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TYPES & REPRESENTATION of GRAPHS

CS224W - Machine Learning with Graphs Stanford / Fall 2019 Jure Leskovec

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REPRESENTATIONS

1. Adjacency Matrix

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Aij=	{ ι	if	there	۶i	an	edge	be	twee	n	i 8	k j	
J	lo	ot	nerwis	e		•						
							V ₁	V ₂	V ₃	V4	V ₅	V ₆
	\bigcirc	(v ₁	0	1	0	0	0	0
	v_2	-('	^{'3}			V ₂	1	0	1	1	0	0
(\searrow_{v}			V ₃	0	1	0	1	0	0
V_1						V ₄	0	1	1	0	1	1
	$\left(v_{6}\right)$	(v_5			۷5	0	0	0	1	0	0
								-	_	_		

· Social media networks are very sparse adjacency matrices

V₆

0 0 0 1

2. Adjacency list

· List usually sorted based on preferences



Node	Connected To
v_1	v_2
v_2	v_1 , v_3 , v_4
v_3	v_2 , v_4
v_4	v_2, v_3, v_5, v_6
v_5	v_4
v_6	v_4

3. Edge list



TYPES

- 1. Null graph
 - · G(V,E) where $V = E = \phi$
- 2. Empty graph
 - · G(V, E) where $V \neq \phi$ but $E = \phi$
- 3. Directed and Undirected Graphs
 - For directed graphs,
 A_{ij} ≠ A_{ji} (A ≠ A^T)







4. Simple and Multigraphs

- Simple graphe : graphe where only single edge can be between any pair of nodes
- · Multi graphs: multiple edges between two nodes
 - eg: web graphs (multiple hyperlinks between 2 webpages)
 - adjacency matrix: numbers larger than I as entries





- s. weighted graphs
 - · Weights: could be distances



- 6. Web graph
 - · Directed multigraph
 - · Nodes: sites, edges: links
 - · Two sites can have multiple links and loops



• Bipartite: nodes belong to 2 sets such that there is no relation among members of a set; relations only between members of sets

- eg: users ve items (recommendation system)

· Monopartite: only one type of node

· Bipartite graph can be projected into mono partite graphs with inferred connections





10. Cyclic and Acyclic Graphs

 Acyclic: impossible to start and end on same node without retracing steps





- 11. Affiliation Networks
 - · Unipartite networks: network of friends
 - · Bipartite networks:
 - (a) Affiliation network: people not connected to each other, organisations not connected to each other; people individually affiliated to one or more organisations
 - Co Membership of people on corporate board: members not connected, boards not connected; members connected to one or more boards

· Tripartite networks

- users, communities, interest terms
 - A network of LiveJournal users
 - users (part 1), communities (part 2), and interest terms (part 3).
 - A user belongs to a community (1-> 2 type edge)
 - A user is interested in a term (a 1-> 3 type edge)
 - A community declares a term as an interest (a 2 -> 3 type edge)

- 12. Heterogeneous graphs
 - · Nodes & edges of diff types handled differently
- 13. Homogeneous graphs
 - · Nodes & edges instances of single type
- 14. Dynamic and static Graphs
 - · Dynamic graphs change over time
- is. Knowledge Graph
 - Directed multi relational graph where an edge represents
 a tuple Ch,r,t> head , relation, tail
 - · Eq: Lstar Trek, Genre, Science Fiction>

16. Hypergraph

- Generalisation of undirected graphs in which edges are subsets of 2 or more vertices
- · Hyperedges connect arbitrary number of nodes
- · size of vertex set: order of hypergraph
- · No. of hyperedges: size of hypergraph





- $\cdot X = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$
- $\cdot \in \{e_1, e_2, e_3, e_4\}$
- $\cdot V = \{\{v_{1}, v_{2}, v_{3}\}, \{v_{2}, v_{3}\}, \{v_{3}, v_{5}, v_{6}\}, \{v_{4}\}\}$
- · Order = 7 Cno. of nodes)
- · Size = 4 (no. of hyperedges)

felection & focial Infuence

- · Homophily: similarity
- · Selection: friend selection
- · Social influence · peer influence (eg: junk food, drinking etc)
- · context dependent
- Either pure social, pure selection or combination of social + selection



- in ego networks, ego is central node that all other nodes are connected to, and alters are all the surrounding nodes directly connected to the ego

- · Real-life interpretation of brokerage opportunity
- 1. If A, B and C are in the same group
 - coordination Broker: B brokers between members of the same group - Eg: manager of a team
- 2. A and C in the same group, B different consultant Broker: B connects members of the group together who want 2 different ends of a service/task
 - Eq: stock broker connecting a buyer and a seller
- 3. A and c are in different groups
 - Representative Broker: B negotiates on behalf of A to C
 - Gatekeeper Broker: transaction begins at A, passes to c's group's gatekeeper B
 - Eg cgatekeeper): B-census bureau, C-govt dept, A-public
- 4. A, B, C different groups Liason Broker: B plays neutral role between A & C
 - eq: A-actor, B-agent, c-producer

Measures Related to Structural Holes

1. Effective size: number of alters that ego has minus average number of ties each alter has to other alters

A

A : ego B,C,D: altere

- A has 3 ties, each tied to 2 others (many redundant ties)
- Average degree of other alters is 2
- Effective size of A's ego network = 3-2=1
- If no alters interconnected, effective size of A's ego network is 3-0 = 3



- 2. Efficiency: portion of ego's ties that are non-redundant
 - Efficiency = <u>Effective size of A's ego net</u> size of A's ego net
 - For first graph, size = 3 (3 alters) and efficiency = 43
 - For second graph, size = 3 and efficiency =1

EGO NETWORKS

- · Focus on individual
- · Ego network data commonly arises in 2 ways
 - 1. Collect data from ego (respondent) about interactions with alters in diff social settings & ask about ties between alters
 - 2. Snowball method : ask ego to identify alters, then ask those alters to identify their ties/alters

- · Use ego nets to make predictions about ego Lhealth, longevity, economic success etc.)
- Effect of social context on individual attributes, behaviours and conditions
- · sum of ego networks = social network

Homophily in Ego Networks

- · Portion of ties in ego net that are homophilous
 - <u>count of ties where ego and alter share same attr</u> total no. of ties in ego net
 - correlation between ego attr and alter attr

A

- Eg: nodes are either members of class red (A,B) homophily = <u>1</u>

· Ascortative mixing/accortavity is a bias in favour of connections between network nodes with similar characteristics

 \odot

- Homophily

Density of Ego Network

- · Size = no. of alters
- · Density = fraction of total no. of possible ties in the ego net that are actually present, excluding the ego
- · consider an ego connected to n alters
- · Assume ego net has L connections between alters
- Assuming undirected graph, total no. of possible edges b/w
 the alters = <u>n(n-1)</u>

Assuming directed graph, total no. of possible edges b/w
 the alters = n(n-1)

Strength of Weak Tics

- · Mark Granovetter
- People with many weak ties can gain speedy advantages in learning about and cashing in on new entrepreneurial opportunities
- · Irony: weak ties provide stronger form of social capital for career advancements

· Eq: LinkedIn - connect to weak ties to get opportunity

Strong Ties

- Determined by 3 characteristics
 1. Long duration of relationship
 2. Closeness of relationship close/very close
 3. Frequency of contact frequent

· In network maps, strong ties are solid lines

- · Benefits
 - 1. Generally trustworthy
 - 2. Provides depth of information

Weak Ties

- Determined by 3 characteristics
 1. short duration of relationship

 - 2. Closeness of relationship not close
 - 3. Frequency of contact infrequent
- · In network maps, weak ties are dotted lines
- · Benefits
 - 1. Provide unique perspectives
 - 2. Helpful for identifying opportunities

O. ego · · · O

Clique

- Subset of network in which actors are more closely and intensely tied to one another than they are to other members of the network
- Human tendency: on the basis of age, gender, race, religion, ethnicity etc.
- · Dyad: clique of 2 actors (smallest)

<u>Cliques vs Weak Ties</u>

- Cliques are great at knowledge preservation, not good at knowledge generation Coliques are knowledge reservoirs)
- · Weak ties serve as bridges
- Weak & strong ties are just weighted edges with appropriate weights
- · Eq: finding a job
 - strong: more motivation to help you
 - Weak: less likely overlap with leads
 - study: most job referrals come through those we see varely
- Board of directors: must model such that boards are independent and not influenced by vested interest

Centrality Analysis in Graphs

- · centrality importance of a node in a graph
- · Nodes maybe important from an angle

Normalised Degree Centrality

- Normalised by max possible degree (n-1)
 C_d (v_i) = <u>di</u> } meso-level analysis
 n-1 } by Freeman
- · Normalised by max degree

$$C_d^{\max}(v_i) = \frac{d_i}{\max_j d_j}$$

· Normalised by degree sum

- · Linton Freeman developed basic measures of centrality
- · Degree centrality: for undirected graphs, unweighted graphs cas it biases towards stronger ties)
- Degree centrality only used to make comparisons between actors of the same net or diff nets of same size
 Still should not compare networks that differ greatly in size chigher norm score for smaller graphs)

· Neighbour focused, not global

Indegree centrality : no of ties received by an actor; measure
 of popularity or prestige

$$C_{d}(v_{i}) = d_{i}^{n}$$

• Outdegree centrality: no of ties given by an actor; measure of expansiveness or gregariousness

$$C_d(V_i) = ol_i^{out}$$

· Combination

$$C_d(v_i) = d_i^{in} + d_i^{out}$$

BETWEENNESS CENTRALITY

- Degree centrality only looks at ego network (immediate ties) and does not consider the rest of the network
- Betweenness centrality: how much potential control an actor has over the flow of information
- How many times an actor sits on the geodesic / shortest path between two actors together
- How central vi's role in connecting a pair of nodes s and t is

$$C_{b}(v_{i}) = \underbrace{ \underbrace{ \sigma_{st}(v_{i})}_{s \neq t \neq v_{i}} }_{S \neq t \neq v_{i}} \underbrace{ \sigma_{st}}_{All s t t values}$$

 σ_{st}: no. of shortest paths from s to t (info pathways)

 σ_{st} (v_i): no. of shortest paths from s to t that pass through
 v_i

· Best case: $\sigma_{st}(v_i) = \sigma_{st}$ or v_i lies on all shortest paths

$$\frac{\sigma_{st}(v_i)}{\sigma_{st}} = 1$$

· Max value of Cb in undirected graphs

$$C_{b \max} = \sum_{\substack{s \neq t \neq V_i}} 1 = \frac{n-1}{2} = \frac{(n-1)}{2} = \frac{(n-1)!}{2! (n-3)!}$$

$$s \in t \text{ chosen}$$
from n-1
nodes (nth is V;)

$$C_{b \max} = \frac{(n-1)(n-2)}{2}$$

· max value of Cb in directed graphs

$$C_{b \max} = \sum_{\substack{s \neq t \neq V_i}} 1 = {n^{-1}P_{1}} = \frac{(n-1)!}{(n-3)!} = (n-1)(n-2)$$

$$C_{b \max} = (n-1)(n-2) = 2^{n-1}C_2$$

· Normalised betweenness centrality

$$C_{P}^{\text{norm}}(v_{i}) = \frac{C_{P}(v_{i})}{2(r_{1}C_{2})}$$

Q: calculate C_CV,) for the given graph



- · All paths between s & t go through v, Call values of s & t)
- \therefore $C_{b}(v_{1}) = {}^{8}C_{2}$
- · Normalised Cb CV1) = 1
- Betweenness centrality for any other node in the graph is
 O
- · Higher betweenness centrality characterised by more structural holes



closeness centrality

- · How close a node is from the rest of the graph
- · Closeness centrality = 0 means it has no neighbours and is severed from the rest of the net
- Closeness centrality = 1 means it is directly connected to every other node

$$C_{c}Cv_{i}) = \underbrace{I}_{v_{i}} \quad \text{where} \quad \overline{L}_{v_{i}} = \underbrace{I}_{n-1} \underbrace{\sum}_{v_{j} \neq v_{i}} \underbrace{L}_{v_{j} \neq v_{i}}$$

Q: calculate C, CV3), C, CV1), C, CV2), C, CV4), C, CV5)



 $C_{c}(V_{4}) = 1/((1+2+2+3)/4) = 0.8$ $C_{c}(V_{4}) = 1/((2+1+2+1)/4) = 0.67$ $C_{c}(V_{4}) = 1/((3+2+1+1)/4) = 0.57$

Harmonic Centrality

· Mean reciprocal distance

PAGE RANK

Discrete Markov Process Crecall MI)

- · Series of experiments performed at regular time intervals
- · Always same set of possible outcomes
- · Discrete steps of time
- · Outcomes called states
- · Model can be in any one state at any given timestep
- Next step: can stay in same state or move to another state
 Movement blw states: probability

Stochastic Transition Probability Matrix

$$\cdot \quad \alpha_{ij} = P(Q_{t+i} = S_j | Q_t = S_i)$$

- · Sum of column = 1
- · Stochastic: all row sums = 1, all values non-negative

			Time	t+1		
7-	tate	S,	52	Sz	S4	Total
	s,	٩,,	٩,2	A 13	٩14	1
Time	Sz	a21	922	٩٦٤	a24	I
t	S3	Q 31	0.32	Q33	a ₃₄	١
	S4	۵۴۱	942	٥	٩	1

Eigen Decomposition Theorem

- Square matrix can be decomposed into eigen vectors & eigen values
- · Let $C_{m\times m}$ be a matrix, x_R be a column vector and λ_R be a constant

- The n column vectors x_R and the n values of λ_R are the right eigenvectors and eigenvalues respectively
- Principle right eigenvector: corresponds to eigenvalue of largest magnitude
- · Left eigenvector is a row vector

$$X_{L}C = \lambda X_{L}$$

Steady State

- · Probability for transitioning to a state reaches a limiting value as $t \rightarrow \infty$
- Probability vector × Transition matrix = Probability vector
- · Steady state: eigenvector for stochastic matrix

ERGODIC MARLOV CHAIN

- · let Markov chain start at t=0 in state i
- If there exists a timestamp value To and a state j such that for all t>To the probability of being in state j is >0, the chain is ergodic
- · conditions for engodicity
 - 1. Irreducibility: sequence of transitions of non-zero probability from any state to any other
 - 2. Aperiodicity: states are not partitioned into sets such that all state transitions occur cyclically from one set to another

STEADY STATE THEOREM

 For any Ergodic Markov chain, there is a unique steady state probability vector TI (left principle eigenvector of transition Matrix P)

$$\pi P = \lambda \pi \qquad \lambda = I$$

Page Rank Formula

- · Web: network of web pages
- · Page rank: numeric value representing importance of a page m the web
- · One hyperlink from one page to another: one vote
- · Needs to be immune to link spamming
- · See : Big Data unit 2

· Model www as a directed graph

Pagel Linksto 2 3	Page 2 Links to 1 3 4
Page 3	Page 4
υ- -	
Linksto 4	Links to



SPECTRAL ANAYSIS TO EXPLAIN PAGE RANK

- Eigenvector centrality: generalise degree centrality Cglobal centrality) – undirected graphs
- Think: which edge A-B or B-C should be severed to make B
 safe from STDs?
 - recursive collepends on probability of being infected by A or c, their neighbours, so m)



- · Degree centrality: uses no. of neighbours
- · We want centrality of v; to be a function of its neighbours' centralities
- · Proposal: centrality of v. & Scentrality of neighbour
- · Assume everyone has an initial score (rank) of I and update centralities recursively
- · Let X = popularity vector

$$X_j(0) = popularity of j at t=0$$

Xj (1) = E A_{ij} Xj(0) for all nodes i ≠ j where A_{ij} is the number of links between i & j Cadjacency matrix>

· Vector form

X(I) = A.X(D)

· At time t

$$X(t) = A X(t-1) = A^2 X(t-2) = \dots = A X(0)$$

$$X(t) = A^{t}X(0)$$

- · For some large value of t, it will stabilise
- · Let XLO) be a linear combination of eigenvectors of A

$$X(0) = \mathcal{L}_{i} v_{i}$$

- · Plugging in, X(2) = At E (i vi
- We know $AV = \lambda V (V eigenvector)$ $\therefore A^{t} V = \lambda^{t} V$
- · Plugging in,

$$X(t) = \Sigma \lambda_i^t c_i v_i$$

· Divide by principle eigenvector λ_1^{t}

$$\frac{X(t)}{\lambda^{t}} = \sum \frac{\lambda_{i}^{t} c_{i} v_{i}}{\lambda^{t}}$$

 $\lim_{t \to \infty} \frac{\chi(t)}{\lambda_i^*} = C_i v_i \qquad (all other \frac{\lambda_i}{\lambda_i} \rightarrow 0)$

 Popularity value converges to principle eigenvector of adjacency matrix

For directed graphs

- · An initial popularity & is added to the centrality values for all nodes
- · X depends on neighbourhood

$$C_{kat_2}(v_i) = d \begin{cases} S & A_{ji} \\ S & J_{ji} \end{cases}$$

- · Vector Form vector of all 1's
 - easier to _____ C = & A^T C Katz + B(1) solve this iteratively

harder to ____ C katz =
$$\beta (I - \alpha A^T)^{-1} \cdot 1$$

 Page Rank – divide value of passed centrality by number of outgoing links

$$C_{p}(v_{i}) = \propto \sum_{j=1}^{n} A_{ji} \frac{C_{p}(v_{j})}{d_{j}^{owt}} + \beta$$

RANDOM SURFER TO EXPLAIN PAGE RANK

- · Model of user behaviour
 - 1. Initially every web page chosen uniformly at random
 - 2. Choose a hyperlink on the page with probability &
 - 3. With probability 1-d, perform random walk on web by randomly choosing a node and then restart at step 1

Algorithm - Basic Page Rank

- In a network of n nodes, we assign all nodes same initial PageRank 1/n
- 2. We choose no of steps k
- 3. We then perform a sequence of k updates as
 - 1. Each page divides its current PageRank equally across its outgoing links and passes that to the pages it points to
 - 2. Each page updates its PageRank to be sum of the shares that it receives
- So, the PageRank remains constant (no scaling needed) neither created nor destroyed but is just moved around
- As K -> ∞, the PageRank of all nodes converge to limiting values (don't change any further)

Algorithm - Scaled Page Rank

- 1. First: apply basic PR update rule, second: scale down by a factor of s so that total PR is down from 1 to s (s <1)
- 2. Divide residual PR (1-s) into n nodes as <u>1-s</u>

Limitations OF Basic Page Rank

- 1. Rank Sinks
 - · Page has no outgoing edges, only incoming edges
 - · Monopolise scores
- 2. Hoarding/Circular Reference · Group of pages that only link between each other
- 3. Dangling nodes · Isolated node (no links at all)

folution

Teleporting: random surfer will teleport to random URLs for a proportion of hops (I-2)

Usually: ~= 0.85, 1-2=0.15

Basic PR



	Iteration O	Iteration 1	Iteration 2	Rank
Α	1/4	412	1/8 = 0.125	4
B	Y 4	5/24	5/24 = 0.208	3
С	V4	3/8	3/8 = 0.375	I
D	4	43	43 = 0.333	ຊ

Iteration 1

	PRCA) =	<u>PRCC)</u> out(C)	2	<u>1/4</u> 3	= _	1			
	PRCB) =	<u>PR(A)</u> out(A)	ł	<u>PR(c)</u> out(c)	= _	<u>/4</u> + 2	· <u>\/ự</u> 3	= <u>5</u> 24	
	PRCC) =	<u>PR(A)</u> out(A)	+	<u>PR(D</u>) out(D)) =)	<u>/4</u> 2	+ <u>Yu</u> 1	= 3 8	
	PRLC) =	<u>PRCB)</u> out(B)	+	PR(C) out(C)	<u>)</u> =	<u>74</u> 1	+ <u>Yu</u> 3	<u>k = 1</u> 3	
Itero	tim	2								
	PR(A)) =	<u>PRCC)</u> out(C)	=	<u>3/8</u> 3	= <u>1</u> 8	5			
	PRLB) =	<u>PR(A)</u> out(A)	t	<u>PR(c)</u> ou+(c)	= \	/ <u>12</u> + 2	<u>3/8</u> 3	= <u> </u> 6	
	PRCC) =	<u>PRLA)</u> out(A)	+	PR(D) out(D	_ =	<u> /12</u> 2	+ <u>13</u>	= 3 8	
	PRLD) =	PRCB) out(B)	+	PRCC) out(C)	=	5 <u>124</u> 1	+ 3/8	<u>= 1</u> 3	

Google PR - no need to divide I-a by n



Transition matrix (divide by no of outlinks)

		so	nuc		
	[0	0	1	Y2]	
dest	43	Ο	0	0	=T
	43	σ	0	42	
	L73	1	0	۲ ه	

Initial page rank

$$X = \begin{bmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix} = X(0)$$

Iteration

$$X(1) = (1 - a) + a T X(0)$$



X(1) =	0.6875]
	0.5417
	0.6042
	L 0.6667 J