Randomness and Computation

or, "Randomized Algorithms"

Mary Cryan

School of Informatics
University of Edinburgh

Markov processes

- A *Markov process* is a r.v $\mathbf{X} = \{X(t) : t \in T\}$, usually $T = \mathbb{N}^0$.
- $X(t)$ (sometimes written as X_t) is the state of the process at time $t \in T$, this is an element of some state set Ω, usually a discrete finite set, sometimes countably infinite.
- A Markov process with the *memoryless property* is one where X_{t+1} will depends on the previous state X_t, but on none of the previous states.

Markov chains

Definition (Definition 7.1)

A discrete-time stochastic process on the state space Ω is said to be a *Markov chain* if

$$\Pr[X_t = a_t \mid X_{t-1} = a_{t-1}, \ldots, X_0 = a_0] = \Pr[X_t = a_t \mid X_{t-1} = a_{t-1}].$$

We will often denote the Markov chain by the name M, and write $M[a_{t-1}, a_t]$ to denote the probability $\Pr[X_t = a_t \mid X_{t-1} = a_{t-1}]$.

Markov chains

We can think about the *Markov chain M* in terms of a matrix of dimensions $|\Omega| \times |\Omega|$ (if Ω is finite) or of infinite dimension if Ω is countably infinite.

$$\begin{bmatrix} M[a_1,a_1] & M[a_1,a_2] & \ldots & M[a_1,a_j] & \ldots \\ M[a_2,a_1] & M[a_2,a_2] & \ldots & M[a_2,a_j] & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ M[a_j,a_1] & M[a_j,a_2] & \ldots & M[a_j,a_j] & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

This is often called the *transition matrix* of the Markov chain.

Transition matrix

This representation assumes that the *states* of the Markov chain have been put in 1-1 correspondance with $\mathbb{N}$. This is certainly possible (as we assume Ω is countably infinite at worst) but it's not *always* the case that this ordering is particularly *natural*. In many situations (especially when Ω is finite but exponentially sized), we'll avoid writing down the *transition matrix* at all - as an example, see the description of the contingency tables 2×2 chain later.

Note that for every $a \in \Omega$, we have $\sum_{b \in \Omega} M[a, b] = 1$ (a's row sums to 1).

Iterations of the Markov chain

Suppose we start our Markov process with the initial state $X(0)$ being some fixed $a \in \Omega$.

- The “next state" $X(1)$ is distributed according to a's row of the transition matrix M (with probability $M[a, b]$ of $X(1)$ becoming b).
- If we define $\bar{p}(0)$ to be the row vector with $\bar{p}_a(0) = 1$ and all other entries 0, then we can define the probability distribution $\bar{p}(1)$ by

  $$\bar{p}(1) \;=\; \bar{p}(0) \cdot M,$$

  and the probability that $X(1)$ is b at the next step is $p_b(1)$ (which equals $M[a, b]$), for every $b \in \Omega$.
- The “next state" $X(1)$ is a *random variable*, and its distribution is the vector $\bar{p}(1)$ above (with values summing to 1).

Iterations of the Markov chain

- If we then carry out a second step of the Markov chain, the random variable $X(2)$ will then be distributed according to $\bar{p}(2)$, where

  $$\bar{p}(2) \;=\; \bar{p}(1) \cdot M \;=\; \bar{p}(0) \cdot M \cdot M \;=\; \bar{p}(0) \cdot M^2.$$

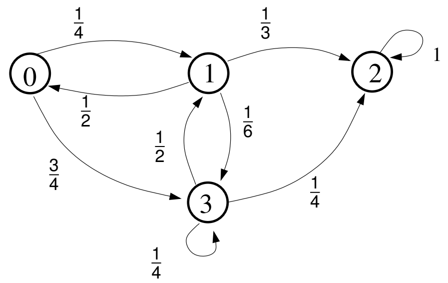
- And so on . . .
  After t steps of the Markov chain M, the random variable $X(t)$ will then be distributed according to $\bar{p}(t)$, where

  $$\bar{p}(t) \;=\; \bar{p}(0) \cdot M^t.$$

Example Markov chain

Let's look at a concrete example of a Markov chain on the *state set* $\Omega = \{0, 1, 2, 3\}$, with probabilities given by the following *transition matrix*:

$$M \;=\; \begin{bmatrix} 0 & \frac{1}{4} & 0 & \frac{3}{4} \\ \frac{1}{2} & 0 & \frac{1}{3} & \frac{1}{6} \\ 0 & 0 & 1 & 0 \\ 0 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}$$



Example Markov chain

- Notice that every row of the matrix sums to 1, as required.
- Not the case for the columns (and doesn't have to be).
- In the graph representation, the "states" are vertices and the "transitions" of the chain are directed edges (labelled with the appropriate probability).
- Consider running this Markov chain from $3 \in \Omega$. Then we set $\bar{p}(0) = (\begin{array}{cccc} 0 & 0 & 0 & 1 \end{array})$.
- Evaluating $\bar{p}(1) = \bar{p}(0) \cdot M$, we note it will be $(\begin{array}{cccc} 0 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \end{array})$.
- Evaluating $\bar{p}(2) = \bar{p}(0) \cdot M^2$, we can compute it as $(\begin{array}{cccc} \frac{1}{4} & \frac{1}{8} & \frac{23}{48} & \frac{7}{48} \end{array})$.
- And so on ...
- We would expect these $\bar{p}(t)$ values to be different if we had started with a different initial state.

  However, these alternate t-step distributions can be easily calculated/compared, if we have pre-computed M^t.

Markov chains for Randomized Algorithms

The graph (and transition matrix) on slide is just a "toy" example. In our world, we will want to exploit Markov chains to obtain randomized algorithms.

- In the 2SAT example of Section 7.1, [MU], we are concerned with *assignments* (functions) A of boolean values to the n logical variables (and which will achieve the max number of satisfied clauses).
- The transitions of the modified Markov chain for 2SAT (Y) are designed to model transitions back and forth between "better" and "worse" assignments.
- However, the *states* of the Markov chain (Y) are the natural numbers $0, 1, \ldots, n$, with n being the number of variables. This is a fairly small state space.
- Next Tuesday we will prove that for a 2SAT instance which *does have* a satisfying assignment, the *expected number of steps* before the Markov chain finds one is at most n^2. This is expected "hitting time".

Markov chains for Sampling and Counting

Another application of Markov chains arises when we want to *randomly sample* (or *approximately count*) the number of combinatorial structures satisfying some constraint.

- In these cases the elements of the state space Ω are individual combinatorial structures themselves, and this space is often very large (potentially exponential in the size of the input).
- One example we can imagine is the set of *contingency tables* $\Sigma_{r,c}$ for given row sums $r = (r_1, \ldots, r_m)$ and column sums $c = (c_1, \ldots, c_n)$.
- With large state spaces of combinatorial elements, we don't explicitly "write down" the transition matrix of a Markov chain on the space - we just give (randomized) rules explaining how we move (randomly) from one element to another.
- We would then want to prove that the "2×2" Markov chain converges to the uniform distribution on $\Omega = \Sigma_{r,c}$.

Markov chains for Sampling Contingency tables

We are given row sums $r = (r_1, \ldots, r_m)$ and $c = (c_1, \ldots, c_n)$. A *contingency table* is a table $X = [X_{i,j}]$ of non-negative integers of dimensions $m \times n$ that satisfies those row/column sums.

$X_{1,1}$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$X_{1,n}$	r_1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\ldots$	$\ldots$	$\mathbf{X}_{i,j}$	$\ldots$	$\mathbf{X}_{i,j'}$	$\ldots$	$\ldots$	r_i
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\ldots$	$\ldots$	$\mathbf{X}_{i',j}$	$\ldots$	$\mathbf{X}_{i',j'}$	$\ldots$	$\ldots$	$r_{i'}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$X_{m,1}$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$X_{m,n}$	r_m
c_1	$\ldots$	c_j	$\ldots$	$c_{j'}$	$\ldots$	c_n	

- The "2×2" Markov chain selects random rows $i, i' \in [m], i \neq i'$ and random columns $j, j' \in [n], j \neq j'$ at each step, calculates the mini-sums for the 2×2 table ... then chooses a uniform random *replacement* that "fits" these mini-sums.

Irreducibility, recurrence, aperiodicity

To analyse the behaviour (both temporary and long-term) of a Markov chain M on the state space Ω, we often work from the *graph representation* of Ms transitions.

Definition (Definition 7.2)

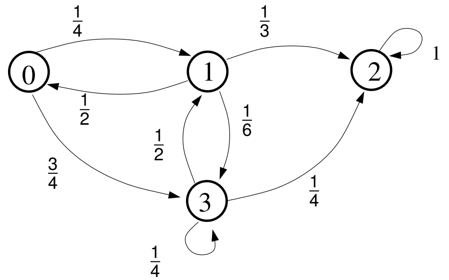
For $a, b \in \Omega$, we say that state b is accessible from state a if there is some $n \in \mathbb{N}$ such that $M^n[a, b] > 0$. If a, b are both accessible from one another, we say that they *communicate*, and write $a \leftrightarrow b$.

Definition (Definition 7.3)

A Markov chain M on the finite state space Ω is said to be *irreducible* if all states of Ω belong to the same communicating class.
Or *equivalently*, if we can show that for every $X, Y \in \Omega$, there is some path $Z^0 = X, Z^1, \ldots, Z^\ell = Y$ of states from Ω connecting X and Y, such that $M[Z^j, Z^{j+1}] > 0$ for every $0 \le j \le \ell - 1$.

Irreducibility, recurrence, aperiodicity

Let's consider our example chain:



- $\{0, 1, 3\}$ forms a maximal communicating class in the graph.
- $\{2\}$ is an isolated communicating class - we can reach 2 from $\{0, 1, 3\}$, but 2 has no outgoing transitions.
- Our example is *not* irreducible.

Irreducibility, recurrence, aperiodicity

We define the concept of "recurrence" in terms of a parameter $r^t_{Z,W}$, where

$$r^t_{Z,W} =_{def} \Pr[X(t) = W \text{ and for all } 1 \le s \le t-1,\ X(s) \ne W \mid X(0) = Z].$$

Definition (Definition 7.4)

If M is a Markov chain and $Z \in \Omega$ a state of that chain, we say Z is *recurrent* if $\sum_{t=0}^{\infty} r^t_{Z,Z} = 1$, and it is *transient* if $\sum_{t=0}^{\infty} r^t_{Z,Z} < 1$.
A Markov chain is recurrent if every state is recurrent.

In our example, the only recurrent state is 2.

Irreducibility, recurrence, aperiodicity

The expected "time to travel" will be important for some analyses. For a pair of given states $Z, W \in \Omega$, we define this value as

$$h_{Z,W} =_{def} \sum_{t=0}^{\infty} t \cdot r^t_{Z,W}.$$

Definition (Definition 7.5)

A *recurrent state* Z of a Markov chain M is *positive recurrent* if $h_{Z,Z} < \infty$. Otherwise, it is *null recurrent*.

Lemma (Lemma 7.5)

In a Markov chain M on a finite *state space* Ω*,*

1. *At least one state is recurrent;*
2. *All recurrent states are positive recurrent.*

Irreducibility, recurrence, aperiodicity

Definition (Definition 7.6)

A state Z of a Markov chain M is *periodic* if there exists an integer $k \geq 2$ such that $\Pr[X(t+s) = Z \mid X(t) = Z]$ is non-zero *if and only if s* is divisible by k.
A discrete Markov chain is *periodic* is any of its states are periodic. Otherwise (all states aperiodic), we say that M is *aperiodic*.

Definition (Definition 7.7)

An aperiodic, positive recurrent state $Z \in \Omega$ of a Markov chain M is said to be an *ergodic* state.
The Markov chain is said to be *ergodic* if *all* its states are ergodic.

Corollary (Corollary 7.6)

Any finite, irreducible and aperiodic Markov chain is an ergodic chain.

Ergodic Markov chains

Corollary (Corollary 7.6)

Any finite, irreducible and aperiodic Markov chain is an ergodic chain.

Proof.

By Lemma 7.5 every chain with a finite state space has *at least one* recurrent state.
If the chain is irreducible, then all states can be reached from one another (with positive probability), so *all states are hence recurrent*.
By Lemma 7.5, this means all states are positive recurrent.
Hence by Definition 7.7 (we have positive recurrence, irreducibility and aperiodicity) the chain is ergodic. □

Take-away: For Markov chains over a *finite* state space, we only need to check *aperiodicity* and *irreducibility* (for all pairs of states) to show *ergodicity*.

Ergodic Markov chains

Why do we care about states/Markov chains being ergodic?

Because an ergodic Markov chain has a *unique stationary distribution*.

Definition (Definition 7.8)

A *stationary distribution* of a Markov chain M on Ω is a probability distribution $\bar{\pi}$ on Ω such that

$$\bar{\pi} = \bar{\pi} \cdot M.$$

Stationary distributions are essentially “settling-down" distributions (in the limit). The “settling-down" is to a *distribution*, not a particular state.

Ergodic Markov chains

Theorem (Theorem 7.7)

Any finite, irreducible and aperiodic Markov chain has the following properties:

1. *The chain has a* unique *stationary distribution* $\bar{\pi} = (\pi_1, \ldots, \pi_{|\Omega|})$.
2. *For all* $X, Y \in \Omega$, $\lim_{t\to\infty} M^t[X, Y]$ *exists and is* independent of X.
3. $\pi_Y = \lim_{t\to\infty} M^t[X, Y] = \frac{1}{h_{Y,Y}}$.

We are not going to prove Theorem 7.7 in this course.
We will later see some ways of *bounding the number of steps needed* for the chain to approach its stationary distribution.

Reading and Doing

Reading

- You will want to read Sections 7.1, 7.2, and 7.3 from the book.

  I have used M (name of the Markov chain) to refer to the transition matrix, as opposed to the book's P.

Doing

- Consider an example of contingency tables where we have $r = (2, 2, 4), c = (2, 3, 3)$. Suppose that we take the following table as our starting state X:

$$X = \begin{array}{ccc||c} \hline 2 & 0 & 0 & \mathbf{2} \\ \hline 0 & 2 & 0 & \mathbf{2} \\ \hline 0 & 1 & 3 & \mathbf{4} \\ \hline\hline \mathbf{2} & \mathbf{3} & \mathbf{3} & \end{array}$$

  Work out the subset of contingency tables which can be reached from X in *one transition* of the 2×2 Markov chain. Also work out the probability of each such transition.

- Tutorial sheet for week 11.