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The Finite State Markov Chain, Its Transition Matrix and Stationary Distribution

1. The Stochastic Process

A stochastic process can be defined as a collection or a set of infinite random variables ordered by an index variable such as time. A stochastic process can also be interpreted as a random element in a functional space. In written forms, it is just

$$\{X_0, X_1, X_2, \ldots\ldots\}$$

Stochastic processes are seldom i.i.d in reality. Temporal dependencies are quite common. Among all such possible dependencies, the simplest one is called the Markov property.

2. The Markov Property

The Markov property is a property that all Markov processes possess. The Markov property can be described as:

$$P(X_{t+1} = x_{t+1} | X_t = x_t, X_{t-1} = x_{t-1}, \ldots, X_0 = x_0) = P(X_{t+1} = x_{t+1} | X_t = x_t)$$

In other words, the future value of X_{t+1} depends only on the present value of X_t or the future is independent of the past given present. Because of this, we can define a probability of transition between two states.

3. The Finite State Markov Process

A finite Markov process is a Markov process which only involves a finite number of states. For an N state finite Markov process $\{X_0, X_1, \ldots, X_{N-1}\}$, there are only N^2 possible transitions and the transition probability can be described by an $N \times N$ matrix P called transition matrix. A Markov process is usually called a Markov Chain. Markov processes are used to model a variety of decision processes in areas such as biology, weather, finance, manufacturing, business, and games etc.

4. The Transition Matrix of a Finite State Markov Chain

The transition matrix P of a finite Markov Chain completely describes the dynamics of the chain. The (i, j)th element P_{ij} of the matrix represents the transition probability from the current state i to the next state j. Therefore, the matrix contains elements only in the range [0,1] and the sum of each row of the matrix is always 1.

$$\sum_{j=0}^{N-1} P_{ij} = 1\,, \quad 0 \leq P_{ij} \leq 1, \quad i, j \in \{0,1, \dots, N-1\}$$

Transition matrix is also known as a stochastic matrix. In our case the transition matrix of the Markov chain is a right stochastic matrix which means it is a real square matrix, with each row summing up to 1.

Let $\pi(t)$ denote any probability distribution of the states of the chain at time t, then based on the definition of the transition matrix the probability distribution of the states at time $t + 1$ is given by

$$\pi(t + 1) = \pi(t)P$$

5. The Basic Theory of Markov Chain

Start with any probability distribution $\pi(0)$ of the states, apply the transition matrix repeatedly, that is simulating an infinitely long chain, what end distribution of the states can we get? That is what will $\lim_{n\to\infty} \pi(0)P^n$ be? To answer this question, we must delve into some basic theory of the Markov chain.

We start with the concept of *communication*. We say state j is *reachable* from state i if $Pr(X_n = j|X_0 = i) > 0$ for some $n \geq 0$. If state j is reachable from i and vice versa, then we call states i and j ***communicate***. Denoted by $i \leftrightarrow j$. Apparently,

1. All states communicate with themselves: $P_{ii}^0 = 1 > 0$
2. Symmetry: If $i \leftrightarrow j$, then $j \leftrightarrow i$
3. Transitivity: If $i \leftrightarrow k$ and $k \leftrightarrow j$, then $i \leftrightarrow j$

This shows communication is an equivalence relationship.

For each Markov chain, there exists a unique decomposition of the state space S (can be infinite) into a sequence of disjoint subset $C_1, C_2, \cdots$

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$$S = \bigcup_{i=1}^{\infty} C_i$$

in which each subset has the property that all states within it *communicate*. Each such subset is called a *communication class* of the Markov chain. This property basically says that every Markov chain can be decomposed into a set of independent and disjoint sub-Markov chains each with one communication class. If a Markov chain contains only one such communication class, then it is called an ***irreducible*** Markov chain and all states in it communicate. So, *every Markov chain is composed of one or more irreducible Markov chains*. We only need to study the irreducible Markov chain and apply the same theory to other irreducible chains if they exist.

Let τ_{ii} denote the return time to state i given $X_0 = i$: $\tau_{ii} \triangleq min\{n \geq 1: X_n = i | X_0 = i\}$. So, a return occurs if and only if $\tau_{ii} < \infty$. Define $f_i \triangleq Pr(\tau_{ii} < \infty)$ which is the probability of ever returning to state i given that it starts in state i. A state i is called ***recurrent*** if $f_i = 1$; ***transient*** if $f_i < 1$. By the Markov property, once the chain revisits state i, the future is independent of the past, and it is as if the chain is starting all over again in state i for the first time. Each time state i is visited, it will be revisited with the same probability f_i independent of the past. If $f_i = 1$ then the chain will return to state i repeatedly, an infinite number of times (recurrent). If state i is transient ($f_i < 1$), then it will only be visited a finite (random) number of times (after which only the remaining states $j \neq i$ can be visited by the chain). Counting through the time, the total number of visits to state i, given that $X_0 = i$, is given by an infinite sequence of indicator RVs:

$$N_i = \sum_{n=0}^{\infty} I\{X_n = i | X_0 = i\}$$

which has a geometric probability distribution,

$$Pr(N_i = n) = f_i^{n-1}(1 - f_i),\ \ n \geq 1$$

Note, the definitive initial visit $X_0 = i$ is counted as the first visit.
The expected number of total visits can be calculated as follows:

$$E(N_i) = \sum_{n=1}^{\infty} nPr(N_i = n) = \sum_{n=1}^{\infty} nf_i^{n-1}(1 - f_i) = \sum_{n=1}^{\infty} nf_i^n \frac{(1 - f_i)}{f_i}$$

Let $x = \sum_{n=1}^{\infty} nf_i^n$, then

$$x = f_i + f_i \sum_{n=1}^{\infty} (n+1) f_i^n = f_i + f_i \left(\sum_{n=1}^{\infty} nf_i^n + \sum_{n=1}^{\infty} f_i^n \right) = f_i + f_i \left(x + \sum_{n=1}^{\infty} f_i^n \right)$$

$\sum_{n=1}^{\infty} f_i^n$ is an infinite sum of a geometric series which equals $f_i/(1 - f_i)$. So

$$(1 - f_i)x = f_i + f_i^2/(1 - f_i) = f_i/(1 - f_i)$$

or $x = f_i/(1-f_i)^2$. Put this back we have

$$E(N_i) = \frac{1}{1-f_i}$$

From this we can conclude that a state i is recurrent ($f_i = 1$) if and only if $E(N_i) = \infty$, or a state i is transient ($f_i < 1$) if and only if $E(N_i) < \infty$. Taking the expectation on both sides of $N_i = \sum_{n=0}^{\infty} I\{X_n = i | X_0 = i\}$ we have

$$E(N_i) = \sum_{n=0}^{\infty} E[I\{X_n = i | X_0 = i\}] = \sum_{n=0}^{\infty} Pr(X_n = i | X_0 = i) = \sum_{n=0}^{\infty} P_{ii}^n$$

So, a state i is recurrent if and only if $\sum_{n=0}^{\infty} P_{ii}^n = \infty$, transient otherwise.

For any communication class C, all states in C are either recurrent or all states in C are transient. Thus, if $i \leftrightarrow j$ and i is recurrent, then so is j. Equivalently if $i \leftrightarrow j$ and i is transient, then so is j. For an irreducible Markov chain, either all states are recurrent, or all states are transient. This is because, suppose $i \neq j$ communicate, choose an appropriate n so that $p = P_{ij}^n > 0$. Now if i is recurrent, then so must be j because every time i is visited there will be the same positive probability $p = P_{ij}^n > 0$ that j will be visited n steps later. But i being recurrent means it will be visited repeatedly, an infinite number of times, so eventually there will be a success of revisiting j repeatedly, meaning j is also recurrent. For an irreducible Markov chain, if all states are recurrent, then we say that the Markov chain is recurrent; transient otherwise. Clearly if the state space is finite for a given Markov chain, then not all the states can be transient, for otherwise after a finite number of steps (time) the chain would leave every state and never return; so where would it go? So, *a Markov chain on a finite state space must contain at least one irreducible recurrent class there all states are recurrent*.

A recurrent state j is called ***positive recurrent*** if the expected amount of time to return to state j given that the chain started in state j has finite first moment: $E(\tau_{jj}) < \infty$. A recurrent state j for which $E(\tau_{jj}) = \infty$ is called ***null recurrent***. So, only positive recurrent states have any practical meaning. Define more generally for $i \neq j$, $\tau_{ij} \triangleq min\{n \geq 1 : X_n = j | X_0 = i\}$, be the time to reaching state j given $X_0 = i$. Then we can say that if i and j communicate and if j is positive recurrent ($E(\tau_{jj}) < \infty$), then i is positive recurrent ($E(\tau_{ii}) < \infty$) and also $E(\tau_{ij}) < \infty$. That is, *all states in a communication class are all together positive recurrent, null recurrent or transient*. This is because given that j is positive recurrent, $E(\tau_{jj}) < \infty$. Choose the smallest $n \geq 1$ such that $P_{ji}^n > 0$. With $X_0 = j$, let $A = \{X_k \neq j, 1 \leq k \leq n, X_n = i\}$; then $Pr(A) > 0$, and we have

$$\infty > E(\tau_{jj}) = E[E(\tau_{jj}|A)] \geq E(\tau_{jj}|A)Pr(A) = [n + E(\tau_{ij})]Pr(A)$$

hence $E(\tau_{ij}) < \infty$, which of course implies $E(\tau_{ii}) < \infty$, because $E(\tau_{ii}) \le E(\tau_{ij}) + E(\tau_{ji}) < \infty$, so i is also positive recurrent.

Now we can define the meaning of a stationary distribution of a Markov chain. Let π_j denote the *long run proportion of time that the chain spends in state* j:

$$\pi_j \triangleq \lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} I\{X_m = j | X_0 = i\} \qquad \forall i \in S \tag{1}$$

Taking expected values, $E(I\{X_m = j|X_0 = i\}) = Pr(X_m = j|X_0 = i) = P_{ij}^m$, we see that if π_j exists then it can be computed by

$$E(\pi_j) = \pi_j = \lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} P_{ij}^m \qquad \forall i \in S \tag{2}$$

If for each $j \in S$, π_j exists as defined in (1) and is independent of the initial state i and $\sum_{j\in S} \pi_j = 1$, then the probability distribution (a row vector) $\pi = (\pi_0, \pi_1, \dots)$ on the state space S is called the limiting or *stationary* or steady-state distribution of the Markov chain.
Recalling that P_{ij}^m is precisely the $(ij)^{th}$ component of matrix P^m, (2) can be written in matrix form as

$$\lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} P^m = \begin{pmatrix} \pi \\ \pi \\ \vdots \end{pmatrix} = \begin{pmatrix} \pi_0 & \pi_1 & \cdots \\ \pi_0 & \pi_1 & \cdots \\ & \vdots & \end{pmatrix}$$

That is, when we average the m-step transition matrices, each row converges to the vector of stationary probabilities $\pi = (\pi_0, \pi_1, \dots)$. The ith row refers to the initial condition $X_0 = i$ in (2) and for each such fixed row i, the jth element of the averages converges to π_j.
If $\{X_n\}$ is a positive recurrent Markov chain, then a unique stationary distribution π exists and is given by

$$\pi_j = \frac{1}{E(\tau_{jj})} > 0 \qquad \forall j \in S$$

This is because on average the chain visits state j once every $E(\tau_{jj})$ amount of time, thus $\pi_j = 1/E(\tau_{jj})$. This establishes a direct relationship between the π_j and $E(\tau_{jj})$ which is very intuitive. For transient or null recurrent states, $E(\tau_{jj}) = \infty$, so $\pi_j = 0$.
Theorem: Suppose $\{X_n\}$ is an irreducible Markov chain with transition matrix P. Then $\{X_n\}$ is positive recurrent if and only if there exists a non-negative, summing to 1 solution, $\pi =$

$(\pi_0, \pi_1, \ldots)$, to the set of linear equations $\pi = \pi P$, in which case π is precisely the unique stationary distribution for the Markov chain.

Based on this, we can algebraically solve for the stationary distribution π for a finite (N) state Markov chain by the following overdetermined system of linear equations, $N + 1$ equations with N unknowns:

$$\begin{cases} (I_N - P^T)\pi^T = \mathbf{0}_N \\ e^T\pi^T = 1 \end{cases}$$

where e is an N-dimensional column vector with unit elements. This system of equations can be solved with the reduced form of QR decomposition.

In summary, every irreducible finite state Markov chain is positive recurrent and thus has a stationary distribution determined by the above equations. The equation $\pi = \pi P$ apparently means the state distribution does not change under any numbers of transition, therefore representing a stationarity, or does not change with time. If a Markov chain starts with the stationary distribution, then the whole Markov chain becomes a stationary random process.

Let

$$M \triangleq \lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} P^m = \begin{pmatrix} \pi \\ \pi \\ \vdots \end{pmatrix}$$

be the stationary transition matrix whose rows are the same stationary distribution π.

Apparently for any state distribution ν we have $\nu M = \pi$. However, if $X_0 \sim \nu$, then $X_1 \sim \nu P$, $X_2 \sim \nu P^2$, …, $X_n \sim \nu P^n$, $n \geq 1$. This indicates that we also require that $\lim_{n\to\infty} P^n = M$. However, it is easily seen that in general the stronger convergence $\lim_{n\to\infty} P^n = M$ will not hold. For example, with $S = \{0,1\}$ and $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ being an antidiagonal identity matrix, then $P^{2n} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $P^{2n+1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. So, it oscillates even though the average converges to $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$.

For a state $j \in S$, consider the set $Q = \{n \geq 1: P_{jj}^n > 0\}$. If there exist an integer $d \geq 2$ such that $Q = \{kd: k \geq 1\}$, then state j is said to be ***periodic*** of period d. This implies that $P_{jj}^n = 0$ whenever n is not a multiple of d. If no such d exists, then the state j is said to be ***aperiodic***. It can be shown that periodicity is a class property: all states in a communication class are either aperiodic, or all are periodic with the same period d. Thus, an irreducible Markov chain is either periodic or aperiodic.

A positive recurrent Markov chain converges to M via the convergence $\lim_{n\to\infty} P^n = M$ if and only if the chain is aperiodic. Historically, a positive recurrent and aperiodic Markov chain is sometimes called an *ergodic* chain. However, the exact meaning of ergodicity has nothing to do with aperiodicity. Therefore, the historical use of ergodic in the context of aperiodic Markov chains is misleading and unfortunate.

6. Finite State Markov Chain in the Context of VAE-SOM

When a finite state Markov chain is used in the context of a VAE-SOM architecture to model reduced and encoded hidden states transitions, an obvious problem is that the state space S may not be irreducible! For example, for 2D presentation reasons of the SOM state transitions, the number of states will be $|S| = W * H$, where $W > 1,\ H > 1$ represents the width and height of the SOM map. Therefore $|S|$ can never match a prime number of actual states. Therefore, it is fundamental that the designed solution can assist to find out the actual effective number of states hidden in the data.
In addition, a mechanism should also be provided to check if the chain is periodic or not.

7. The Algorithm, An Empirical Approach

Since there is no predetermined theoretical model for the dynamic system at hand, we take an empirical approach to handle the state transition problem, meaning regardless of any given initial conditions, the result will converge to the true state of the Markov chain as more data is provided and processed. For this purpose, we, by default, construct the Markov chain object with the number of possible states $N_0 \geq N$ (N being the unknown number of actual positive recurrent states of the Markov chain), the initial state update count matrix $U = \mathbf{0}_{N_0 \times N_0}$, the actual state count vector $AC = \mathbf{0}_{N_0}$, and empty state history. Then via a method call update_transition(i, j), representing a $i \to j$ state transition, we increment (+1) the actual count AC_i for the state i and the U_{ij} element of U. The states are cached in the internal state history. At any time t into the simulation, the Markov chain object can be queried to return a true transition matrix P ($L \times L$, with $L \leq N$ being the number of states seen so far) or a full transition matrix F ($N_0 \times N_0$) which includes all the possible states together with the internal U matrix, AC vector and state history. The returned U matrix, AC vector and state history are used to initialize continued simulation sessions as the corresponding parameters of Markov chain object constructor. The actual transition matrix P ($L \times L$) is the one that should be used in any calculations.

Since we do not know in advance how many communication classes exist, we can, by the above-mentioned theory, assume without loss of generality, that there is one positive recurrent class and one transient or null recurrent class. We therefore must prune some short-lived transient states after sufficient amount of simulation by deleting them from the state history and properly update the U matrix and AC vector. This action is totally under user's discretion. This way, we can dynamically identify the actual irreducible and recurrent states in the finite positive recurrent communication class of the Markov chain.

The full transition matrix F is an affine combination of the identity matrix I ($N_0 \times N_0$) and the actual state update count matrix U ($N_0 \times N_0$) by the following formulae

$$F_{i*}(t) = \frac{1}{1+AC_i(t)}\left[I_{i*} + U_{i*}(t)\right] \quad \forall i \in \{0,1,\ldots,N_0-1\}$$

where $F_{i*}(t)$ is the ith row of F at time t, I_{i*} is the ith row of I, and $U_{i*}(t)$ is the ith row of U at time t. $AC_i(t)$ is the actual state count of state i at time t. The actual transition matrix P is then a proper $L \times L$ slice of F corresponding to all the states whose AC count is larger than zero. As more data come in and the chain progresses or after some persist/continue cycles with some proper pruning, eventually $L \to N$ and $P \to P^{true}$.

For the actual transition matrix P, the stationary state distribution associated with it is algebraically provided via the reduced QR decomposition solver. We also provide a brute-force stationary distribution calculator for P by taking P to the mth power where m is a positive integer argument. By comparing the results of this brute force calculated stationary distributions of different ms with the algebraically calculated one, one can detect whether the chain is periodic or not and even the actual period of the chain.

8. Code and Test Results

The code and test results can be found in the provided git-repo.

Reference : Karl Sigman, 2009 : "Recurrence and Stationary distributions for a Markov Chain", url : http://www.columbia.edu/~ks20/stochastic-I/stochastic-I-MCII.pdf