

## Markov Chains

Markov chains:

- Powerful tool for sampling from complicated distributions
- rely only on local moves to explore state space.
- Many use Markov chains to *model* events that *arise* in nature.
- We *create* Markov chains to *explore* and *sample from* problems.

2SAT:

- Fix some assignment  $A$
- let  $f(k)$  be expected time to get all  $n$  variables to match  $A$  if  $n$  currently match.
- Then  $f(n) = 0$ ,  $f(0) = 1 + f(1)$ , and  $f(k) = 1 + \frac{1}{2}(f(k+1) + f(k-1))$ .
- Rewrite:  $f(0) - f(1) = 1$  and  $f(k) - f(k+1) = 2 + f(k-1) - f(k)$
- So  $f(k) - f(k+1) = 2k + 1$
- deduce  $f(0) = 1 + 3 + \dots + (2n-1) = n^2$
- so, find with probability  $1/2$  in  $2n^2$  time.
- With high probability, find in  $O(n^2 \log n)$  time.

More general formulation: *Markov chain*

- State space  $S$
- markov chain begins in a *start state*  $X_0$ , moves from state to state, so output of chain is a sequence of states  $X_0, X_1, \dots = \{X_t\}_{t=0}^{\infty}$
- movement controlled by matrix of *transition probabilities*  $p_{ij}$  = probability next state will be  $j$  given current is  $i$ .
- thus,  $\sum_j p_{ij} = 1$  for every  $i \in S$
- implicit in definition is *memorylessness property*:

$$\Pr[X_{t+1} = j \mid X_0 = i_0, X_1 = i_1, \dots, X_t = i] = \Pr[X_{t+1} = j \mid X_t = i] = p_{ij}.$$

- Initial state  $X_0$  can come from any probability distribution, or might be fixed (trivial prob. dist.)
- Dist for  $X_0$  leads to dist over sequences  $\{X_t\}$
- Suppose  $X_t$  has distribution  $q$  (vector,  $q_i$  is prob. of state  $i$ ). Then  $X_{t+1}$  has dist  $qP$ . Why?

- Observe  $\Pr[X_{t+r} = j \mid X_t = i] = P_{ij}^r$

Graph of MC:

- Vertex for every state
- Edge  $(i, j)$  if  $p_{ij} > 0$
- Edge weight  $p_{ij}$
- weighted outdegree 1
- Possible state sequences are paths through the graph

Stationary distribution:

- a  $\pi$  such that  $\pi P = \pi$
- left eigenvector, eigenvalue 1
- steady state behavior of chain: if in stationary, stay there.
- note stationary distribution is a sample from state space, so if can get right stationary distribution, can sample
- lots of chains have them.
- to say which, need definitions.

Things to rule out:

- infinite directed line (no stationary)
- 2-cycle (no stationary)
- disconnected graph (multiple)

Irreducibility

- any state can reach any other state
- i.e. path between any two states
- i.e. single strong component in graph

Persistence/Transience:

- $r_{ij}^{(t)}$  is probability first hit state  $j$  at  $t$ , given start state  $i$ .
- $f_{ij}$  is probability *eventually* reach  $j$  from  $i$ , so  $\sum r_{ij}^{(t)}$
- expected time to reach is *hitting time*  $h_{ij} = \sum tr_{ij}^{(t)}$

- If  $f_{ij} < 1$  then  $h_{ij} = \infty$  since might never reach. Converse not always true.
- If  $f_{ii} < 1$ , state is *transient*. Else *persistent*. If  $h_{ii} = \infty$ , *null persistent*.

Persistence in finite graphs:

- graph has strong components
- *final* strong component has no outgoing edges
- Nonfinal components:
  - once leave nonfinal component, cannot return
  - if nonfinal, nonzero probability of leaving in  $n$  steps.
  - so guaranteed to leave eventually
  - so, vertices in nonfinal components are transient
- Final components
  - if final, will stay in that component
  - If two vertices in same strong component, have path between them
  - so nonzero probability of reaching in (say)  $n$  steps.
  - so, vertices in final components are persistent
  - geometric distribution on time to reach, so expected time finite. Not null-persistent

Conclusion:

- In finite chain, no null-persistent states
- In finite irreducible chain, all states non-null persistent (no transient states)

Periodicity:

- Periodicity of a state is max  $T$  such that some state only has nonzero probability at times  $a + Ti$  for integer  $i$
- Chain *periodic* if some state has periodicity  $> 1$
- In graph, all cycles containing state have length multiple of  $T$
- Easy to eliminate: add self loops
- slows down chain, otherwise same

Ergodic:

- aperiodic and non-null persistent
- means might be in state at any time in (sufficiently far) future

Fundamental Theorem of Markov chains: Any irreducible, finite, aperiodic Markov chain satisfies:

- All states ergodic (reachable at any time in future)
- unique stationary distribution  $\pi$ , with all  $\pi_i > 0$
- $f_{ii} = 1$  and  $h_{ii} = 1/\pi_i$
- number of times visit  $i$  in  $t$  steps approaches  $t\pi_i$  in limit of  $t$ .

Justify all except uniqueness here.

Finite irreducible aperiodic implies ergodic (since finite irreducible implies non-null persistent)

Intuitions for quantities:

- $h_{ii}$  is expected return time
- So hit every  $1/h_{ii}$  steps on average
- So  $h_{ii} = 1/\pi_i$
- If in stationary dist,  $t\pi_i$  visits follows from linearity of expectation

## Random walks on undirected graphs:

- general Markov chains are directed graphs. But undirected have some very nice properties.
- take a connected, non-bipartite undirected graph on  $n$  vertices
- states are vertices.
- move to uniformly chosen neighbor.
- So  $p_{uv} = 1/d(u)$  for every neighbor  $v$
- stationary distribution:  $\pi_v = d(v)/2m$
- uniqueness says this is only one
- deduce  $h_{vv} = 2m/d(v)$

Definitions:

- Hitting time  $h_{uv}$  is expected time to reach  $u$  from  $v$
- commute time is  $h_{uv} + h_{vu}$
- $C_u(G)$  is expected time to visit all vertices of  $G$ , starting at  $u$
- *cover time* is  $\max_u C_u(G)$  (so in fact is max over any starting distribution).

- let's analyze max cover time

Examples:

- clique: commute time  $n$ , cover time  $\Theta(n \log n)$
- line: commute time between ends is  $\Theta(n^2)$
- lollipop:  $h_{uv} = \Theta(n^3)$  while  $h_{vu} = \Theta(n^2)$  (big difference!)
- also note: lollipop has edges added to line, but higher cover time: adding edges can increase cover time even though improves connectivity.

general graphs: adjacent vertices:

- lemma: for adjacent  $(u, v)$ ,  $h_{uv} + h_{vu} \leq 2m$
- proof: new markov chain on *edge traversed following vertex MC*
  - transition matrix is *doubly stochastic*: column sums are 1 (exactly  $d(v)$  edges can transit to edge  $(v, w)$ , each does so with probability  $1/d(v)$ )
  - In homework, show such matrices have *uniform* stationary distribution.
  - Deduce  $\pi_e = 1/2m$ . Thus  $h_{ee} = 2m$ .
- So consider suppose original chain on vertex  $v$ .
  - suppose arrived via  $(u, v)$
  - expected to traverse  $(u, v)$  again in  $2m$  steps
  - at this point will have commuted  $u$  to  $v$  and back.
  - so conditioning on arrival method, commute time  $2m$  (thanks to memorylessness)

General graph cover time:

- theorem: cover time  $O(mn)$
- proof: find a spanning tree
- consider a dfs of tree-crosses each edge once in each direction, gives order  $v_1, \dots, v_{2n-1}$
- time for the vertices to be visited in this order is upper bounded by commute time
- but vertices adjacent, so commute times  $O(m)$
- total time  $O(mn)$
- tight for lollipop, loose for line.

Tighter analysis:

- analogue with electrical networks

- Assume unit edge resistance
  - Kirchoff's law: current (rate of transitions) conservation
  - Ohm's law
  - Gives effective resistance  $R_{uv}$  between two vertices.
- Theorem:  $C_{uv} = 2mR_{uv}$
  - (tightens previous theorem, since  $R_{uv} \leq 1$ )
  - Proof:
    - Suppose put  $d(x)$  amperes into every  $x$ , remove  $2m$  from  $v$
    - $\phi_{uv}$  voltage at  $u$  with respect to  $v$
    - Ohm: Current from  $u$  to  $w$  is  $\phi_{uw} - \phi_{vw}$
    - Kirchoff:  $d(u) = \sum_{w \in N(u)} \text{currents} = \sum_{w \in N(u)} \phi_{uw} - \phi_{vw} = d(u)\phi_{uv} - \sum \phi_{vw}$
    - Also,  $h_{uv} = \sum (1/d(u))(1 + h_{vw})$
    - same soln to both linear equations, so  $\phi_{uv} = h_{uv}$
    - By same arg,  $h_{vu}$  is voltage at  $v$  wrt  $u$ , if insert  $2m$  at  $u$  and remove  $d(x)$  from every  $x$
    - add linear systems, find  $h_{uv} + h_{vu}$  is voltage difference when insert  $2m$  at  $u$  and remove at  $v$ .
    - now apply ohm.