l > 0$.*

. A proof of the Claim above is given in [Ha02], we briefly sketch the proof idea in a somewhat different way than done in [Ha02]. Let $M = (X_i)_{i \geq 0}$, with state space Ω be an ergodic Markov chain, and let P be its transition matrix. We recall that $G(P)$ is used to denote the underlying transition graph of the chain. We shall use the following fact repeatedly in the proof sketch below:

Fact 3 *For every two vertices u, v in $G(P)$, and for every walk w from u to v of length $|w| \geq 1$ in $G(P)$, and for every $n \geq 0$, by definition of $G(P)$, $\Pr(X_{n+|w|} = v | X_n = u) > 0$.*

Next, for any state $i \in \Omega$, let A_{ii} , a set of positive integers:

$$A_{ii} = \{|w| | w \text{ is a walk from } i \text{ to } i, |w| \geq 1\}$$

We note that since the chain is aperiodic, by definition, the gcd of the numbers in A_{ii} is 1. Further, the set of numbers in A_{ii} is closed under addition: if $G(P)$ has two walks w_1, w_2 , each from vertex i back to i , which means that $|w_1|, |w_2| \in A_{ii}$; we can concatenate the two walks to get a longer walk from i back to i , and therefore $|w_1| + |w_2|$ will also be in A_{ii} .

We can now use the following number theoretic fact (Lemma 4.1 of [Ha02]):

Fact 4 ([Bré68]) *Let $A = \{a_1, a_2, \dots\}$ be a set of positive integers which is*

²Consider the two state chain with the state space $\{0, 1\}$, in each move, if the chain is currently in state i , it moves with probability 1 to the other state, namely the state $1 - i$. This chain has the unique stationary probability distribution $[0.5, 0.5]$, but the stationary distribution is never attained.

1. *nonlattice*, meaning the $\gcd\{a_1, a_2, \dots\} = 1$, and
2. *closed under addition*, meaning that if $a \in A$ and $a' \in A$ then $a + a' \in A$

then there exists an integer $N < \infty$ such that $n \in A$ for all $n \geq N$.

Clearly, the above Fact applies to the set A_{ii} , and let N_i denote the number such that for all $n \geq N_i$, there will be a walk of length n from vertex i back to i , which implies by Fact 3 that with a positive probability the Markov chain M can move from state i back to state i in n steps.

Next, let j be an arbitrary state of the Chain M . As the Chain M is assumed to be irreducible, there exists at least one path from vertex i to j in the transition graph $G(P)$, we consider one such path which is of length, say, l_{ij} .

Let $K_{ij} \stackrel{\text{def}}{=} N_i + l_{ij}$. It is clear that for any $m \geq K_{ij}$, there is a walk in $G(P)$ of length m from i to j : first use the first $m - l_{ij}$ steps to go from i back to i , and then use the last l_{ij} steps to move from i to j . It follows from Fact 3 that for every $m \geq K_{ij}$, the (i, j) th entry of $P_{ij}^m > 0$. Let K denote

$K \stackrel{\text{def}}{=} \max\{K_{ij} | i, j \in \Omega\}$. We have therefore, that for every $l \geq K$, the matrix P^l is positive. This completes our proof sketch of the above Claim 2.

Therefore, for the purpose of proving the fundamental theorem, we lose no generality by assuming the transition probability matrix to be positive, an assumption we often make here in our proofs.

3 A simple and elementary proof

The first proof that we discuss is an elementary and a very simple proof, which is due to Alessandro Panconesi [Pa05], who in turn credits the proof idea to David Gilat. Interestingly, the same proof idea was used by Markov himself in his original 1906 paper on Markov chains, see Theorem 4.1 of the survey on Markov's life and his work [Ba04]. The proof also implies a bound which we provide on how quickly an ergodic Markov chain comes close to its stationary distribution; we also discuss how good the bound is.

3.1 The proof

Let P be the transition matrix of an ergodic Markov chain, we assume that P is positive.

$$P^\infty \stackrel{\text{def}}{=} \lim_{n \rightarrow \infty} P^n$$

Proposition 5 For any $n \times n$ positive stochastic matrix P , there exist $\pi_1, \pi_2, \dots, \pi_n$, with each i , $0 < \pi_i < 1$ and $\sum_{i=1}^n \pi_i = 1$ such that

$$P^\infty = \begin{bmatrix} \pi_1 & \pi_2 & \dots & \pi_n \\ \pi_1 & \pi_2 & \dots & \pi_n \\ \cdot & \cdot & \dots & \cdot \\ \pi_1 & \pi_2 & \dots & \pi_n \end{bmatrix}$$

Further, $\pi \stackrel{\text{def}}{=} (\pi_1, \pi_2, \dots, \pi_n)$ is a stationary distribution of P , and for any initial distribution $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_n)$, the sequence $(\sigma^{(i)})_{i \geq 1}$, defined as $\sigma^{(1)} \stackrel{\text{def}}{=} \sigma$ and $\sigma^{(i+1)} \stackrel{\text{def}}{=} \sigma^{(i)} P$, reaches π as i goes to infinity.

Proof. That, for any column of P^∞ , every element in the column has the same value follows from the following Claim:

Claim 6 Let P be a stochastic matrix with each entry positive. For an arbitrary fixed column, say k , of P , let $m^{(i)}$ and $M^{(i)}$ denote respectively the minimal and the maximal entry of the column k of P^i , the i th power of P . Then,

- (a) the sequence $(m^{(i)})_{i \geq 1}$ is non-decreasing,
- (b) the sequence $(M^{(i)})_{i \geq 1}$ is non-increasing, and,
- (c) $\Delta^{(i)} \stackrel{\text{def}}{=} M^{(i)} - m^{(i)}$ goes to 0 as i goes to infinity.

The following Corollary is immediate from the Claim above.

Corollary 7 If P is a positive, stochastic matrix then there exists a value, say π_k , such that each element of the k th column of $P^{(i)}$ approaches π_k as i goes to infinity.

The corollary above follows from Proposition 6 because as P is a positive, stochastic matrix, each P^i too is positive and stochastic for all $i > 0$. Therefore, $0 < m^{(i)}$ and $M^{(i)} < 1$, for each $i \geq 1$. As every bounded non-decreasing (or, non-increasing) sequence has a limit, the sequences in (a) and (b) of the Proposition 6 each has a limit. These two limits must be equal as (c) implies that for any $\epsilon > 0$, there will be some i such that $\Delta^{(i)} < \epsilon$. As noted by Panconesi, (c) alone does not guarantee the Corollary; consider the case where the sequences of (a) and (b) are identical but oscillating, say, each sequence being $((-1)^i)_{i \geq 1}$.

Now we prove Claim 6.

Proof. Proofs of (a):

$$\begin{aligned}
m^{(i+1)} &\stackrel{\text{def}}{=} \min_r P_{rk}^{i+1} \\
&= \min_r \sum_s P_{rs} P_{sk}^i \\
&\geq \min_r \sum_s P_{rs} m^{(i)} \\
&= m^{(i)} \min_r \sum_s P_{rs} \\
&= m^{(i)}
\end{aligned}$$

Thus, $m^{(i+1)} \geq m^{(i)}$, proving (a). A proof of (b) of Claim 6 can be given in a similar manner.

Proof of (c):

As before, our attention is on the k th column of the powers of the transition matrix P . Consider the rk entry of P^{i+1} , for an arbitrary r . As $P^{i+1} = PP^{(i)}$,

$$P_{rk}^{i+1} = \sum_l P_{rl} P_{lk}^i$$

Let a maximal entry of the k th column of P^i , viz., $M^{(i)}$, occur as the s th entry in the column. Then

$$\begin{aligned}
P_{rk}^{i+1} &= P_{rs} M^{(i)} + \sum_{l \neq s} P_{rl} P_{lk}^i \\
&\geq P_{rs} M^{(i)} + (1 - P_{rs}) m^{(i)} \\
&= m^{(i)} + P_{rs} (M^{(i)} - m^{(i)}) \\
&\geq m^{(i)} + p_{\min} (M^{(i)} - m^{(i)})
\end{aligned}$$

where p_{\min} denotes the minimum of all entries in the transition matrix P . (This is positive, as P is assumed to be positive.) As the above inequality is satisfied by an arbitrary entry of the k th column of $P^{(i+1)}$, it will be satisfied by $m^{(i+1)}$. Therefore, we have,

$$m^{(i+1)} \geq m^{(i)} + p_{\min} (M^{(i)} - m^{(i)}) \quad (1)$$

In a similar manner, next we get an upper bound on $M^{(i+1)}$. We focus again on an arbitrary entry of the k th column of $P^{(i+1)}$, this time we will take out the minimal element. Let a minimal entry of the k th column of P^i , viz., $m^{(i)}$, occur as the t th entry in the column.

Then

$$\begin{aligned}
P_{rk}^{i+1} &= P_{rt}m^{(i)} + \sum_{l \neq t} P_{rl}P_{lk}^i \\
&\leq P_{rt}m^{(i)} + (1 - P_{rt})M^{(i)} \\
&= M^{(i)} - P_{rt}(M^{(i)} - m^{(i)}) \\
&\leq M^{(i)} - p_{\min}(M^{(i)} - m^{(i)})
\end{aligned}$$

As the above inequality is satisfied by an arbitrary entry of the k th column of $P^{(i+1)}$, it will be satisfied by $M^{(i+1)}$. Therefore, we have,

$$M^{(i+1)} \leq M^{(i)} - p_{\min}(M^{(i)} - m^{(i)}) \quad (2)$$

Subtracting inequality 1 from the inequality 2, we obtain

$$M^{(i+1)} - m^{(i+1)} \leq M^{(i)} - m^{(i)} - 2p_{\min}(M^{(i)} - m^{(i)})$$

That is,

$$M^{(i+1)} - m^{(i+1)} \leq (1 - 2p_{\min})(M^{(i)} - m^{(i)})$$

In terms of Δ , we get

$$\Delta^{(i+1)} \leq (1 - 2p_{\min})\Delta^{(i)}$$

Noting that $\Delta^{(1)} \leq 1$, we get

$$\Delta^{(n)} \leq (1 - 2p_{\min})^{n-1} \quad (3)$$

Assuming that the state space of the Markov chain has three or more states ensures that $0 < (1 - 2p_{\min}) < 1$. Thus, the inequality 3 proves that $\Delta^{(n)}$ goes (*exponentially fast*) to 0 as n goes to infinity, thereby proving (c) of Claim 6. This completes the proof of the Claim 6, which, as we have seen, establishes that P^∞ is of the form

$$\begin{bmatrix} \pi_1 & \pi_2 & \dots & \pi_n \\ \pi_1 & \pi_2 & \dots & \pi_n \\ \cdot & \cdot & \dots & \cdot \\ \pi_1 & \pi_2 & \dots & \pi_n \end{bmatrix}$$

□

Let us now prove the remaining assertions of Proposition 5. We prove first that π is a distribution. This follows from the fact that for each $i \geq 1$, P^i is a stochastic matrix. The proof is by induction on i : suppose P^i is stochastic. Consider $P^{i+1}\mathbf{1}$ where $\mathbf{1}$ is the column vector of all 1's.

$$\begin{aligned}
P^{i+1}\mathbf{1} &= P(P^i\mathbf{1}) \\
&= P\mathbf{1} \\
&= \mathbf{1}
\end{aligned}$$

Further, for each i , P^i remains a positive matrix as P is positive. Therefore, π is a probability distribution with full support.

Next we show that π is a stationary distribution of P . Consider

$$\begin{aligned} P^\infty P &\stackrel{\text{def}}{=} \lim_{i \rightarrow \infty} P^i P \\ &= \lim_{i \rightarrow \infty} P^{i+1} \\ &= \lim_{i \rightarrow \infty} P^i \\ &\stackrel{\text{def}}{=} P^\infty \end{aligned}$$

Therefore we have

$$\begin{bmatrix} \pi_1 & \pi_2 & \dots & \pi_n \\ \pi_1 & \pi_2 & \dots & \pi_n \\ \cdot & \cdot & \dots & \cdot \\ \pi_1 & \pi_2 & \dots & \pi_n \end{bmatrix} P = \begin{bmatrix} \pi_1 & \pi_2 & \dots & \pi_n \\ \pi_1 & \pi_2 & \dots & \pi_n \\ \cdot & \cdot & \dots & \cdot \\ \pi_1 & \pi_2 & \dots & \pi_n \end{bmatrix}$$

Which shows that

$$[\pi_1 \pi_2 \dots \pi_n] P = [\pi_1 \pi_2 \dots \pi_n]$$

proving that π is a stationary distribution of P .

Next we show that the Markov chain, started with any initial distribution σ will reach the stationary distribution π in the limit. Let $\sigma^{(i)}$ be as defined in the statement of the Proposition 5. We need to show that $\lim_{i \rightarrow \infty} \sigma^{(i)} = \pi$. This follows easily using the inductive definition of $\sigma^{(i)}$:

$$\begin{aligned} \lim_{i \rightarrow \infty} \sigma^{(i)} &= \lim_{i \rightarrow \infty} \sigma P^{i-1} \\ &= \sigma \lim_{i \rightarrow \infty} P^{i-1} \\ &= \sigma P^\infty \\ &= \pi \end{aligned}$$

This completes the proof of the fundamental theorem. \square

(It will be instructive to figure out where in the proof we have made an essential use of the assumption that the chain is aperiodic.)

A simplification: Yogesh Dahiya³ suggested that instead of proving the two inequalities 1 and 2 to establish (c) of Claim 6, either of the two inequalities would suffice. For example, the inequality 1 gives

$$m^{(i+1)} \geq m^{(i)} + p_{\min} \Delta^{(i)}$$

³As an MS student at that time, Dept. of Computer Science, IIT Kanpur.

Now, taking the limits of both the sides of the above as i goes to infinity, we get

$$\lim_{i \rightarrow \infty} \Delta^{(i)} \leq 0$$

Since $\Delta^{(i)}$'s are non-negative by definition, we get

$$\lim_{i \rightarrow \infty} \Delta^{(i)} = 0$$

thereby establishing (c) of Claim 6. Further, an exponential convergence similar to 3 can also be obtained using only either of the two inequalities:

$$\begin{aligned} \Delta^{(i+1)} &\stackrel{\text{def}}{=} M^{(i+1)} - m^{(i+1)} \\ &\leq M^{(i)} - m^{(i+1)} \\ &\leq M^{(i)} - m^{(i)} - p_{\min} \Delta^{(i)} \\ &= (1 - p_{\min}) \Delta^{(i)} \end{aligned}$$

3.2 Convergence rate as implied by the proof

Finite Markov chains have been used for obtaining approximate solutions of $\#P$ -hard counting problems [Si93] and in combinatorial optimization problems [SRB10], [SBK20]. Whether the resulting algorithms are efficient or not depends on whether or not the underlying Markov chains come *close* to their stationary distributions *quickly*. This issue is also of importance in a recent application of Markov chains that models evolution of a population of closely related virus species with a view to design drugs against certain diseases like AIDS [PV16]. The notion of *mixing time* is generally used to formally capture how quickly does a Markov chain come close to its stationary distribution. The proof of the fundamental theorem given above provides a bound on mixing time; we see in this section what the bound is and whether it is a good bound or not. First, we state the necessary definitions [LPW09].

The *total variational distance* between two probability distributions μ and ν on state space Ω , denoted as $\|\mu - \nu\|_{\text{TV}}$ is defined as

$$\|\mu - \nu\|_{\text{TV}} \stackrel{\text{def}}{=} \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|$$

For a chain with transition probability matrix P , the *distance* $d(t)$ of the chain, after t steps from the stationary distribution π , is the maximum of the total variational distances between π and the distribution resulting after t steps, starting the chain from any state of Ω , that is,

$$d(t) \stackrel{\text{def}}{=} \max_{x \in \Omega} \|P^t(x, \cdot) - \pi\|_{\text{TV}}$$

where $P^t(x, \cdot)$ denotes the distribution that results after t steps of starting the chain from the state x . We note that the distribution $P^t(x, \cdot)$ is the row of the matrix P^t that corresponds to the state x . The *mixing time* within a given ϵ , denoted as $t_{\text{mix}}(\epsilon)$, is defined as

$$t_{\text{mix}}(\epsilon) \stackrel{\text{def}}{=} \min\{t \mid d(t) \leq \epsilon\}$$

Mixing time t_{mix} conventionally denotes the mixing time within $1/4$, i.e., $t_{\text{mix}}(1/4)$.

The above defined $d(t)$ easily relates to $\Delta^{(t)}$ defined in Claim 6. Consider the element P_{ij}^t . Fixing our attention to the column j , clearly, $|P_{ij}^t - \pi_j| \leq M^{(t)} - m^{(t)}$, that is, $|P_{ij}^t - \pi_j| \leq \Delta^{(t)}$. This is true of any state i , therefore, $d(t) \leq n\Delta^{(t)}$, where n is the number of states.

Next, for $d(t)$ to be less than or equal to ϵ , it suffices to have $n\Delta^{(t)} \leq \epsilon$. In the proof of Claim 6, we had established that

$$\Delta^{(t)} \leq (1 - 2p_{\min})^{t-1}$$

(We recall that p_{\min} denotes the minimum entry in the (positive) matrix P .) This gives us the condition

$$t \geq \frac{1}{2p_{\min}} \ln \frac{n}{\epsilon} + 1 \Rightarrow d(t) \leq \epsilon$$

Therefore,

$$t_{\text{mix}}(\epsilon) = O\left(\frac{1}{2p_{\min}} \ln \frac{n}{\epsilon}\right)$$

The above analysis assumes the transition probability matrix P to be positive. Let us consider the general case of an ergodic Markov chain M with transition probability matrix Q . We define m as $m \stackrel{\text{def}}{=} \min\{k \geq 1 : Q^k > 0\}$. (Ergodicity of M ensures that m will be defined.) After the first m steps, if we consider moves of M in sequences of m steps each, then actions of these move sequences are of course defined through Q^m , which is a positive matrix. For the chain M , therefore, we have

$$t_{\text{mix}}(\epsilon) = O\left(\frac{m}{2p_{\min}} \ln \frac{n}{\epsilon}\right) \tag{4}$$

In many applications, we would like the underlying Markov chain to be *rapidly mixing*. A chain is rapidly mixing if it is the case that $t_{\text{mix}} = O(p(n))$ where n is the length of the description of the chain, and $p(\cdot)$ is a fixed polynomial, that is, the chain mixing time is bounded by a fixed polynomial in the size of the input to describe the chain. The size can of course be taken as the size of the state space. However, in many applications, the input chain is implicitly described such that input size is logarithmic in the state space. For example, consider random walks on an n -dimensional hypercube, the walk can be modeled by a Markov chain for which a state is an n -dimensional 0 – 1 vector that describes the current position of the walk. The Markov chain can be described by specifying what the

transitions will be, with their probabilities, given a state. As there are only $O(n)$ neighbours of any state, the description of the Markov chain is of size $O(n)$ whereas the state space size is 2^n .

Before we put the relation 4 to use to check rapid mixing, we need to comment upon the parameter m in the equation. Trivially, m is bounded by the number of states, but in many applications where the chain state space is exponential in the size of its description, m turns out to be polynomially bounded by the chain description. For the hypercube random walk example, notice that m is equal to n , as the chain has a path from any state to any other of length n or less, with paths from $[00 \dots 0]$ to $[11 \dots 1]$ being of length n . Similarly, for the case of card shuffle where a move consists of picking a card from the deck uniformly at random and then placing the chosen card on top of the deck, for a deck with n cards, there are $n!$ states but we can get to any state from any other in at most n moves. Thus, for both these examples where the number of states is exponential in the (implicit) input size, m is of the size of the input, rather than of the size of the state space.

In reasonable descriptions of the input chain, the description size is no less than logarithmic in the size of the states. Assuming such descriptions, We see from the relation 4 that a sufficient condition for a chain to be rapidly mixing is that both m and $\frac{1}{p_{\min}}$ are bounded by a fixed polynomial in the size of the chain description. This condition immediately implies rapid mixing of random walks on a graph because p_{\min} is no less than $1/n$ for an n -vertex graph. However, the condition is too weak to prove rapid mixing in many cases. Consider the case of random walks on n -dimensional hypercube. Although as we have remarked, the value of m poses no problem, p_{\min} is too small: the probability of moving from $[00 \dots 0]$ to $[11 \dots 1]$ is $n!/n^n$. Using Stirling's approximation $n! \sim \sqrt{2\pi n}(n/e)^n$, we see that the probability is inverse exponential in n .⁴ Therefore, the relation 4 does not prove rapid mixing of the chain, though the chain does mix rapidly, using a coupling argument, one can prove that the chain will mix in $O(n \log n)$ steps.

4 Stationarity: Existence, Convergence

A common approach ([LPW09], [Ha02], [MU05]) to prove the fundamental theorem is to prove separately the following:

- (a) if a chain is irreducible then it has a stationary distribution in which every state has a non-zero probability,
- (b) if π is a stationary distribution of an ergodic chain with with transition probability matrix P , then starting with any initial distribution, the chain reaches π in the limit.

An easy consequence of (b) above is that, a stationary distribution, if it exists, is unique. (Theorem 5.3 of [Ha02]). For proof, suppose that π and π' are two stationary distributions,

⁴In order to make the chain aperiodic, the chain is made lazy, thereby the value is further reduced by a factor of 2^n which is ignored for the sake of simplicity.

we show that $\pi = \pi'$. Let us start the chain with π as its initial distributions. Then, denoting πP^n as $\pi^{(n)}$, we have from (b) that $\lim_{n \rightarrow \infty} \pi^{(n)} = \pi'$. However, as π is stationary, $\pi = \pi P$, so, $\lim_{n \rightarrow \infty} \pi^{(n)} = \pi$. Therefore, $\pi = \pi'$.

Clearly then, proving (a) and (b) together will prove the fundamental theorem.

We note first that irreducibility is both a necessary and sufficient condition for the existence of a stationary distribution. We had seen in Section 2 the necessity, and (a) above guarantees sufficiency. We note that the converse of (a) is not true, a trivial counter example is that of a chain with the identity matrix as its transition probability matrix. Further, it is easy to see that a periodic chain can have stationary distribution: a trivial example is a chain with state space $\{s_0, s_1\}$ and transition probabilities are given by the rule: if in state s_i , with probability 1 go to the other state, namely, s_{1-i} . Clearly, the underlying transition graph is bipartite, but the chain has the unique stationary distribution $[0.5, 0.5]$.

Actually, irreducibility guarantees not just existence, but also the *uniqueness* of the positive stationary distribution, [LPW09] (Corollary 1.17), ([Sa06] (Lemma 1.2.2). We briefly sketch the proof as given in [LPW09] ([Sa06] proof is essentially the same).

Let us call a function h from the state space Ω to \mathbb{R} to be *harmonic* if, regarding h as a column vector, we have $h = Ph$. If P is the transition matrix of an irreducible chain, then h must be a constant function. The proof: since Ω is finite, there exists an $x_0 \in \Omega$ such that h is maximal at x_0 . Let $h(x_0)$ be equal to M . Let $z \in \Omega$ be such that $P(x_0, z) > 0$ and $h(z) < M$. Now, h being harmonic,

$$h(x_0) = P(x_0, \cdot)h = P(x_0, z)h(z) + \sum_{w \neq z} P(x_0, w)h(w)$$

Clearly, the RHS of the second equality is strictly less than M , which then gives $h(x_0) < M$, a contradiction. This implies that $h(z) = M$. Irreducibility implies that for every $y \in \Omega$, there is some q such that there is a sequence $x_0, x_1, \dots, x_q = y$ with $P(x_i, x_{i+1}) > 0$. Repeating the argument tells us that $M = h(x_0) = \dots = h(x_{q-1}) = h(y)$. Therefore, h is a constant function. Now, by definition, $(P - I)h = 0$. As h is a constant (column) vector, the kernel of $(P - I)$ is 1. Therefore, the column rank of $P - I$ is $\Omega - 1$. As the row and the column ranks of a matrix are the same, the solution space of the matrix equation $\sigma = \sigma P$ is also one dimensional. Normalizing the solutions to have all entries of a solution summing to 1, there will be a unique solution to $\sigma = \sigma P$.

The following subsection deals with proving (a), and (b) is dealt with in the next subsection.

4.1 Existence of stationary distribution

We provide two proofs, the first is probability based, and the other one uses only graph theoretic argument. Of course, linear algebra based proofs are also there, as the one given in [Sa06], making essential use of Perron's theorem. However, since Section 5 details a complete proof of the fundamental theorem entirely based on linear algebra and matrix

analysis, which too uses Perron's theorem, we do not discuss in this subsection linear algebra based proofs of existence of positive stationary distributions.

4.1.1 Stationarity using probability argument

We sketch the proof given in [LPW09].

Proof Sketch. The intuition is that the probability π_y corresponding to a state y in a stationary distribution is the fraction of time the chain spends in state y in the “long-term”. As the chain runs, if we consider successive sequences, each of which starts at (a specific but arbitrary) state z and ends when the chain revisits z for the first time after the start of that sequence, then these sequences are identically distributed. Therefore, the average number of times a state y is visited per sequence should be proportional to π_y .

Let M be a Markov chain $(X_i)_{i \geq 0}$ with state space Ω and the transition probability matrix P . Let z be an arbitrary state. We follow the notation in [LPW09] to denote $\mathbf{Pr}_z(\mathcal{E})$, $\mathbf{Ex}_z(Y)$ respectively as the probability of the event \mathcal{E} , and the expectation of Y , when the initial distribution has the state z with probability 1. Also, define $\tilde{\pi}_y$ as

$\tilde{\pi}_y \stackrel{\text{def}}{=} \mathbf{Ex}_z(\text{number of visits to } y \text{ before returning to } z \text{ for the first time})$. Let τ_z^+ denote $\min\{t \geq 1 | X_0 = z, X_t = z\}$, i.e., the first return time to z . Let I_t denote the indicator variable which is 1 if $X_t = y$ and $\tau_z^+ > t$. Then,

$$\tilde{\pi}_y = \mathbf{Ex}\left(\sum_{t=0}^{\infty} I_t\right) = \sum_{t=0}^{\infty} \mathbf{Pr}_z(X_t = y, \tau_z^+ > t)$$

Next, we verify that $\tilde{\pi}$ is stationary: we show that for arbitrary $y \in \Omega$, $\tilde{\pi}_y = \sum_{x \in \Omega} \tilde{\pi}_x P(x, y)$. Using the definition of $\tilde{\pi}_x$,

$$\sum_{x \in \Omega} \tilde{\pi}_x P(x, y) = \sum_{x \in \Omega} \sum_{t=0}^{\infty} \mathbf{Pr}_z(X_t = x, \tau_z^+ > t) P(x, y) \quad (5)$$

We use below the fact that the event $\tau_z^+ \geq t + 1$, i.e., $\tau_z^+ > t$ is determined entirely by X_0, X_1, \dots, X_t in obtaining the third equality in the following:

$$\begin{aligned} & \mathbf{Pr}_z(X_t = x, X_{t+1} = y, \tau_z^+ \geq t + 1) \\ &= \mathbf{Pr}_z(\tau_z^+ \geq t + 1 | X_t = x, X_{t+1} = y) \mathbf{Pr}_z(X_t = x, X_{t+1} = y) \\ &= \mathbf{Pr}_z(\tau_z^+ \geq t + 1 | X_t = x) \mathbf{Pr}_z(X_t = x, X_{t+1} = y) \\ &= \mathbf{Pr}_z(\tau_z^+ \geq t + 1 | X_t = x) \mathbf{Pr}_z(X_t = x) P(x, y) \\ &= \mathbf{Pr}_z(\tau_z^+ \geq t + 1, X_t = x) P(x, y) \end{aligned}$$

Reversing the order of summation in 5, and using the above,

$$\begin{aligned}
& \sum_{x \in \Omega} \tilde{\pi}_x P(x, y) \\
&= \sum_{t=0}^{\infty} \sum_{x \in \Omega} \mathbf{Pr}_z(X_t = x, X_{t+1} = y, \tau_z^+ > t) \\
&= \sum_{t=0}^{\infty} \mathbf{Pr}_z(X_{t+1} = y, \tau_z^+ \geq t+1) \\
&= \sum_{t=1}^{\infty} \mathbf{Pr}_z(X_t = y, \tau_z^+ \geq t)
\end{aligned}$$

The right hand side of the above syntactically is almost the same as in the definition of $\tilde{\pi}_y$, in fact with a little work it can be shown that the right hand side of the above *is* $\tilde{\pi}_y$, which establishes that $\tilde{\pi}$ is stationary: $\tilde{\pi}P = \tilde{\pi}$. To obtain a probability distribution from $\tilde{\pi}$, we normalize it by $\sum_x \tilde{\pi}_x$, which is $\mathbf{E}\mathbf{x}_z(\tau_z^+)$. Thus, the distribution is π where

$$\pi_x = \frac{\tilde{\pi}_x}{\mathbf{E}\mathbf{x}_z(\tau_z^+)}$$

As z was arbitrary, we can set z to be x , to get

$$\pi_x = \frac{1}{\mathbf{E}\mathbf{x}_x(\tau_x^+)}$$

We note that, by construction, each $\pi_x > 0$. We also note that proof above does not need the chain to be aperiodic, though irreducibility is needed— we have made use of the tacit assumption that $\tilde{\pi}_x < \infty$ for all states x which would not hold for a reducible chain. \square

4.1.2 Stationarity using graph theoretic argument

The proof we give here is based on one given in [Kar08] which is the unpublished notes on Markov chains by Rajeeva Karandikar.⁵

As before, let Ω be the state space and P be the transition probability matrix of a Markov chain M , which is assumed to be irreducible. For $x, y \in \Omega$, we use p_{xy} as an abbreviation of $P(x, y)$.

Suppose we are able to define a $\gamma : \Omega \rightarrow \mathbb{R}^+$, satisfying, for every $y \in \Omega$

$$\sum_{x \in \Omega} \gamma(x) p_{xy} = \gamma(y)$$

⁵Karandikar communicated to us that his proof was adapted from [FW12].

then γ is stationary for P (though not necessarily a distribution). The equation above is equivalent to

$$\begin{aligned} \sum_{x \in \Omega, x \neq y} \gamma(x) p_{xy} &= \gamma(y) - \gamma(y) p_{yy} \\ &= (1 - p_{yy}) \gamma(y) \\ &= \sum_{x \in \Omega, x \neq y} p_{yx} \gamma(y) \end{aligned}$$

That is, we need to establish, for each $y \in \Omega$,

$$\sum_{x \in \Omega, x \neq y} \gamma(x) p_{xy} = \sum_{x \in \Omega, x \neq y} \gamma(y) p_{yx} \quad (6)$$

Intuitively, the equation captures a balance condition, *viz.*, attaining stationarity means that for every y , 'flow' into y equals the 'flow' out of y .

Such a γ is defined from G_M , the underlying directed graph capturing P . G_M has Ω as its set of vertices, and for every pair of vertices, x, y , there is an edge from x to y of weight p_{xy} . For a vertex x , let $\tau(x)$, a subgraph of G_M , be called an *upward spanning tree rooted at x* , if $\tau(x)$ satisfies the following:

- $\tau(x)$ spans G_M : every vertex of G_M occurs once and only once in $\tau(x)$,
- From every vertex in $\tau(x)$, except x , there is exactly one outgoing edge, and the outdegree of x is zero.
- From every vertex y of G_M other than x , there is one and exactly one path from y to x in $\tau(x)$.

For every vertex x , we define $\mathcal{T}(x)$ as

$$\mathcal{T}(x) \stackrel{\text{def}}{=} \{\tau(x) \mid \tau(x) \text{ is an upward spanning tree rooted at } x\}$$

The weight $W(H)$ of a subgraph H is defined to be the product of the weights of the edges in G , and the weight of a set S of subgraphs is the sum of the weights of its elements. In particular, the *weight* $W(\mathcal{T}(x))$ is the sum of the weights of the upward spanning trees in $\mathcal{T}(x)$, where the weight of the upward spanning tree $\tau(x)$ is the product of its edge weights. Thus,

$$W(\mathcal{T}(x)) \stackrel{\text{def}}{=} \sum_{\tau(x) \in \mathcal{T}(x)} \prod_{(y,z) \in \tau(x)} p_{yz}$$

For each $x \in \Omega$, we define $\gamma(x)$ as

$$\gamma(x) \stackrel{\text{def}}{=} W(\mathcal{T}(x))$$

Clearly, the Markov chain being irreducible, for every $x \in \Omega$, there is at least one upward spanning tree rooted at x , so, $\gamma(x)$ is positive. Next,

Claim 8 $\gamma(x)$'s, as defined above satisfy the stationarity condition Eqn. 6.

A proof of the above is as follows.

The LHS of the balance condition, Eqn. 6, can be seen as the weight of the following set A of subgraphs of G_M : $A \stackrel{\text{def}}{=} \cup_{x \in \Omega, x \neq y, \tau(x) \in \mathcal{T}(x)} (\tau(x) \cup \{(x, y)\})$. Similarly, the RHS of Eqn. 6 can be seen as the weight of the following set B of subgraphs of G_M : $B \stackrel{\text{def}}{=} \cup_{x \in \Omega, x \neq y, \tau(y) \in \mathcal{T}(y)} (\tau(y) \cup \{(y, x)\})$. We show that the two sets, A and B are same, because each is contained in the other. To see that $A \subseteq B$, consider an element of A , which is, for some $x, x \neq y$, an upward spanning tree rooted at x , say $\tau'(x)$, with the edge (x, y) added to it. Since $\tau'(x)$ is spanning, the vertex y occurs in $\tau'(x)$, and let z be the vertex that immediately follows y in the unique directed path from y to x in $\tau'(x)$. By removing the edge (y, z) from $\tau'(x)$ and adding instead the edge (x, y) , we get a subgraph which is an upward spanning tree now rooted at y . The union of this new upward spanning tree with the edge (y, z) is clearly a member of B , being the subgraph which is the union of an upward spanning tree rooted at y along with the edge (y, z) . To check the containment of B in A , consider an element of B , which is some upward spanning tree rooted at y , say $\tau''(y)$ along with an edge (y, w) for some $w, w \neq y$. Consider the unique path from w to y in $\tau''(y)$, and let u be the vertex which immediately precedes y in this path. By deleting the edge (u, y) from $\tau''(y)$ and adding instead the edge (y, w) , we get an upward spanning tree now rooted at u , say, $\tau'''(u)$. This tree, along with the edge (u, y) , is indeed a member of A . Karandikar gives a succinct description of the set $A(= B)$: it is the set of all minimally spanning sets with exactly one cycle that contains y and in which every vertex has outdegree exactly 1.

As $A = B$, they will have identical weights. This ends the proof of the above claim.

Defining $\pi(x)$ as $\gamma(x) \sum_{y \in \Omega} \gamma(y)$, we get a stationary distribution for the Markov chain M .

The proof above uses irreducibility, but aperiodicity has not been assumed.

4.2 Proofs of convergence to stationarity

As stated earlier, what we wish to prove here is: if an ergodic Markov chain M admits a stationary distribution π then the chain attains π in the limit, starting from any distribution. Formally, we prove:

Theorem 9

$$\lim_{n \rightarrow \infty} \|P^n(x, \cdot) - \pi\|_{\text{TV}} = 0$$

for all $x \in \Omega$. or, equivalently, $\lim_{n \rightarrow \infty} P^n(i, j) = \pi_j$ for all $i, j \in \Omega$

We discuss here two types of proofs of the above, one uses coupling, the other type uses matrix analysis.

4.2.1 Convergence using coupling

Coupling is a technique which has been widely used in establishing upper bounds on the mixing times of Markov chains [LPW09], [MU05]. It is therefore not surprising that this technique can be used for proving the convergence result, which is a weaker result than proving, given any $\epsilon \geq 0$, starting from an arbitrary initial distribution, an upper bound on the number of steps a chain will take to come ϵ -close to its stationary distribution, which is what is used to establish an upper bound on mixing time of the chain.

We first explain the notion of coupling and indicate how the notion is used in establishing upper bounds on mixing time. We shall define coupling of a Markov chain in a manner different from the usual ones, say, as found in [LPW09], and refer to relevant literature as to why our definition is more appropriate. Actually, the coupling notion used in practice is a restricted notion called the *faithful coupling*, we shall briefly indicate why the restricted notion is used rather than the general notion as given in the [LPW09]

Next, we prove Theorem 9 and the proof we shall provide, is by Karandikar, given in [Kar08]. Although it is a coupling based proof, it assumes no knowledge of coupling, and hence can be read independently without first going through the next two subsections.

4.2.2 Coupling of two distributions

Let μ and ν be two distributions on the same set, say, Ω . A coupling of these two distributions is a pair (X, Y) of random variables X and Y , defined on the same probability space, therefore, one can define a joint distribution of X and Y . Let θ be such a joint distribution, (clearly, θ is a distribution on $\Omega \times \Omega$). For (X, Y) to be a coupling of μ and ν , θ needs to satisfy the property that the marginal distribution of X in θ is μ and the marginal distribution of Y is ν .

For the same pair of distributions, in general, there will be many couplings, i.e., there will be many joint distributions of two random variables (X, Y) such that the marginal distribution of X is μ and the marginal distribution of Y is ν . For examples, we refer to the discussion preceding Proposition 4.7 of [LPW09]. Also, there is an example given in the [DDB17] of two distributions with exactly one coupling.

The importance of coupling of two distributions stems from the following fact: if (X, Y) is a coupling of two distributions μ and ν , then $\mathbf{Pr}(X \neq Y)$ is an upper bound of the total variational distance between μ and ν , $\|\mu - \nu\|_{\text{TV}}$. Further, the infimum of all couplings is exactly the total variational distance, and this coupling, called the *optimal coupling*, can be defined constructively, given any two distributions. We refer to Proposition 4.7 of [LPW09]

for a proof.

4.2.3 Coupling of a Markov chain

Let M be a Markov chain with its state space as Ω , and transition matrix P . We define the coupling notion of M in the following way: a coupling of M is given by an infinite sequence $(X_i, Y_i)_{i \geq 0}$ of pairs of random variables, each taking values from Ω , and the sequence satisfies the property that for some two distributions μ_0 and ν_0 , both on Ω , (X_i, Y_i) is a coupling of $\mu_0 P^i$ and $\nu_0 P^i$, for all $i \geq 0$. Such a coupling can be constructed by defining a transition matrix Q and a joint distribution θ_0 of μ_0 and ν_0 , such that denoting, for all $i \geq 0$, θ_i as $\theta_0 Q^i$, then θ_i is a coupling of $\mu_0 P^i$ and $\nu_0 P^i$. Thus the distribution of X_i is $\mu_0 P^i$ and the distribution of Y_i is $\nu_0 P^i$, for all $i \geq 0$. Therefore, both $(X)_{i \geq 0}$, and $(Y)_{i \geq 0}$ are two evolutions of the chain M , for certain initial distributions, but crucially, what we are *not* saying is that $(X)_{i \geq 0}$ and $(Y)_{i \geq 0}$ are Markov chains.

If we compare the definition above with the one given in [LPW09], ours appears unnecessarily complicated, as our definition is in terms of specific initial distributions for the two copies of the chain, as well as it is in terms of a specific joint distribution of the two initial distributions of the Markov chain. The reason why our definition is the appropriate definition is given in [HM18], [DDB17].

In any case, a coupling of a Markov chain M can be seen as a process $(X_i, Y_i)_{i \geq 0}$ where each of $(X_i)_{i \geq 0}$ and $(Y_i)_{i \geq 0}$ follows the evolution of the chain M . We say that such a coupling has *coupled at time T* if $X_T = Y_T$, further we say that the coupling has the *now-equals-forever* property [Ro97] if for any j , $X_j = Y_j$, then for every $k \geq j$, $X_k = Y_k$. One way which has been used for turning a coupling $(X_i, Y_i)_{i \geq 0}$ into a coupling with the now-equals-forever property is by replacing $(Y_i)_{i \geq 0}$ by $(Z_i)_{i \geq 0}$ where

$$Z_i = \begin{cases} Y_i & \text{if } i \leq T \\ X_i & \text{otherwise} \end{cases} \quad (7)$$

where $T \stackrel{\text{def}}{=} \inf\{i | X_i = Y_i\}$. In other words, the process $(Y_i)_{i \geq 0}$ starts following the process $(X_i)_{i \geq 0}$ once the coupling has happened. [HM18] called replacing Y_i s by Z_i s as the *sticking* operation.

Rosenthal [Ro97] proved that the sticking operation *does not guarantee* that the two processes $(X_i, Y_i)_{i \geq 0}$ and $(X_i, Z_i)_{i \geq 0}$ will be equivalent. Rosenthal then proved that if the coupling is what he defined as *faithful*, then the two processes are guaranteed to be equivalent.

If the coupling has (or made to have through sticking) the now-equals-forever property, then it can be shown that the following holds:

Lemma 10

$$\|\mu_0 P^i - \nu_0 P^i\|_{\text{TV}} \leq \Pr(T > i)$$

where T is as defined above, and (as we defined in the beginning of our discussion on the Markov chain coupling), μ_0 and ν_0 are the two initial distributions, and P is the transition matrix of the Markov chain being coupled. This follows from Lemma 11.2 of [MU05], the lemma is known as the *coupling lemma*. For an explicit proof of 10, we refer to [DDB17].

Let us now indicate how coupling is used to obtain an upper bound on the mixing time. Suppose μ_0 is the stationary distribution of M , say π , and let ν_0 be an *arbitrary* initial distribution. By providing an upper bound on $\Pr(T > i)$ for some i , we get an upper bound on the variational distance between the stationary distribution and the distribution obtained after running the chain for i steps. Therefore, given an $\epsilon \geq 0$, we can determine an i such that $\Pr(T > i) \leq \epsilon$, which will provide an upper bound on the number of steps the chain, starting with an arbitrary distribution, needs to run so that the chain distribution comes ϵ -close to the stationary distribution. Of course, how good the bound is will depend on the coupling that is defined.

For the sake of completeness, we give the definition of faithful coupling:

Definition 11 (Faithful coupling) *Let $(M_i)_{i \geq 0}$ be a Markov chain M with the state space Ω . Then a coupling of M , $(X_i, Y_i)_{i \geq 0}$ is a faithful coupling if $(X_i, Y_i)_{i \geq 0}$ is itself a Markov chain on state space $\Omega \times \Omega$ satisfying:*

$$\Pr(X_{t+1} = x' | (X_t, Y_t) = (x, y)) = \Pr(M_{t+1} = x' | M_t = x)$$

$$\Pr(Y_{t+1} = y' | (X_t, Y_t) = (x, y)) = \Pr(M_{t+1} = y' | M_t = y)$$

for all $t \geq 0$ and for all $x, y, x', y' \in \Omega$.

In terms of the matrix Q defined earlier, the conditions above is equivalent to: that the transition matrix Q satisfies the following:

for all $i, j, i', j' \in \Omega$,

$$\sum_{j' \in \Omega} Q((i, j), (i', j')) = P(i, i'), \text{ and}$$

$$\sum_{i' \in \Omega} Q((i, j), (i', j')) = P(j, j')$$

Recall that P is the transition matrix of the Markov chain M . Faithfulness appears to be a natural property, all coupling examples in [LPW09] are said to be faithful.

4.2.4 An coupling based proof of convergence

We provide here a coupling based proof of the convergence theorem, the proof we provide is by Karandikar citerajeeva. ⁶ Although the proof is coupling based, the proof assumes

⁶Karandikar informed us that his proof is adapted from a proof given in [Bi95]

no background knowledge of coupling, it develops all the necessary concepts from the first principles. Such a 'simple' coupling based proof was possible because the coupling used is the trivial coupling where two independent copies of a chain are coupled. The discerning reader will see that the proof indeed uses the concepts etc. we discussed in the last subsection. *These connections are pointed out in remarks which are given in parentheses, these parenthetical remarks are not necessary for understanding the proof.*

Let M be a Markov chain with state space Ω and transition matrix P . M is assumed to be irreducible and aperiodic. Let π be a stationary probability of M . We prove convergence to π by showing that for all $i, j \in \Omega$,

$$\lim_{n \rightarrow \infty} P^n(i, j) = \pi_j$$

Let $(X_i)_{i \geq 0}$ and $(Y_i)_{i \geq 0}$ be two independent copies of M , that is, for all $i, i', j, j' \in \Omega$, $\mathbf{Pr}(X_i = i', Y_j = j') = \mathbf{Pr}(X_i = i')\mathbf{Pr}(Y_j = j')$

Consider now $N = (X_i, Y_i)_{i \geq 0}$. (Clearly, N defines a coupling of the simplest kind, called an *independent coupling* which can easily shown to be a faithful coupling.)

Using independence, it is easy to prove that

- N is a Markov chain with state space $\Omega \times \Omega$,
- the transition matrix of N is given by Q where for all $i, j, k, l \in \Omega$, $Q((i, k), (j, l)) = P(i, j) \times P(k, l)$,
- N is aperiodic and irreducible.⁷

Let $t \in \Omega$ be any fixed state of M . Because the chain N is irreducible, for any arbitrary $i, j \in \Omega$, with $X_0 = i$ and $Y_0 = j$, there will be infinitely many finite n 's such that $X_n = t$ and $Y_n = t$. Let τ denote the least of these n 's.

We define a new sequence of random variables $(Z_i)_{i \geq 0}$ where

$$Z_i = \begin{cases} Y_i & \text{if } i \leq \tau \\ X_i & \text{otherwise, that is, for all } i > \tau \end{cases} \quad (8)$$

(This sticking operation turns the chain N to a new chain which has now-equals-forever property.)

Claim 12 $(Z_i)_{i \geq 0}$ is a Markov chain with transition matrix P .

Proof. The Claim is proved by showing that for any $n \geq 0$, and for all i_0, i_1, \dots, i_n , where each of the i s is in Ω ,

$$\mathbf{Pr}(Y_0 = i_0, \dots, Y_n = i_n) = \mathbf{Pr}(Z_0 = i_0, \dots, Z_n = i_n) \quad (9)$$

⁷The chain N will not be irreducible unless M is both aperiodic and irreducible. The proof below will break down if N is not irreducible. This is where we make essential use of ergodicity of M . We are grateful to Rajeeva Karandikar for pointing this out to us.

Proving the equality establishes the Claim is because $(Z_i)_{i \geq 0}$ behaves exactly the same way as $(Y_i)_{i \geq 0}$ does which we know to be a Markov chain. For a more formal argument, one can invoke Theorem 1.1.1 of [No97]. In turn, it suffices to prove that for all $m \geq 0$,

$$\mathbf{Pr}(Y_0 = i_0, \dots, Y_n = I_n, \tau = m) = \mathbf{Pr}(Z_0 = i_0, \dots, Z_n = i_n, \tau = m) \quad (10)$$

We note that if $m \geq n$ then 10 is true by definition of $(Z_i)_{i \geq 0}$. On the other hand, if $n > m$ and if $i_m \neq t$, then both LHS and RHS of 10 are zero. Therefore, the only interesting case to be considered is when $n > m$ and $i_m = t$. In that case, the RHS of 10 is then

$$\mathbf{Pr}(Z_0 = i_0, \dots, Z_n = i_n, \tau = m)$$

Using the definition of Z , the above is equal to

$$Y_0 = i_0, \dots, Y_m = t, \tau = m, X_{m+1} = i_{m+1}, \dots, X_n = i_n$$

Using independence of X_i 's and Y_i 's, we get

$$\mathbf{Pr}(Y_0 = i_0, \dots, Y_m = t, \tau = m) \times \mathbf{Pr}(X_{m+1} = i_{m+1}, \dots, X_n = i_n | X_m = t)$$

Now, using the fact that, by definition, if $\tau = m$, then $X_m = Y_m = t$, we get from the above $= \mathbf{Pr}(Y_0 = i_0, \dots, Y_m = t, \tau = m) \cdot p_{t,m+1} \cdots p_{n-1,n}$

The LHS of 10 can, a little more easily, be proved to be the same expression as above. Hence, $(Z_i)_{i \geq 0}$ is also a Markov chain with P as its transition matrix, being identical to $(Y_i)_{i \geq 0}$, which proves the Claim 12. \square

(Because the coupling used here is the simplest, independent coupling, the independence of the two chains $(X_i)_{i \geq 0}$ and $(Y_i)_{i \geq 0}$ made the proof above quite easy. For a general faithful coupling, such a proof, somewhat more complex, can be found in [Ro97], [DDB17].)

Finally, we are ready to prove convergence by showing that in P^n as n tends to infinity, each column entry for any $k \in \Omega$ has the same value π_k , the k th component of the stationary distribution π which was assumed to exist for P .

We use the following notation: for any event A , and for any $i, j \in \Omega$, $\mathbf{Pr}_{i,j}(A)$ will denote $\mathbf{Pr}(A | X_0 = i, Y_0 = j)$, or equivalently, $\mathbf{Pr}(A | X_0 = i, Z_0 = j)$. When P is a transition matrix, we recall that the (i, j) th entry of the matrix P^n is denoted by $p_{ij}^{(n)}$. For the Markov chain M as P its transition matrix, we know that

$$p_{jk}^{(n)} = \mathbf{Pr}_{ij}(Y_n = k) = \mathbf{Pr}_{ij}(Z_n = k). \text{ Therefore,}$$

$$\begin{aligned}
|p_{ik}^{(n)} - p_{jk}^{(n)}| &= |\mathbf{Pr}_{ij}(X_n = k) - \mathbf{Pr}_{ij}(Z_n = k)| \\
&= |\mathbf{Pr}_{ij}(X_n = k, Z_n \neq k) + \mathbf{Pr}(X_n = k, Z_n = k) \\
&\quad - \mathbf{Pr}_{ij}(Z_n = k, X_n = k) + \mathbf{Pr}_{ij}(Z_n = k, X_n \neq k)| \\
&= |\mathbf{Pr}_{ij}(X_n = k, Z_n \neq k) - \mathbf{Pr}(Z_n = k, X_n \neq k)| \\
&\leq \mathbf{Pr}_{ij}(X_n = k, Z_n \neq k) + \mathbf{Pr}_{ij}(Z_n = k, X_n \neq k) \\
&\leq \mathbf{Pr}_{ij}(X_n \neq Z_n) = \mathbf{Pr}_{ij}(\tau > n)
\end{aligned}$$

We have already argued that the chain $(X_i, Y_i)_{i \geq 0}$, that is $(X_i, Z_i)_{i \geq 0}$, is irreducible, and therefore, for any $i, j \in \Omega$, τ is finite. Therefore,

$$\lim_{n \rightarrow \infty} |p_{ik}^{(n)} - p_{jk}^{(n)}| \leq \mathbf{Pr}_{ij}(\tau > n) = 0$$

From the above, we conclude that $\lim_{n \rightarrow \infty} |p_{ik}^{(n)} - p_{jk}^{(n)}| = 0$. Since the limit is zero, we the above is equivalent to

$$\lim_{n \rightarrow \infty} (p_{ik}^{(n)} - p_{jk}^{(n)}) = 0 \tag{11}$$

This shows that, in the limit n tending to infinity, all entries in any column k of P^n will have all its entries identical. Next, we show that this value is π_k , the k th entry of the of π , the stationary distribution of the chain M the existence of which we have assumed. As π is a stationary distribution for the chain M , $\pi P^n = \pi$ for all $n \geq 0$. Therefore,

$\sum_{i \in \Omega} \pi_i p_{ik}^{(n)} = \pi_k$, the k th component of π .

Now consider

$$\sum_{i \in \Omega} \pi_i (p_{ik}^{(n)} - p_{jk}^{(n)}) = \pi_k - p_{jk}^{(n)} \tag{12}$$

Using Equation 11

$$\lim_{n \rightarrow \infty} \sum_{i \in \Omega} \pi_i (p_{ik}^{(n)} - p_{jk}^{(n)}) = 0 \tag{13}$$

Using Equations 12 and 13, we get the result we wanted to prove:

$$\lim_{n \rightarrow \infty} (\pi_k - p_{jk}^{(n)}) = 0$$

Further, the proof also shows that the stationary distribution is unique, as $\lim_{n \rightarrow \infty} p_{jk}^{(n)}$ will be a unique value.

4.2.5 Convergence through matrix analysis

First proof:

We consider first the proof given in [LPW09]⁸ and provide the proof idea. Let π be a stationary distribution for P and let Π be (as in Section 2) the square matrix each row of which is π . First, we note

Fact 13 (a) $M\Pi = \Pi$ holds for any stochastic matrix M , and (b) $\Pi M = \Pi$ holds for any stochastic matrix M for which π is a stationary distribution.

As P is positive, there exists a δ strictly between 0 and 1 such that for every pair x, y , $P(x, y) \geq \delta\Pi(x, y)$ holds. Let $\theta \stackrel{\text{def}}{=} 1 - \delta$. A key ingredient of the proof is to define a stochastic matrix Q through the equation

$$P = (1 - \theta)\Pi + \theta Q \quad (14)$$

The above gives

$$P - \Pi = \theta(Q - \Pi) \quad (15)$$

The left hand side of the above is the “error” to begin with. This error reduces exponentially as we power P ; making crucial use of Fact 13, we prove that for all n *geq* 1

$$P^n - \Pi = \theta^n(Q^n - \Pi Q^{n-1}) \quad (16)$$

The proof is by induction, let us show the induction step. Suppose we have for some k

$$P^k - \Pi = \theta^k(Q^k - \Pi Q^{k-1})$$

We post-multiply the two sides of the above by the two sides of (15), and then simplify using Fact 13:

$$\begin{aligned} (P^k - \Pi)(P - \Pi) &= \theta^k(Q^k - \Pi Q^{k-1})\theta(Q - \Pi) \\ P^{k+1} - P^k\Pi - \Pi P + \Pi^2 &= \theta^{k+1}(Q^{k+1} - Q^k\Pi - \Pi Q^k + \Pi(Q^{k-1}\Pi)) \\ P^{k+1} - \Pi &= \theta^{k+1}(Q^{k+1} - \Pi - \Pi Q^k + \Pi^2) \\ P^{k+1} - \Pi &= \theta^{k+1}(Q^{k+1} - \Pi Q^k) \end{aligned}$$

This proves the induction step. In the derivation above, besides Fact 13, we have also used the fact that the product of two stochastic matrices is also stochastic, and therefore, any power of a stochastic matrix is also stochastic. Also, for a matrix Q , we have taken Q^0 by definition to be the identity matrix I .

The last step is to consider the x th row of of the resultant matrix on each side of

$$P^n - \Pi = \theta^n(Q^n - \Pi Q^{n-1})$$

⁸a similar proof is there in [Sa06]

summing the absolute values of the elements on each side, then dividing by two to get

$$\|P^n(x, \cdot) - \pi\|_{\text{TV}} = \theta^n \|Q^n(x, \cdot) - \Pi Q^{n-1}(x, \cdot)\|_{\text{TV}}$$

Noting that 1 is the largest value that a total variational distance can take, we get

$$\|P^n(x, \cdot) - \pi\|_{\text{TV}} \leq \theta^n$$

This completes the proof sketch of the Convergence theorem.

Second proof that uses an interesting matrix norm

5 Linear algebra proof of the Fundamental Theorem

The proof we provide makes use of Perron's theorem of 1907, a result that applies to all real, positive square matrices. Perron's result was (somewhat weakly) extended to real, non-negative square matrices by Frobenius in 1912. Perron-Frobenius results have many applications, we refer to [Ma00] for a survey. The proof below essentially details the proof sketch given there.

Proof. The statement of Perron's theorem is:

Theorem 14 ((Perron)) *Let A be a positive real square matrix. The largest eigenvalue λ of A is real, with algebraic (and therefore, geometric) multiplicity of 1, and with an associated eigenvector which is both real and positive. All other eigenvalues of A are strictly smaller than λ in absolute value.*

Let M be a finite ergodic Markov chain with Ω as its set of states, and P as its transition probability matrix. Without loss of generality, we assume P to be positive. We note that 1 is an eigenvalue of P , because $P\mathbf{1} = \mathbf{1}$ as P is stochastic. In fact, we show next that 1 is the largest real eigenvalue of P . Suppose otherwise, let $\lambda > 1$ be the largest real eigenvalue of P . As the spectra of P and its transpose P^T are same, λ is the largest real eigenvalue of P^T as well. Perron's theorem says that there will be a positive eigenvector corresponding to λ , let this eigenvector, after normalization so that its components add to 1, be⁹ μ^T . Then, $P^T \mu^T = \lambda \mu^T$. Taking transposes, we get $\mu P = \lambda \mu$. Thus, P transforms a probability distribution to something which is not a probability distribution. This is a contradiction because P , being stochastic, always transforms probability distributions to probability distributions: suppose ρ is a probability distribution on Ω then so is $\sigma \stackrel{\text{def}}{=} \rho P$, for, $\sum_{x \in \Omega} \sigma_x = 1$ as $\sigma \cdot \mathbf{1} = \rho(P\mathbf{1}) = \rho \cdot \mathbf{1} = 1$, and no element of $\sigma = \rho P$ can be negative as P is positive, and

⁹We remind that, as per the non-standard convention we are following here, μ denotes a row vector.

ρ , being a probability distribution, cannot have any negative element. Therefore, 1 is the largest real eigenvalue of P .

We have it from Perron's theorem that the eigenvalue 1 is of multiplicity one, and it strictly dominates all other eigenvalues. Casting P in Jordan canonical form, $P = MJM^{-1}$, J being a Jordan matrix where the first Jordan block corresponds to the largest eigenvalue of P , namely, 1. Since this eigenvalue is of multiplicity 1, the first block of J consists of a single element, namely, 1. Next, we show that

$$J^\infty \stackrel{\text{def}}{=} \lim_{n \rightarrow \infty} J^n = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} \quad (17)$$

That is, J^∞ is a square matrix with only one non-zero element, 1, which is at the left, top corner. This is so because as the power n goes to infinity, every Jordan block of J , except the first one, goes to a zero matrix. Proof: consider such a Jordan block J_i , corresponding to the eigenvalue λ_i , and suppose it is a $k \times k$ matrix. Therefore,

$$J_i = \begin{bmatrix} \lambda_i & 1 & 0 & \dots & 0 \\ 0 & \lambda_i & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \lambda_i & 1 \\ 0 & 0 & \dots & 0 & \lambda_i \end{bmatrix}$$

Now, the matrix J_i^n can be shown¹⁰ to be

$$J_i^n = \begin{bmatrix} \lambda_i^n & \binom{n}{1} \lambda_i^{n-1} & \binom{n}{2} \lambda_i^{n-2} & \dots & \binom{n}{k-1} \lambda_i^{n-k+1} \\ 0 & \lambda_i^n & \binom{n}{1} \lambda_i^{n-1} & \dots & \binom{n}{k-2} \lambda_i^{n-k+2} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \lambda_i^n & \binom{n}{1} \lambda_i^{n-1} \\ 0 & 0 & \dots & 0 & \lambda_i^n \end{bmatrix}$$

That is, the first row of J_i^n is the first k terms of the binomial expansion of $(\lambda_i + 1)^n$, and the other rows are obtained by right shifting the first row successively and placing zeros initially. Perron guarantees that each $|\lambda_i| < 1$. Therefore, each non-zero element in J_i goes to 0 as n goes to infinity, each such term element being a ratio of a polynomial in n to an exponential in n . Thus, we have 17.

Let us define P^∞ as

$$\mathbf{P}^\infty \stackrel{\text{def}}{=} \lim_{n \rightarrow \infty} P^n$$

We note that J^∞ is a rank 1 matrix, therefore P^∞ , being equal to $MJ^\infty M^{-1}$, is also of rank 1. Next, we note that P^∞ is a stochastic matrix, as P is stochastic, and the product

¹⁰by induction, alternatively, noting that $J_i = D_i + U_i$, D_i diagonal and U_i nilpotent, and noting that these two commute.

of two stochastic matrices is also stochastic. Therefore, being stochastic, every row of P^∞ is stochastic, and being of rank 1, all the rows are identical. Thus, for some probability distribution on Ω , $\pi = [\pi_1 \pi_2 \cdots \pi_{|\Omega|}]$,

$$P^\infty = \begin{bmatrix} \pi_1 & \pi_2 & \cdots & \pi_{|\Omega|} \\ \pi_1 & \pi_2 & \cdots & \pi_{|\Omega|} \\ \cdot & \cdot & \cdots & \cdot \\ \pi_1 & \pi_2 & \cdots & \pi_{|\Omega|} \end{bmatrix} \quad (18)$$

Next, we show that π as above is a stationary distribution of P , i.e., $\pi P = \pi$.

$$P^\infty P \stackrel{\text{def}}{=} \lim_{n \rightarrow \infty} P^n P = \lim_{n \rightarrow \infty} P^{n+1} \stackrel{\text{def}}{=} P^\infty$$

We have thus $P^\infty P = P^\infty$. Equating the first row of the LHS matrix product with that of the RHS matrix we get $\pi P = \pi$, establishing π as a stationary distribution of P .

Next, we see that π is the unique stationary distribution of P and the support of π is the entire state space. Repeating an earlier argument, taking the transpose of $\pi P = \pi$, we see π^T to be¹¹ a (right) eigenvector of π which corresponds to the eigenvalue 1 of P^T . Since P^T has the same spectra as P , and as we have proved 1 to be the largest eigenvalue of P , we have 1 to be the largest eigenvalue of P^T as well. From Perron's theorem then, since 1 is of multiplicity 1, π^T is, after normalization, the unique eigenvector corresponding to the eigenvalue 1. So, π is the unique stationary distribution of P . Further, Perron's theorem also guarantees that π^T is positive. Therefore, the support of π is the entire state space. Finally, if we run the chain with any initial distribution σ , as $\sigma P^\infty = \pi$, the chain will converge to the unique stationary distribution π in the limit. This completes the present proof of the fundamental theorem. \square

6 Concluding remarks

An elementary proof need not be simple, and simplicity in many simple proofs is due to the use of some advanced concepts. The first proof that we have seen in this note is remarkable because it is both elementary and simple. Moreover, although the result is about a stochastic process, the proof does not use any probabilistic idea. The key idea that is used is that when we take the dot product of a row of a stochastic matrix with a column of a positive matrix, we perform a weighted averaging of the column entries— the result will be a value between the smallest and the largest entry of the column, and the betweenness is strict when the stochastic matrix is positive. The second proof that we have seen makes essential use of probability arguments. Though the presentation here (following [LPW09]) is elementary, the proof originally emanates, as noted in [MU05], from renewal theory. The third proof

¹¹we note again that we are abusing the standard notation in writing π^T as a column vector.

rests on Perron’s theorem which is usually proved making use of Gelfand’s spectral radius formula, a result from the theory of Banach algebras, though elementary proofs of Perron-Frobenius theorem do exist, see, e.g., [Su83]. One may therefore say that the three proofs rest on three different intuitions. The hallmark of a great result is that it can be arrived at through different points of view—indeed then, the fundamental theorem of Markov chains possesses this hallmark.

Acknowledgements: I express my indebtedness to all the authors whose proofs I have surveyed in this paper. I am grateful to Manindra Agrawal, Rajeeva Karandikar, Satyadev Nandakumar, Nandini Nilakantan, and Nisheeth Vishnoi for helpful discussions.

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