## Discrete Time Markov Chains

• An extremely pervasive probability model

## Random Walks on Graphs

• One of the most important special cases of DTMC

## Why cover them in this course?

- DTMC is the first non-trivial probability model we discuss
- Lots of fundamental probabilistic reasoning
- Lots of applications in Computer Science

- A gambler has \$100, bets \$1 each game, wins with probability 1/2.
- He stops if he gets broke or wins \$1000
- Questions: what's the probability that he gets broke? On average how many games are played?



# Example 2: Slow Sort

- Given an array  $A = (a_1, \ldots, a_n)$  of numbers
- SLOW-SORT: as long as A is not sorted, swap two random elements
- Question: what's the running time?



n! orderings of  $a_1, \ldots, a_n$ 

## Shuffling a Deck of Cards

 $\bullet\,$  What's the number of shuffles until the ordering is "almost" uniform?

## Single Server Queue

- At each time slot, an Internet router's buffer gets an additional packet with probability p, or releases one packet with probability q, or remains the same with probability r.
- Starting from an empty buffer, what is the distribution of the number of packets after *n* slots?
- As  $n \to \infty$ , will the buffer be overflowed?
- As  $n \to \infty$ , what's the typical buffer size?

# Examples 5 & 6: 2-SAT and P2P Networks

2-SAT: find a satisfying assignment if there's any

- Assign  $x_i = \text{TRUE}/\text{FALSE}$  with probability 1/2
- If there's an unsatisfied clause, flip value of one of the two literals randomly
- If there is a satisfying assignment, how long does it take?

## Searching on P2P Networks

- The initial node sends k independent queries out
- Each query sent to a random neighbor
- Upon receiving a query, an intermediate node forwards it to its random neighbor
- Questions: how long does it take until all nodes receive one of the queries? What's the trade-off between k and this speed?

• Stochastic process: a collection of random variables (on some probability space) indexed by some set *T*:

 $\{X_t, t \in T\}$ 

When  $T \subseteq \mathbb{R}$ , think of T as set of points in time

- State space, denoted by I, is the set of all possible values of the  $X_t$
- When T is countable: discrete-time stochastic process
- When T is an interval of the real line: continuous-time stochastic process

# Examples of Stochastic Processes

Bernoulli process: a sequence  $\{X_0, X_1, X_2, ...\}$  of *independent* Bernoulli random variables with parameter p.

• In assignment 1, we have derived statistics on

 $S_n = X_1 + \dots + X_n$   $T_n = \text{number of slots from the } (n-1)\text{th } 1 \text{ to the } n\text{th } 1$  $Y_n = T_1 + \dots + T_n$ 

In practice, things are not that easy. We often see processes whose variables are correlated.

- Stock market and exchange rate fluctuations
- Signals (speech, audio and video)
- Daily temperatures
- Brownian motion or random walks
- etc.

# Discrete-Time Markov Chain

- A DTMC is a discrete-time stochastic process  $\{X_n\}_{n\geq 0}$
- State space I is countable (often labeled with a subset of  $\mathbb{N}$ )
- For all states i, j there is a given probability  $p_{ij}$  such that

$$P[X_{n+1} = j \mid X_n = i, X_{n-1} = i_{n-1}, \dots X_0 = i_0] = p_{ij},$$

for all  $i_0, \ldots, i_{n-1} \in I$  and all  $n \ge 0$ .

$$p_{ij} \geq 0, \quad \forall i, j \in I,$$
$$\sum_{j \in I} p_{ij} = 1, \quad \forall i \geq 0.$$

•  $\mathbf{P} = (p_{ij})$  is called the *transition probability matrix* of the chain

#### Given a DTMC **P** with state space $I, A \subset I$

- Starting from  $X_0 = i \notin A$ 
  - What's the probability A is ever "hit"?
  - What's the probability  $X_n \in A$  for a given n?
  - $\bullet\,$  What's the expected number of steps until A is hit
  - What's the probability we'll come back to i?
  - What's the expected number of steps until we come back?
  - What's the expected number of steps until all states are visited?
  - As n → ∞, what's the distribution of where we are? Does the "limit distribution" even exist? If it does, how fast is the convergence rate?
- Given an initial distribution  $\lambda$  of  $X_0,$  repeat the above questions
- And many more, depending on the application

- A measure on I is a vector  $\lambda$  where  $\lambda_i \ge 0$ , for all  $i \in I$ .
- A measure is a distribution if  $\sum_i \lambda_i = 1$ .
- For any event F, let

$$\Pr_i[F] = \Pr[F \mid X_0 = i]$$

• For any random variable Z, let

$$\mathsf{E}_i[Z] = \mathsf{E}[Z \mid X_0 = i]$$

• If we know  $\lambda$  is the distribution of  $X_0$ , then we also write

$$(X_n)_{n\geq 0} = \operatorname{Markov}(\mathbf{P}, \lambda).$$

# Multistep Transition Probabilities and Matrices

- Define the probability of going from i to j in n steps  $p_{ij}^{(n)} = \Pr_i[X_n = j]$
- And the *n*-step transition probability matrix  $\mathbf{P}^{(n)} = (p_{ij}^{(n)})$

# Chapman-Kolmogorov Equations $p_{ij}^{(m+n)} = \sum_{k \in I} p_{ik}^{(n)} p_{kj}^{(m)}, \quad \forall n, m \ge 0, i, j \in I.$

It follows that

$$\mathbf{P}^{(n)} = \mathbf{P}^n$$

## Corollary

If  $\lambda$  (a row vector) is the distribution of  $X_0$ , then  $\lambda \mathbf{P}^n$  is the distribution of  $X_n$ 

- j is reachable from i if  $p_{ij}^{(n)} > 0$  for some  $n \ge 0$ . We write  $i \rightsquigarrow j$ .
- *i* and *j* communicate if  $i \rightsquigarrow j$  and  $j \rightsquigarrow i$ . We write  $i \leftrightarrow j$ .
- Communication is an *equivalence relation*, partitioning *I* into *communication classes*
- Communication classes are *strongly connected components* of the directed graph corresponding to for **P**
- A chain is *irreducible* if there is only one class
- A *closed* class C is a class where  $i \in C$  and  $i \rightsquigarrow j$  imply  $j \in C$  (no escape!)
- A state i is absorbing if  $\{i\}$  is a closed class

# Illustration of Communication Classes



## • First passage time

$$T_i = \min\{n \ge 1 \mid X_n = i\} \quad (X_0 = i \text{ doesn't count!})$$

## Define

$$\begin{array}{lll} f_{ij}^{(n)} & = & {\rm Pr}_i[X_n = j \ \land \ X_s \neq j, \forall s = 1, ..., n-1] = {\rm Pr}_i[T_j = n] \\ \\ f_{ij} & = & \sum_{n=1}^{\infty} f_{ij}^{(n)} \end{array}$$

- Note that  $f_{ij} = \Pr_i[T_j < \infty]$
- State *i* is
  - recurrent (also called persistent) if  $f_{ii} = \Pr_i[T_i < \infty] = 1$
  - transient if  $f_{ii} = \mathsf{Pr}_i[T_i < \infty] < 1$

- Let  $V_i$  be the number of visits to i, namely  $V_i := \sum_{n=0}^{\infty} \mathbb{1}_{\{X_n = i\}}$ .

#### Theorem

Given a DTMC  $\mathbf{P}$  and a state i, the following are equivalent

i is recurrent

$$f_{ii} = \mathsf{Pr}_i[T_i < \infty] = 1$$

**3** 
$$\Pr_i[X_n = i \text{ for infinitely many } n] = 1$$

• 
$$\mathsf{E}_i[V_i] = \infty$$

$$\bigcirc \sum_{n\geq 0} p_{ii}^{(n)} = \infty$$

Given a DTMC  $\mathbf{P}$  and a state i, the following are equivalent

i is transient

$$f_{ii} = \mathsf{Pr}_i[T_i < \infty] < 1$$

**3** 
$$\Pr_i[X_n = i \text{ for infinitely many } n] = 0$$

• 
$$\mathsf{E}_i[V_i] < \infty$$

$$\mathbf{S} \, \sum_{n \ge 0} p_{ii}^{(n)} < \infty$$

To prove the last two theorems, we need the strong Markov property

• A r.v. T taking values in  $\mathbb{N}$  is called a stopping time of a DTMC  $(X_n)_{n\geq 0}$  if the event  $\{T=n\}$  can be determined by looking at  $X_0, \cdots, X_n$ 

(Need measure theory to be rigorous on this definition.)

- Examples:
  - First passage time  $T_i = \min\{n \ge 1 : X_n = i\}$  is a stopping time
  - Last exit time  $L_A = \max\{n : X_n \in A\}$  is not a stopping time

## Theorem (Strong Markov Property)

Suppose T is a stopping time of a DTMC  $(X_n)_{n\geq 0}$ . Then, conditioned on  $T < \infty$  and  $X_T = i$ , the sequence  $(X_{T+n})_{n\geq 0}$  behaves exactly like the Markov chain with initial state i.

## Proof.

By strong Markovian:

$$\mathsf{E}_{i}[V_{i}] = \sum_{n=1}^{\infty} n f_{ii}^{n-1} (1 - f_{ii}) = \frac{1}{1 - f_{ii}}.$$

On the other hand,

$$\mathsf{E}_{i}[V_{i}] = \mathsf{E}_{i}\left[\sum_{n=0}^{\infty} \mathbb{1}_{\{X_{n}=i\}}\right] = \sum_{n=0}^{\infty} \mathsf{E}_{i}[\mathbb{1}_{\{X_{n}=i\}}] = \sum_{n=0}^{\infty} p_{ii}^{(n)}.$$

Recurrence and transience are class properties, i.e. in a communication class C either all states are recurrent or all states are transient

Why is it true? Suppose i and j belong to the same class. If i is recurrent and j is transient, each time the process returns to i there's a positive chance of going to j. Thus, the process cannot avoid j forever.

- (i) Every recurrent class is closed
- (ii) Every finite, closed class is positive recurrent
- Why does (i) hold?
- If the class is not closed, there's an escape route, and thus the class cannot be recurrent.
- Why does (*ii*) hold?
- In a finite and closed class, it cannot be the case that every state is visited a finite number of times. So, the chain is recurrent.

# Infinite Closed Class Could be Transient or Recurrent

- Consider a random walk on  $\mathbb{Z}$ , where  $p_{i,i+1} = p$  and  $p_{i+1,i} = 1 p$ , for all  $i \in \mathbb{Z}$ , 0
- The chain is an infinite and closed class.
- For any state *i*, we have

$$p_{ii}^{(2n+1)} = 0$$
  
$$p_{ii}^{(2n)} = {\binom{2n}{n}} p^n (1-p)^n$$

Hence,

$$\sum_{n=0}^{\infty} p_{ii}^{(2n)} = \sum_{n=0}^{\infty} {\binom{2n}{n}} p^n (1-p)^n$$
$$\approx \sum_{n \ge n_0} \frac{1}{\sqrt{\pi n}} (4p(1-p))^n (1+o(1)).$$

which is  $\infty$  if p = 1/2 and finite if  $p \neq 1/2$ .

In an irreducible and recurrent chain,  $f_{ij} = 1$  for all i, j

Why is it true? If  $f_{ij} < 1$ , there's a non-zero chance of the chain starting from j, getting to i, and never come back to j. However, j is recurrent!

Consider a DTMC on state space  $\ensuremath{\mathbb{N}}$  where

• 
$$p_{i,i+1} = a_i, p_{i,i-1} = b_i, p_{ii} = c_i$$

- $a_i + b_i + c_i = 1$ ,  $\forall i \in \mathbb{N}$ , and implicitly  $b_0 = 0$
- $a_i, b_i > 0$  for all i, except for  $b_0$

## Question

When is this chain transient/recurrent?

To answer this question, we need some results about computing hitting probabilities

# Hitting Times and Hitting Probabilities

- Let  $\mathbf{P}$  be a DTMC on I. Let  $A \subseteq I$ .
- The hitting time  $H^A$

$$H^A := \min\{n \ge 0 : X_n \in A\}.$$

• The probability of hitting A starting from i

$$h_i^A := \mathsf{Pr}_i[H^A < \infty].$$

• If A is a closed class, the  $h_i^A$  are called the *absorption probabilities* • The *mean hitting time*  $\mu_i^A$  is defined by

$$\mu_i^A := \mathsf{E}_i[H^A] = \sum_{n < \infty} n \mathsf{Pr}[H^A = n] + \infty \mathsf{Pr}[H^A = \infty]$$

The vector  $(h^A_i:i\in I)$  is the minimal non-negative solution to the following system

$$\begin{cases} h_i^A = 1 & \text{for } i \in A \\ h_i^A = \sum_{j \in I} p_{ij} h_j^A & \text{for } i \notin A \end{cases}$$

## Back to the Birth-and-Death Chain

• Note that 
$$f_{00} = c_0 + a_0 h_1^{\{0\}} = 1 - a_0 (1 - h_1^{\{0\}})$$
  
The system: 
$$\begin{cases} h_0^{\{0\}} = 1\\ h_i^{\{0\}} = a_i h_{i+1}^{\{0\}} + c_i h_i^{\{0\}} + b_i h_{i-1}^{\{0\}} & \text{for } i \ge 1 \end{cases}$$

Define d<sub>n</sub> := b<sub>1...b<sub>n</sub>/a<sub>1...a<sub>n</sub></sub>, n ≥ 1, and d<sub>0</sub> = 1
When ∑<sub>n=0</sub><sup>∞</sup> d<sub>n</sub> = ∞, h<sub>i</sub><sup>{0}</sup> = 1, ∀i is the solution
When ∑<sub>n=0</sub><sup>∞</sup> d<sub>n</sub> < ∞, we have the following solution</li>
</sub>

$$\begin{cases} h_0^{\{0\}} = 1 \\ h_i^{\{0\}} = \frac{\sum_{j=i}^{\infty} d_j}{\sum_{j=0}^{\infty} d_j} < 1 \quad \text{for } i \ge 1 \end{cases}$$

Thus,

- the DTMC is recurrent  $(f_{00}=1)$  when  $\sum_{j=0}^{\infty} d_j = \infty$
- the DTMC is transient  $(f_{00} < 1)$  when  $\sum_{j=0}^{\infty} d_j < \infty$

- We often only need to look at closed classes (that's where the chain will eventually end up).
- We can then consider irreducible chains instead.
- Let  $\mathbf{P}$  be an irreducible chain.
  - If **P** is finite, then **P** is recurrent.
  - If  $\mathbf{P}$  is infinite, then  $\mathbf{P}$  could be either transient or recurrent.

• A distribution  $\lambda$  is a stationary (also equilibrium or invariant) distribution if  $\lambda^T \mathbf{P} = \lambda$ 

#### Theorem

(i) Let  $(X_n)_{n\geq 0} = \mathsf{Markov}(\mathbf{P}, \lambda)$ , where  $\lambda$  is stationary, then  $(X_{n+m})_{n\geq 0} = \mathsf{Markov}(\mathbf{P}, \lambda)$  for any fixed m.

(ii) In a finite DTMC, suppose for some  $i \in I$  we have

$$\lim_{n \to \infty} p_{ij}^{(n)} = \pi_j, \forall j \in I,$$

then  $\pi = (\pi_j : j \in I)$  is an invariant distribution.

- In an infinite DTMC, it is possible that  $\lim_{n\to\infty} p_{ij}^{(n)}$  exists for all i, j, producing a vector  $\pi$  for each i, yet  $\pi$  is **not** a distribution.
- $\bullet$  Consider the DTMC with state space  $\mathbb Z$  and

$$p_{i,i+1} = p = 1 - q = 1 - p_{i,i-1}, \quad \forall i \in \mathbb{Z}.$$

(This is a random walk on  $\mathbb{Z}$  we have considered.)

$$\lim_{n \to \infty} p_{ij}^{(n)} = 0, \forall i, j.$$

#### Define

$$\mu_{ij} = \sum_{n=1}^{\infty} n f_{ij}^{(n)} = \mathsf{E}_i[T_j]$$

## Definition

A recurrent state i is positive recurrent if  $\mu_{ii} < \infty$ 

## Definition

A recurrent state i is null recurrent if  $\mu_{ii} = \infty$ 

## Example of Positive Recurrent States

$$\mathbf{P} = \begin{bmatrix} p & 1-p \\ 1-p & p \end{bmatrix}, \text{ for } 0$$

Let the states be 0 and 1, then

$$\begin{array}{rcl} f_{00}^{(1)} & = & f_{11}^{(1)} = p \\ f_{00}^{(n)} & = & f_{11}^{(n)} = (1-p)^2 p^{n-2}, & n \geq 2 \end{array}$$

Both states are recurrent. Moreover,

$$\mu_{00} = \mu_{11} = p + \sum_{n=2}^{\infty} n(1-p)^2 p^{n-2} = 2.$$

Hence, both states are positive recurrent states.

# Example of Null Recurrent States

Consider a Markov chain with  $I = \mathbb{N}$  where  $p_{01} = 1$ , and

$$P_{m,m+1} = \frac{m}{m+1}, \quad \forall m \ge 1$$
$$P_{m,0} = \frac{1}{m+1}, \quad \forall m \ge 1.$$

Then,

$$f_{00}^{(1)} = 0$$
  

$$f_{00}^{(n)} = \frac{1}{n(n-1)}$$
  

$$f_{00} = \sum_{n=1}^{\infty} f_{00}^{(n)} = 1$$
  

$$\mu_{00} = \sum_{n=1}^{\infty} n f_{00}^{(n)} = \sum_{n=1}^{\infty} \frac{1}{n} = \infty.$$

Consequently, 0 is a null recurrent state.

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Positive and null recurrence are class properties, i.e. in a recurrent communication class either all states are positive recurrent or all states are null recurrent. Consider a DTMC on state space  $\ensuremath{\mathbb{N}}$  where

• 
$$p_{i,i+1} = a_i$$
,  $p_{i,i-1} = b_i$ ,  $p_{ii} = c_i$ 

- $a_i + b_i + c_i = 1$ ,  $\forall i \in \mathbb{N}$ , and implicitly  $b_0 = 0$
- $a_i, b_i > 0$  for all i, except for  $b_0$

#### Question

When is this chain positive/null recurrent?

To answer this question, we need a result on computing mean hitting times

# Mean Hitting Times

- Let  $\mathbf{P}$  be a DTMC on I. Let  $A \subseteq I$ .
- The hitting time  $H^A$

$$H^A := \min\{n \ge 0 : X_n \in A\}.$$

• The probability of hitting A starting from i

$$h_i^A := \mathsf{Pr}_i[H^A < \infty].$$

If A is a closed class, the h<sup>A</sup><sub>i</sub> are called the *absorption probabilities*The *mean hitting time* μ<sup>A</sup><sub>i</sub> is defined by

$$\mu_i^A := \mathsf{E}_i[H^A] = \sum_{n < \infty} n \mathsf{Pr}[H^A = n] + \infty \mathsf{Pr}[H^A = \infty]$$

The vector  $(\mu_i^A:i\in I)$  is the minimal non-negative solution to the following system

$$\begin{cases} \mu_i^A = 0 & \text{for } i \in A \\ \mu_i^A = 1 + \sum_{j \notin A} p_{ij} \mu_j^A & \text{for } i \notin A \end{cases}$$

# Back to the Birth-and-Death Chain

• Note that 
$$\mu_{00} = c_0 + a_0(1 + \mu_1^{\{0\}}) = 1 + a_0\mu_1^{\{0\}}$$
  
The system: 
$$\begin{cases} \mu_0^{\{0\}} = 0\\ \mu_1^{\{0\}} = 1 + a_1\mu_2^{\{0\}} + c_1\mu_1^{\{0\}}\\ \mu_i^{\{0\}} = 1 + a_i\mu_{i+1}^{\{0\}} + c_i\mu_i^{\{0\}} + b_i\mu_{i-1}^{\{0\}} & \text{for } i \ge 2 \end{cases}$$
• Define  $e_n := \frac{a_0 \dots a_{n-1}}{b_1 \dots b_n}, n \ge 1$ .  
• When  $\sum_{n=1}^{\infty} e_n = \infty, \mu_i^{\{0\}} = \infty, \forall i \ge 1$  is the solution  
• When  $\sum_{n=1}^{\infty} e_n < \infty$ , we have the following solution  

$$\begin{cases} \mu_0^{\{0\}} = 0\\ \mu_1^{\{0\}} = \frac{1}{a_0} \sum_{n=1}^{\infty} e_n \end{cases}$$

$$\left( \mu_i^{\{0\}} = \frac{d_i}{a_0} (\sum_{j=i}^{\infty} e_j) \quad \text{for } i \ge 2 \right)$$

Thus, (conditioned on the chain being recurrent)

- $\bullet\,$  the DTMC is positive recurrent when  $\sum_{j=1}^\infty e_j < \infty\,$
- the DTMC is null recurrent when  $\sum_{j=1}^{\infty} e_j = \infty$

An irreducible DTMC  $\mathbf{P}$  has a stationary distribution if and only if one of its states is positive recurrent.

Moreover, if  $\mathbf{P}$  has a stationary distribution  $\pi$ , then

$$\pi_i = 1/\mu_{ii}$$

Line of proof

- Every irreducible and recurrent **P** basically has a unique invariant measure (unique up to rescaling)
- Due to positive recurrence, the measure can be normalized to be come an invariant distribution

# Proof of the Existence of a Stationary Distribution

Define the expected time spent in  $\boldsymbol{i}$  between visits to  $\boldsymbol{k}$ 

$$\gamma_i^{(k)} = \mathsf{E}_k \left[ \sum_{n=0}^{T_k - 1} \mathbf{1}_{X_n = i} \right]$$

#### Lemma

If **P** is irreducible and recurrent, then (i)  $\gamma_k^{(k)} = 1$ (ii) the vector  $\gamma^{(k)} = (\gamma_i^{(k)} \mid i \in I)$  is an invariant measure, namely  $\gamma^{(k)}\mathbf{P} = \gamma^{(k)}$ (iii)  $0 < \gamma_i^{(k)} < \infty$  for all  $i \in I$ 

Conversely, if **P** is irreducible and  $\lambda$  is an invariant measure with  $\lambda_k = 1$ , then  $\lambda \geq \gamma^{(k)}$ . Moreover, if **P** is also recurrent, then  $\lambda = \gamma^{(k)}$ 

# Periodicity

- For a state  $i \in I$ , let  $d_i = \gcd\{n \ge 1 : p_{ii}^{(n)} > 0\}$ .
- When  $d_i \ge 2$ , state *i* is periodic with period  $d_i$ .
- When  $d_i = 1$ , state *i* is *aperiodic*.
- A DTMC is periodic if it has a periodic state. Otherwise, the chain is violetaperiodic.

#### Theorem

If  $i \leftrightarrow j$ , then  $d_i = d_j$ . If i is aperiodic, then  $\exists n_0 : p_{ii}^{(n)} > 0$ ,  $\forall n \ge n_0$ .

## Corollary

If **P** is irreducible and has an aperiodic state i, then **P**<sup>n</sup> has all strictly positive entries for sufficiently large n.

- An *ergodic* state is an aperiodic and positive recurrent state.
- An *ergodic Markov chain* is a Markov chain in which all states are ergodic. (Basically, a "well-behaved" chain.)

Suppose  $\mathbf{P}$  is irreducible and ergodic. Then, it has an invariant distribution  $\pi$ . Moreover,

$$\frac{1}{\mu_{jj}} = \pi_j = \lim_{n \to \infty} p_{ij}^{(n)}, \quad \forall j \in I.$$

Thus,  $\pi$  is the unique invariant distribution of **P**.

Note: there is a generalized version of this theorem for irreducible chains with period  $d \ge 2$ . (And the chain is not even required to be positive recurrent.)

# Ergodic Theorem

Let

$$V_i(n) = \sum_{k=0}^{n-1} 1_{\{X_k=i\}}.$$

## Theorem (Ergodic Theorem) Let P be an irreducible DTMC. Then

$$\Pr\left[\lim_{n \to \infty} \frac{V_i(n)}{n} = \frac{1}{\mu_{ii}}\right] = 1$$

Moreover, if **P** is positive recurrent with (unique) invariant distribution  $\pi$ , then for any bounded function  $f: I \to \mathbb{R}$ 

$$\Pr\left[\lim_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} f(X_k) = \sum_{i \in I} \pi_i f_i\right] = 1,$$