Markov chains

Recherche opérationnelle
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In this chapter, we will see how it is possible to model certain specific random behaviors in the form of Markov chains, that are graphs augmented with probabilities. The properties of these graphs will then make it possible to deduce information about the system. Applications of chains are generally fault finding in a system, estimation of the position of a population in a set of states, and, as we will see in the associated chapter, queuing modeling. From the information on these systems, we can deduce an appropriate action which will not depend on the probabilistic aspects of the systems.

1 Definitions

1.1 Stochastic process and Markov chain

Definition 1. A random variable X is a S-valued function where S is a set of **states**. A stochastic process is a family $(X_t)_{t \in T}$ of random variables where $T \subset \mathbb{R}^+$.

For example, you can think of the weather as a random phenomenon. On day t, X_t will be the random variable representing the weather for that day, there will be some probability of seeing this variable occuring in the form of good weather, rain, gloomy weather, ... We consider the sequence of variables as a stochastic process.

Some processes have particular properties. The first is that of a Markovian process, it is a process without memory, where knowing the last state of the process at time t is sufficient to deduce the probabilities of completion at the next time. Before going into the definition, here are three examples.

Suppose you have two bags. The first contains n_1 white and m_1 black balls respectively. The second contains n_2 white and m_2 black balls respectively. In the first round, we draw from bag 1. On each subsequent round, if the last ball drawn is white, we draw from bag 1, otherwise we draw from bag 2. Once a ball has been drawn, we put the ball back in his bag. In this case, we indeed have a Markovian process. Only the last ball is important. If it is white, we have a probability $\frac{n_1}{n_1+m_1}$ of drawing white and $\frac{m_1}{n_1+m_1}$ of drawing black. If it is black, we have a probability $\frac{n_2}{n_2+m_2}$ of drawing white and $\frac{m_2}{n_2+m_2}$ of drawing black. Knowing whether the balls before were white or black gives us no additional information.

Suppose you have a single bag filled with n white and m black balls. You draw from it then put the ball back in the bag before starting again. In this case, each draw is independent, you have the same probability $\frac{n}{n+m}$ of drawing white and $\frac{m}{n+m}$ of drawing black. This example is an extreme version of a Markovian process. It is not even necessary to know the last ball to determine the probability of the next draw.

Finally, suppose you have a single bag filled with n white and m black balls. You draw from it but don't put the ball back in the bag before starting again. In this case, each draw depends on all the previous ones. Without knowledge of these previous draws, you do not know how many balls are left in the bag and therefore you cannot deduce the probabilities of drawing in the next round.

Definition 2. We say a process $(X_t)_{t \in T}$ is a *markov* process if and only if *the futur depends only on the present* :

$$\forall t_1 < t_2 < \cdots < t_n < t_{n+1} \in T, \forall A \subset S$$

$$P(X_{t_{n+1}} \in A |\ X_{t_1} X_{t_2}, \ldots, X_{t_n}) = P(X_{t_{n+1}} \in A |\ X_{t_n})$$

A Markovian process means that the function $P(X_{t_{n+1}} \in A | X_{t_1} X_{t_2}, \ldots, X_{t_n})$ does not depend on the state of the variables $X_{t_1} X_{t_2}, \ldots, X_{t_{n-1}}$. It is a function that only depends on the state of X_{t_n}. It is a memoryless process. It looks at what state it is in at a given time, and this defines the random variable of the next state. Please note, knowing the realization of X_{t_n} is not enough to know that of $X_{t_{n+1}}$ but is enough to know the probabilities of realization of this variable.

The second important property of Markov chains is homogeneity. This means that the probabilities do not vary over time. The first 2 examples with the bags of balls are homogeneous. If, on the other hand, in each round, you add a black ball and a white ball to the bags, the probabilities will vary over time (until reaching approximately 0.5 in this case). This process is therefore not homogeneous. Let's consider another example. If you have a car that breaks down regularly. We model the fact of breaking down with a process: this car, when it breaks down one week, has a probability 0.5 of breaking down again the following week. If it is not broken, then it has a 0.01 probability of breaking down the following week. This process is a Markovian process (only the state of the car the previous week is important) and it is homogeneous (the probabilities do not depend on the week in which we look to see if it will break down). Now suppose that the model is the following: when it breaks down one week t, has a probability $1 - 0.5e^{-}t$ of breaking down again the following week. If it is not broken in week t, then it has probability 0.01 of breaking down the following week. So the later the car breaks down, the more likely it is to stay broken down for a long time. This process is not homogeneous. On the other hand, it is still Markovian.

Definition 3. We say a process $(X_t)_{t\in T}$ is a *time-homogeneous* process if and only if *the conditional probabilities does not change when the time grows* :
$\forall t, t' \in T, s > 0 \backslash t + s, t' + s \in T, A \subset S$

$$P(X_{t+s} \in A | X_t) = P(X_{t'+s} \in A | X_{t'})$$

We can now define a Markov chain.

Definition 4. A *Markov chain* is a time-homogeneous process and a Markov process $(X_t)_{t\ \in T}$.

In the following, we will consider a simple case of Markov chain where the time T is countable and where the state space S is finite and discrete. But it should be noted that the definitions in this course generalize to the case where time is continuous and to the case where the state space is continuous.

1.2 Characterization by a graph

Taking into account the homogeneity and the fact that a Markov chain is a Markovian process, we observe that, knowing the realization of the variable X_t, we can deduce the probabilities of realization of the variable X_{t+1}. This probability does not depend on iteration t.

Definition 5. p_{ij} is the probability for the system to move from the state i to the state j in one step. This probabilty does not depend on the moment $t \in T$ when the state of the system is i.

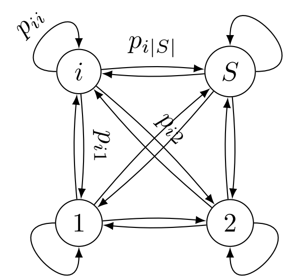
$$\forall i, j \in S, \exists p_{ij} \quad \backslash \quad \forall t \in \mathbb{N} \quad P(X_{t+1} = j | X_t = i) = p_{ij}$$

$$P = \begin{array}{c} \begin{array}{cccccc} 1 & 2 & & j & & |S| \end{array} \\ \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1j} & \cdots & p_{1|S|} \\ p_{21} & p_{22} & \cdots & p_{2j} & \cdots & p_{2|S|} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ p_{i1} & p_{i2} & \cdots & p_{ij} & \cdots & p_{i|S|} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ p_{|S|1} & p_{|S|2} & \cdots & p_{|S|j} & \cdots & p_{|S||S|} \end{pmatrix} \end{array} \begin{array}{c} 1 \\ 2 \\ \\ i \\ \\ |S| \end{array}$$

We can already note an interesting property of the matrix P. It is called stochastic because the sum of the elements of a line is equal to 1.

$$\sum_{j=1}^{|S|} p_{ij} = 1$$

Definition 6. The graph $G = (V, A)$ of a Markov chain is a **directed graph** where every node is a state S (thus $V = S$), and every arc linking i to j is weighted with p_{ij}. An arc is not added if $p_{ij} = 0$.



It is possible to deduce more complex transition probabilities from P.

Theorem 1.1. *Let $k \in \mathbb{N}$ then $P(X_{t+k} = j | X_t = i) = P^k_{ij}$.*

Remark 1. It may seem strange to consider this probability knowing that, in the examples of Markovian processes in the previous section, much emphasis was placed on the fact that only the last realization, X_{t+k-1}, was necessary to know the probability of realization of X_{t+k}. But that's because our examples are imprecise. If we look closely at the definition of Markovian process, we do not say that only the realization of the previous iteration makes it possible to deduce probabilities, we say that if we are aware of several realizations, then only the last one is useful. In other words, if we know the realization of X_t and that of X_{t+k-1} then the knowledge of X_t is superfluous. But if we do not know X_{t+k-1} we will still be able to get (less precise) information from X_t.

Proof. Let us prove this theorem by induction on k. Let us denote $R_{kij} = P(X_{t+k} = j | X_t = i)$. Let us show that $R_k = P^k$ for all k.

If $k = 0$ then the probability of being in state j at iteration t knowing that one is in state i is 1 if $i = j$ and 0 otherwise. So $R_0 = I = P^0$. So the property is well proven for $k = 0$.

Now suppose the property is proven for some value $k - 1$. According to the law of total probabilities:

$$\begin{aligned} R_{kij} &= \sum_{s \in S} P(X_{t+k} = j | X_{t+k-1} = s) \cdot R_{k-1,is} \\ &= \sum_{s \in S} P_{sj} \cdot R_{k-1,is} \end{aligned}$$

By induction hypothesis

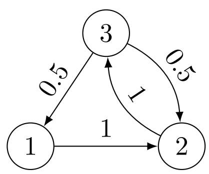
$$\begin{aligned} R_{kij} &= \sum_{s \in S} P_{sj} \cdot P_{is}^{k-1} \\ &= P_{ij}^k \end{aligned}$$

□

1.3 State probability distribution vector

We wish to study $q_i(t) = P(X_t = i)$. We denote by $Q(t)$ the vector of probabilities $q_i(t)$. We can notice that it is not possible to deduce $Q(t)$ from P only. A simple reason is that Q depends on t so P is constant. However, knowing $Q(t)$ allows knowing $Q(t+k)$ for all $k \in \mathbb{N}$.

Consider now the following chain:



Without additional information, it is not possible to know what the probability of $X(t)$ occurring is. Let us suppose that we know, by some indirect means, this probability when $t = 0$. We know that at the start of the chain, we have a probability $q_1(0) = 0.25$ of being in state 1, $q_2(0) = 0.5$ of being in state 2 and $q_3(0) = 0.25$ to be in state 3. Another way to see these probabilities is to suppose that we are studying a population with many individuals, for example 1000000 people. There would then be at the beginning 250,000 people in state 1, 250,000 people in state 3 and 500,000 people in state 2. Obtaining the probabilities $Q(0)$ is then done just with statistical counting, the realization of $X(0)$ is then only a random person from the population. After one iteration of the chain, anyone who was in state 1 moves, with probability 1, to state 2. Likewise, anyone in state 2 moves to 3. Finally, anyone in 3 has a one in two chance of moving to state 1 or state 2. We would therefore have at the end of this move, $125,000$ people in state t1, $375,000$ in state 2 and $500,000$ in state 3, i.e. $Q(1) = (0.125, 0.375, 0.5)$. We can finally note the following property: if we multiply $Q(0)$ by P, we obtain $Q(1)$.

$$\begin{pmatrix} 0.25 & 0.5 & 0.25 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0.5 & 0.5 & 0 \end{pmatrix} = (0.125, 0.375, 0.5)$$

Thus the knowledge of $Q(0)$ allows us to deduce $Q(1)$ using P. This property can be generalized and demonstrated.

Theorem 1.2. *Let $k \in \mathbb{N}$ then $Q(t+k) = Q(t) \cdot P^k$.*

Proof. The proof is very similar to that of theorem 1.1. It is proven by induction and uses the law of total probabilities. □

Warning: to calculate $Q(t+k)$, you must multiply $Q(t)$ by P^k and not the other way around.

2 Stationnary distribution and limit distribution

Thus, by continuing the calculations of the previous example, we can obtain $Q(t)$ for all t starting from $Q(0)$. This property is interesting but requires us to know $Q(0)$ to have information. However, we can notice a surprizing detail. If we calculate $Q(1000)$, we obtain

$$Q(0) \cdot P^{1000} = \begin{pmatrix} 0.2 & 0.4 & 0.4 \end{pmatrix}$$

Now suppose we start with another initial vector, say $Q'(0) = \left(0.33, 0.33, 0.33\right)$. If we calculate $Q'(1000)$, we obtain

$$Q'(0) \cdot P^{1000} = \begin{pmatrix} 0.2 & 0.4 & 0.4 \end{pmatrix}$$

We can start again with other initial vectors, we will always come across the same vector. To be exact, they are not the same vector but very close vectors to the point so that very high precision is necessary to differentiate them. But it seems that, whatever the initial probability vector, the distribution always converges to the same vector. This property is interesting because it is no longer necessary to know the initial population distribution vector, it is enough to execute enough iterations to transform any distribution into its limit distribution. In the rest of this section, we will characterize the chains which have such a limit distribution, and we will describe a method for calculating it. An interesting thing to note is that the characterization goes purely through a characterization of the chain graph, without taking into account the probability values on the arcs.

2.1 States classification

The concepts used in Markov chains that are described here are the same as those used in graph theory, although the vocabulary differs. In the following, we consider a chain whose graph is G.

Definition 7. A state j is *accessible* from i if there is a **path** from i to j in G.

$$\exists k \backslash (P^k)_{ij} > 0$$

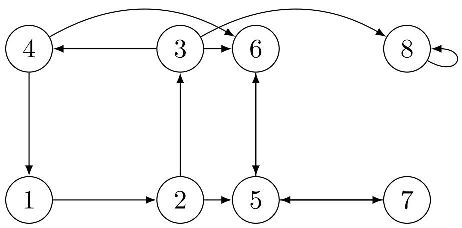
Definition 8. Two states i and j are said *communicating* if i is accessible from j and conversely.

Definition 9. A *communicating class* is a strongly connected component of G. In other words, it is a maximal set of pairwise communicating states.

Definition 10. A state i is *transient* if there is a state j such that j is accessible from i but i is not accessible from j.

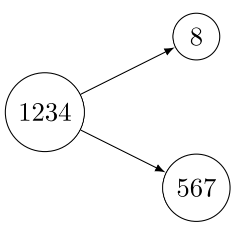
Definition 11. A state i is *recurrent* if for every accessible state j from i, i is accessible from j.

We consider the following example.



- All states are accessible from 1
- Only 5, 6 and 7 are accessible from 5.
- 1 and 3 communicate because each is accessible from the other.
- This chain has three communicating classes: 1234, 567 and 8.
- 1, 2, 3 and 4 are transient. Indeed, from any of these states, we can reach for example state 5. But from state 5 it is impossible to return to these 4 states. **Attention**, one might believe that 1 is not transient because from 1, we must necessarily reach 2, from which we can reach 1 again. But the definition does not speak of direct transition, it speaks of accessibility. From 1, we can reach 2 then 5. So there is a possibility that 5 will be reached, and once this possibility is achieved, it is no longer possible to return to 1.
- 5, 6, 7 are recurrent. Indeed, from each of these states, we can only reach 5, 6 and 7. We can therefore always return to the starting position.
- 8 is also recurrent, because no state is accessible from 8 except itself.

We can quite easily distinguish between transient and recurrent states in the following way. Create a new graph G_c. In this graph, add one node per communicating class of G. Add in G_c an arc between two nodes u and v if there exists in G an arc connecting the class corresponding to u and the one corresponding to v. In the previous chain, this would result in the following graph:



We call G_c the *contraction of* G. This graph has two interesting properties:

Theorem 2.1. *Let G_c be the contraction of G then G_c is acyclic and a state of G is recurrent if and only if the node corresponding to its communicating class in G_c is a well.*

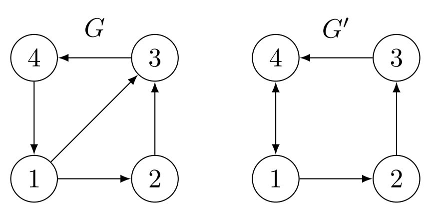
Proof. If G_c contains a circuit between the nodes $u_1, u_2, \ldots, u_p$ whose associated p communicating classes are $C_1, C_2, \ldots, C_p$, then it exists in G a circuit D passing successively through the nodes of $C_1, C_2, \ldots, C_p$ then returning to C_1. Let v be a node of $C_1 \cap D$ and w be a node of $C_2 \cap D$, then, since D is a circuit, v is accessible from w and vice versa. So the two communicate. Since all states of C_1 communicate with v and all states of C_2 communicate with w then all states of C_1 communicate with all states of C_2. So $C_1 \cup C_2$ is a set of communicating states, which means that C_1 and C_2 were not maximal. This contradicts the fact that these were classes of communicating states. There is therefore a contradiction, so G_c is acyclic.

Let a well u of G_c and C be the associated communcating class. Let $v \in C$. Since there is no arc coming out of u in G_c then no state outside of C is accessible from v. So if w is accessible from v, then $w \in C$. But w and v communicate so v is accessible from w. So v is recurrent.

Let a node u of G_c which is not a sink and C be the associated communicating class. Let $v \in C$. Since u is not a sink, there exists a neighbor u' of u in G_c. Let C' be the associated class. There exists between C and C' an arc (w, w'). Since $w \in C$ then v and w communicate. So w is accessible from v. Since there is an arc from w to w' then w' is accessible from v. Since G_c does not contain any circuit, then there does not exist in G_c a path from u' to u. So there cannot exist a path in G from w' to v. So v is not accessible from w', so v is transient. □

2.2 Period of a state

The period of a state measures the ability of a chain to periodically return the population to a state it left. Consider the following two examples.



Assuming that the probabilities are 1 everywhere except for edges leaving state 1 where they are fixed at 0.5, and assuming that the initial state $Q(0)$ (left) and $Q'(0)$ (right) check $q_1(0) = q'_1(0) = 1$ and $q_i(0) = q'_i(0) = 0$ for $i > 1$, we obtain the following results:

$$Q(1000) = (0.28, 0.14, 0.28, 0.28)$$
$$Q(1001) = (0.28, 0.14, 0.28, 0.28)$$
$$Q(1002) = (0.28, 0.14, 0.28, 0.28)$$
$$Q(1003) = (0.28, 0.14, 0.28, 0.28)$$
$$Q'(1000) = (0.67, 0, 0.33, 0)$$
$$Q'(1001) = (0, 0.33, 0, 0.67)$$
$$Q'(1002) = (0.67, 0, 0.33, 0)$$
$$Q'(1003) = (0, 0.33, 0, 0.67)$$

We see that, in Q', a regularity appears with a period 2. We could consider that Q is also regular with a period 1. We nevertheless say that, in this case, Q is aperiodic although Q' is periodic.

To understand this notion of periodicity, it is necessary to understand that we are talking here about a periodicity in the probabilities and not in the realizations of these probabilities. Thus, if a population is placed on state 1 of the chain whose graph is G', then after 1000 iterations, we will see that the population makes a regular movement on the chain. On even iterations, there will be people on states 1 and 3 (with about 2 times as many in state 1). On odd iterations, these people will be in states 2 and 4 (with about twice as many people in state 4). But this does not mean that every member of the population will have periodic movement. On the scale of the individual, we will not be able to see anything. It is only at the population level that we see this period emerging.

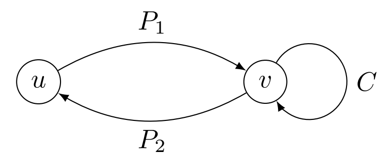
Let us now formally define this period. It can be noted that $(P^k)_{ii} > 0$ if there exists a circuit with k arcs of weight non zero going through i.

Definition 12. Let $d_i = GCD(k|(P^k)_{ii} > 0, k > 0)$ with $d_i = 1$ if $(P^k)_{ii} = 0 \quad \forall k$.) A state i is said to be *periodic* if $d_i > 1$. Otherwise, the state is aperiodic. d_i is the *period* of i.

In other words, the period of a state is the GCD of the sizes of all circuits passing through that state. In the two previous examples, in G, the state 1 is contained in two circuits of size 3 and 4, the circuits 1231 and 12341. There are other circuits containing 1 but the GCD of all these circuits cannot be different from 1 since it is the only common divisor of 3 and 4. In G', there exists an infinity of circuits passing through 2: circuits $23412, 234123412, 2341412, 23414123412, \ldots$. We can see that the sizes of these circuits cover all even numbers starting from 4. There is no circuit of odd size containing 2. So the period of state 2 is $PGCD(4, 6, 8, \ldots)$ =2. By applying the same process, one could show that all the states of G are aperiodic and all the states of G' are periodic with period 2.

Theorem 2.2. *Let u and v be two states of the same communicating class then u and v have the same period.*

Proof. Let d_u be the period of u, let us show that the period d_v of v is greater than d_u. By symmetry, we can deduce that they are equal. Since u and v communicate, there exist paths from u to v and from v to u. For each path P_1 from u to v and each path P_2 from v to u, we can construct a circuit with P_1 followed by P_2. This circuit passes through u therefore $|P_1| + |P_2|$ is divisible by d_u. Now let us consider a circuit C passing through v. Consider the circuit consisting of P_1 then C then P_2, it is a circuit passing through u. So $|P_1| + |P_2| + |C|$ is divisible by d_u. We deduce that $|C|$ is also divisible by d_u. So all the sizes of the circuits passing through v are divisible by d_u so their GCD is at least d_u.



□

2.3 Regular chain

The theorems demonstrated here are not all generalizable to the case where the state space is infinite.

Definition 13. A distribution Q is said to be *stationary* if $Q = QP$. A Markov chain is said to be regular if there exists a stationary distribution Q^* such that, whatever the initial distribution vector $Q(0)$, $\lim_{t\to+\infty} Q(t)$ exists and is worth Q^*.

One can note that only stationary distributions can satisfy the second property. We will show in this last part that it is possible to characterize regular chains.

Lemma 2.1. *A chain that contains two or more recurrent communicating classes is not regular.*

Proof. Suppose the chain has at least two recurrent communicating classes C_1 and C_2. Let $i_1 \in C_1$ and $i_2 \in C_2$. By definition, only the states of C_1 are accessible from (and communicate with) i_1. So if $Q(0)$ is the vector such that $q_{i_1}(0) = 1$ and $q_j(0) = 0$ for any other state j then, for all $t \geq 0$, there exists $j \in C_1$ such that $q_j(t) \neq 0$. Likewise, only the states of C_2 are accessible and communicate with i_2. So if $Q'(0)$ is the vector such that $q'_{i_2}(0) = 1$ and $q'_j(0) = 0$ for any other state j then, for all $t \geq 0$ and all $j \in C_1$, $q_j(t) = 0$. Thus, if these limits exist, we have $\lim_{t\to+\infty} Q(t) \neq \lim_{t\to+\infty} Q'(t)$. The chain is therefore not regular. □

Lemma 2.2. *A chain that contains a recurrent communicating class whose states all have period $d > 1$ is not regular.*

Proof. Suppose the chain has a recurrent communicating class C whose states have period d. Let us assume without loss of generality that $1 \in C$. We denote by $N(i)$ the states whose distance from 1 (the shortest path in number of arcs) is worth i modulo d (it is written $k \cdot d + i$ where $k \in \mathbb{N}$). Thus $1 \in N(0)$, any state at a distance $3 \cdot d$ is in $N(0)$, any state at a distance $d+2$ is in $N(2)$ assuming $d > 2 \ldots$

Note that a state of $N(i)$ can only be connected with an arc to a state of $N(i+1)$. Otherwise there would exist a circuit passing through 1 whose size would not be divisible by d. The proof is similar to that of theorem 2.2.

Now consider $Q(0)$ the vector such that $q_1(0) = 1$ and $q_j(0) = 0$ for all $j \neq 1$. Since C is a recurrent class, the only states that communicate with 1 are those of C. So, for all t, $\sum_{j \in C} q_j(t) = 1$. Finally, we can notice that if $t \equiv i[d]$ then only the states of $N(i)$ can check $q_i(t) > 0$ and therefore $\sum_{j \in N(i)} q_j(t) = 1$. So, for example at iterations $d, 2d, 3d, \ldots, kd$, the entire population is concentrated in $N(0)$. And at iterations $d+1, 2d+1, \ldots, kd+1$, the entire population is concentrated in $N(1)$. Since $N(0) \neq N(1)$, it is therefore not possible that $\lim_{t \to +\infty} Q(t)$ exists. So the chain is not regular. □

Proving that the properties of the two previous lemmas are equally necessary is not very complicated but would require introducing many more notions to be well written. Here we give a very useful intermediate result and the reference to the complete proof.

Lemma 2.3. *If Q is a stationary distribution then, for any transient state i, $q_i = 0$.*

Remark 2. One way to understand this lemma is to notice that, at each step, there is a non-zero probability of moving from the set of transient states to a recurrent state. So, the population in the transient states will be emptied little by little. It is necessary to demonstrate that this decrease converges towards 0.

Proof. Let T be the set of transient states and R be the set of permanent states. Let us divide Q and the transition matrix P into blocks.

$$Q = \begin{pmatrix} Q_T & Q_R \end{pmatrix} \quad P = \begin{pmatrix} P_T & P_{TR} \\ 0 & P_R \end{pmatrix}$$

By definition of transient state, the probability of going from R to T is zero. Since $Q = QP$ then $Q_T = Q_T P_T$. Finally, note that $I - P_T$ is an invertible square matrix (its inverse is equal to $\sum_{n \in \mathbb{N}} P_T^n$). So $Q_T = 0$. □

So it is not necessary to look at the transient states.

Theorem 2.3. *If a chain has a unique aperiodic recurrent communicating class then it is regular.*

Proof. The proof can be found for example in Theorem 4.9 of David A Levin and Yuval Peres. *Markov chains and mixing times.* Vol. 107. American Mathematical Soc., 2017. URL: `https://pages.uoregon.edu/dlevin/MARKOV/`. Taking a look at section 1.5 first may be helpful. □

2.4 Compute Q^*

How to calculate Q^* knowing the regularity of the chain? There are two methods. The first deduction from the proof of theorem 2.3 consists of calculating the limit of P^t. We can then notice that this matrix converges to the matrix where all the rows are equal to Q^*. The second method is to remember that Q^* is stationary. It therefore checks $Q^* = Q^* P$. Such a system has an infinite number of solutions, by adding the constraint that $\sum_i q_i^* = 1$, we obtain a unique solution.

Theorem 2.4. *If Q^* exists then it is solution of* $\begin{cases} Q^* & = Q^* P \\ \sum_i q_i^* & = 1 \end{cases}$