



Network Metrics 3/06/24



- Last class:
 - Causal Inference with text
- Reminders:
 - HW 3 due (next) Friday
 - \circ Midterm in 1 week



Outline

- Introduction and definitions
- Basic Network Metrics
- Advanced Network Methods
- Graph Neural Network







Introduction and Definitions

Motivation: understand relationship

High School Partnership Network



FIG. 3.—Temporally ordered ties in the Jefferson High partnership network

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Motivation: understand epidemic

Sex Partner Network and HIV



Fig. 3. Size of Largest component and bicomponent by average number of sexual partners for short-tailed and scale-free distributions. The curves plot the growth of the largest component and bicomponent as a function of the average degree, based on 100 simulations of a 10,000-node network at each degree setting. The red curve plots the analytic solution for the size of the giant component for the simulated networks with scale-free distributions, and the orange curve plots the largest bicomponent. The dark blue curve plots the analytic solution for the size of the largest component for the simulated low-degree networks, and the light blue curve plots the size of the largest bicomponent. The bicomponent curves are not continuous due to sampling.

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Motivation: understand online "epidemic"

• Lies spread faster than the truth



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Motivation: how to succeed as individual

- Looking for a job? Making Weak Ties.
- Want to be influential? Try something new, but don't go too far.

The Strength of Weak Ties¹

Mark S. Granovetter Johns Hopkins University

> Analysis of social networks is suggested as a tool for linking micro and macro levels of sociological theory. The procedure is illustrated by elaboration of the macro implications of one aspect of small-scale interaction: the strength of dyadic ties. It is argued that the degree of overlap of two individuals' friendship networks varies directly with the strength of their tie to one another. The impact of this principle on diffusion of influence and information, mobility opportunity, and community organization is explored. Stress is laid on the cohesive power of weak ties. Most network models deal, implicitly, with strong ties, thus confining their applicability to small, welldefined groups. Emphasis on weak ties lends itself to discussion of relations *between* groups and to analysis of segments of social structure not easily defined in terms of primary groups.

Atypical Combinations and Scientific Impact

Brian Uzzi,^{1,2} Satyam Mukherjee,^{1,2} Michael Stringer,^{2,3} Ben Jones^{1,4}*

Novelty is an essential feature of creative ideas, yet the building blocks of new ideas are often embodied in existing knowledge. From this perspective, balancing atypical knowledge with conventional knowledge may be critical to the link between innovativeness and impact. Our analysis of 17.9 million papers spanning all scientific fields suggests that science follows a nearly universal pattern: The highest-impact science is primarily grounded in exceptionally conventional combinations of prior work yet simultaneously features an intrusion of unusual combinations. Papers of this type were twice as likely to be highly cited works. Novel combinations of prior work are rare, yet teams are 37.7% more likely than solo authors to insert novel combinations into familiar knowledge domains.

JOHNS HOPKI WHITING SCHOOL of ENGINEERING Granovetter, M. S. (1973). The strength of weak ties. *American journal of sociology*, 78(6), 1360-1380.
 Uzzi, B., Mukherjee, S., Stringer, M., & Jones, B. (2013). Atypical combinations and scientific impact. Science, 342(6157), 468-472.

Motivation: how to promote mobility as society

- <u>https://socialcapital.org/</u>
- Go to the right schools and make the right friends







Chetty, R., Jackson, M. O., Kuchler, T., Stroebel, J., Hendren, N., Fluegge, R. B., ... & Wernerfelt, N. (2022). Social capital I: measurement and associations with economic mobility. *Nature*, *608*(7921), 108-121.

How might we represent network?

Represent connections between vertices/nodes

- Vertex: a node of the graph
- Edge: a link between two vertices

A graph consists of a set of nodes and a set of edges

• G(V, E)





Graph Data: Adjacency Matrix

The matrix of vertices connections
 Encode in a symmetric matrix (for undirected network)
 (n × n) matrix A

The adjacency matrix has elements

$$a_{ij} = \begin{cases} 1 & if i and j are connected \\ 0 & otherwise \end{cases}$$

 $A = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix}$

	Mark	Peter	Bob	Jill	Aaron	
Mar <mark>k</mark>	0	1	0	1	0	
Peter	1	0	1	0	1	
Bob	0	1	0	1	0	
Jill	1	0	1	0	1	
Aaron	0	1	0	1	0	

Graph Data: Edge Lists

Two-column matrices that directly indicate how vertices are connected





Types of Edges

Directed vs. undirected



Directed sociomatrix

	Α	В	С	D	E	F	G
А	-	metric	0	1	0	0	0
В	Ounsy	-	0	1	0	0	0
С	0	0	-	etric	0	0	0
D	0	1	0 sym	-	0	1	0
E	0	0	0	0	-	0	0
F	0	0	0	0	0 ~	Unsymmetric	V O
G	0	0	0	0	1	50	-

Undirected sociomatrix

	A	В	С	D	E	F	G
Α	-	petric1	0	1	0	0	0
В	1 Sym	-	0	1	0	0	0
С	0	0	-	oetrio	0	0	0
D	1	1	osym	-	0	1	0
E	0	0	0	0	-	0 5	1
F	0	0	0	1	0	symmetric	√ o
G	0	0	0	0	1	S 0	-

Types of Edges

- Weighted vs. unweighted
- Multiplex

• Affect in a sorority vs. campaign financing



Organizations: authority, trust, & friendship



Hypergraph Incidence Matrix





Example from: https://sonic.northwestern.edu/

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Example of hypergraph: Lungeanu, A., Carter, D. R., DeChurch, L. A., & Contractor, N. S. (2021). How team interlock ecosystems shape the assembly of scientific teams: A hypergraph approach. In Computational Methods for Communication Science (pp. 95-119). Routledge.





Basic Metrics

Network Parameters

Different Dimensions to Consider

- Entity: Nodes vs. Edges (e.g., degree, path length)
- Scale: Local vs. Global (e.g., cluster, dimensions)
- **Topology:** Structure (e.g., small world network, scale-free network)
- **Quantity:** Volume (e.g., weighted edges)
- **Quality:** Classification (e.g., friends, family, ...)

• ...

Different combinations of dimensions create different network metrics; You can always **create your own**.



Example 1: Network Density

Edges * Global (Ignore multiplex hypergraph topology for all examples)

- For a directed unweighted network with n nodes, the max number of possible edges is: n(n-1)
- For an undirected unweighted network: n(n-1)/2
- Network density:

Number of edges Number of possible edges



Americans are becoming more isolated

Table 5. Structural Characteristics of Core Discussion in	Retworks	
	1985 (N = $1,167^{a}$)	$2004 (N = 788^{b})$
Network Density		
<.25	9.9%	7.3%
.2549	18.5%	11.8%
.50–.74	37.9%	39.5%
>.74	33.7%	41.4%
Mean	.60	.66
SD	.33	.33
Mean Frequency of Contact (days per year)		
6–12	3.7%	3.0%
>12-52	15.3%	10.6%
>52–365	81.0%	86.4%
Mean	208.92	243.81
SD	117.08	114.86
Length of Association (in years)		
>0-4.5	12.1%	10.7%
>4.5-8+	87.9%	89.3%
Mean	6.72	7.01
SD	1.34	1.00

 Table 3.
 Structural Characteristics of Core Discussion Networks



McPherson, M., Smith-Lovin, L., & Brashears, M. E. (2006). Social isolation in America: Changes in core discussion networks over two decades. American sociological review, 71(3), 353-375.

Example 2: Closeness Centrality

Nodes * Global

 Measuring the mean shortest distance from a node to every other nodes in a network with n nodes:



 Where d represent the length of the shortest path between i and j. Here, the path length refers to the number of nodes between i and j (degrees of separation).



How minorities generate impact from a Table 1. Variable Descriptions and Descriptive Statistics Table 1. Variable Descriptions Mean Modia Influence Number of words in press release reproduced verbation 4 500

 Start from periphery and channel through emotions (sentiment analysis)



Figure 1. Idealized Opportunity Structure Created by Cognitive-Emotional Currents

Variable	Description	Mean	SD
Media Influence (Outcome)	Number of words in press release reproduced verbatim or paraphrased by six national media sources.	4.590	18.736
Fringe Media Frames	Euclidean distance between five dummy variables describing civil society organization media frames about Islam in each press release and average for all other organizations during the same year.	.913	.197
Assets	Total assets of organization sponsoring press release at year-end	27.0 (mill.)	68.3 (mill.)
Inter-organizational Networks	Closeness centrality of organization within field (constructed using interlocking directorates by year).	.188	.355
Narrowness of Mission	Dummy variable that describes whether organization's primary goal is influencing media discourse about Islam (1 = yes, 0 = no).	.493	.500
Displays of Fear or Anger	Dummy variable that describes whether civil society organization displays fear or anger in press release $(1 = \text{yes}, 0 = \text{no}).$.654	.478
News Cycle	Number of hits for the term "Muslim" or "Islam" on Google News during month the press release was issued.	8,264	2,830
Previous Media Coverage	Dummy variable that describes whether civil society organization issuing the press release previously influenced media discourse about Islam.	.524	.500
U.S. Government Targeted	Dummy variable that describes whether the press release targets an individual or organization representing the U. S. government (1 = yes, 0 = no).	.283	.451
Public Interest	Dummy variable that describes whether main event described in the press release was one of the top-10 Google searches during the week it was issued $(1 = yes, 0 = no)$.	.061	.239
Violence or Disruptive Activity	Dummy variable that describes whether main event described in the press release involved physical violence, strikes, protests, rallies, or boycotts $(1 = yes, 0 = no)$.	.223	.416
Event in United States	Dummy variable that describes whether main event described in the press release occurred in the United States (1 = yes, 0 = no).	.572	.450

Bail, C. A. (2012). The fringe effect: Civil society organizations and the evolution of media discourse about Islam since the September 11th attacks. *American Sociological Review*, 77(6), 855-879.



Bail, C. A., Brown, T. W., & Mann, M. (2017). Channeling hearts and minds: Advocacy organizations, cognitive-emotional currents, and public conversation. American Sociological Review, 82(6), 1188-1213.

Example 3: Quarter-Power Scaling

Topology * Volume * Scale

Observation: Many biological scaling can be described as

$$Y = aM^b$$

Where Y is a biological variable, such as "*life span*"; a is a constant, b is a scaling exponent; M is a metabolic measurement, such as "*blood circulation time*". The value of b is usually $\frac{1}{4}$ or $\frac{3}{4}$.

We also have similar observations in economic growth, innovation, and pace of life in cities.

West, G. B., Brown, J. H., & Enquist, B. J. (1999). The fourth dimension of life: fractal geometry and allometric scaling of organisms. science, 284(5420), 1677-1679.



Bettencourt, L. M., Lobo, J., Helbing, D., Kühnert, C., & West, G. B. (2007). Growth, innovation, scaling, and the pace of life in cities. Proceedings of the national academy of sciences, 104(17), 7301-7306. 21

 Theory: maximize metabolic capacity - transportation through space-filling fractal networks of branching tubes



Fig. 1. Diagrammatic examples of segments of biological distribution networks: (A) mammalian circulatory and respiratory systems composed of branching tubes; (B) plant vessel-bundle vascular system composed of diverging vessel elements; (C) topological representation of such networks, where k specifies the order of the level, beginning with the aorta (k = 0) and ending with the capillary (k = N); and (**D**) parameters of a typical tube at the *k*th level.

Model

Parameters

West, G. B., Brown, J. H., & Enquist, B. J. (1997). A general model for the origin of allometric scaling laws in biology. *Science*, *276*(5309), 122-126.



Table 1. Values of allometric exponents for variables of the mammalian cardiovascular and respiratory systems predicted by the model compared

with empirical observations. Observed values of exponents are taken from (2, 3); ND denotes that no data are available.

Ca	rdiovascular			Respiratory					
) (aviable	Exponent					Exponent			
variable	Predict	ted	Observed	Variable	Pre	Predicted Ob			
Aorta radius r_0 Aorta pressure Δp_0 Aorta blood velocity u_0 Blood volume V_b Circulation time Circulation distance <i>I</i> Cardiac stroke volume Cardiac frequency ω Cardiac output <i>E</i> Number of capillaries N_c Service volume radius Womersley number α Density of capillaries O_2 affinity of blood P_{50} Total resistance <i>Z</i> Metabolic rate <i>B</i>	3/8 = 0 = 0 = 0 = 0 = 0 = 0 = 0 = 0 = 0 =	0.375 0.00 1.00 0.25 0.25 1.00 -0.25 0.75 0.75 0.75 0.083 0.25 -0.083 -0.083 -0.75 0.75	0.36 0.032 0.07 1.00 0.25 ND 1.03 -0.25 0.74 ND 0.25 -0.095 -0.095 -0.089 -0.76 0.75	Tracheal radius Interpleural pressure Air velocity in trachea Lung volume Volume flow to lung Volume of alveolus V_A Tidal volume Respiratory frequency Power dissipated Number of alveoli N_A Radius of alveolus r_A Area of alveolus A_A Area of alveolus A_A Area of lung A_L O_2 diffusing capacity Total resistance	3/8 0 0 1 3/4 1/4 1 -1/4 3/4 1/4 1/12 1/6 11/12 1 -3/4 3/4	= 0.375 $= 0.00$ $= 0.00$ $= 1.00$ $= 0.75$ $= 0.25$ $= 1.00$ $= -0.25$ $= 0.75$ $= 0.75$ $= 0.75$ $= 0.083$ $= 0.083$ $= 0.92$ $= 1.00$ $= -0.75$ $= 0.75$	0.39 0.004 0.02 1.05 0.80 ND 1.041 -0.26 0.78 ND 0.13 ND 0.95 0.99 -0.70 0.76		

West, G. B., Brown, J. H., & Enquist, B. J. (1997). A general model for the origin of allometric scaling laws in biology. *Science*, *276*(5309), 122-126.



List of Other Metrics

Node Degree (in-degree; out-degree)N-cliquesDegree distributionN-clans

Betweenness centrality

Eigenvector centrality

Page Rank (Google)

Constraint (Structure hole) Hubs and Authorities (HITS)

Clustering coefficient

Components

Subgraphs

N-clans K-plexes K-cores Structural Equivalence Shortcut



For more information, refer to textbooks, Wikipedia or python/R packages (e.g. NetworkX https://networkx.org/)







Advanced Network Methods



 Logistic Regression (Feb 14) assume independence of errors, linearity in the logit for continuous variables, absence of multicollinearity, and lack of strongly influential outliers

Supervised learning





Network "regression"

Problem:

- Analogous to logistic regression: if we want to **predict** the probability that a pair of nodes in a network will **have a tie** between them (0,1).
- Ties between nodes in real social networks are not **independent**.

Solution

- Exponential Random Graph Model (ERGM)
- Through simulation, ERGMs allow dyadic and higher-order dependencies to be modeled. Then it can describe how **interdependent structures** shape a network.

https://eehh-stanford.github.io/SNA-workshop/ergm-intro.html#what-is-an-ergm

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Hunter, D. R., Handcock, M. S., Butts, C. T., Goodreau, S. M., & Morris, M. (2008). ergm: A package to fit, simulate and diagnose exponential-family models for networks. *Journal of statistical software*, *24*(3), nihpa54860.

ERGM Model

Observe the distribution of structural features of interest in simulated networks





Network Statistics: Undirected

ERGM Model

Adding different structural metrics as X into

a "regression".

Parameter	statnet name		Parameter	statnet name	
Edge	edges	• •	Isolates	isolates	•
2-Star	kstar(2)	\leq	3-Star	kstar(3)	\leqslant
Triangle	triangle	\bigtriangleup	K-Star	kstar(k)	

Network Statistics: Directed

Parameter	statnet name		Parameter	statnet name	
Arc	edges	• •	Reciprocity	mutual	•
2-In-Star	istar(2)	•	2-Out-Star	ostar(2)	\leq
Mixed-2-Star (two-path)	m2star				_
3-In-Star	istar(3)	•	3-Out-Star	ostar(3)	
K-In-Star	istar(k)		K-Out-Star	ostar(k)	

ERGM Model

Let **Y** denote an $n \times n$ sociomatrix where $y_{ij} = 1$ if individuals $y_{ij} = i$ and j have a tie. Let **X** denote a matrix of covariates, which includes structural measures of the network as well as nodal and possibly edge-level attributes. A generic ERGM can be written as:

$$P_{\theta,\mathcal{Y}}(\mathbf{Y} = \mathbf{y} | \mathbf{X}) = \frac{exp\{\theta^{\mathsf{T}}g(y, X)\}}{\kappa(\theta, \mathcal{Y})}$$

where θ is a vector of coefficients, $g(y, \mathbf{X})$ is a vector of sufficient statistics, \mathcal{Y} is the space of possible graphs, and $\kappa(\theta, \mathcal{Y})$ is a normalizing constant. That is, it's the numerator summed across all possible graphs \mathcal{Y} . For even moderate-sized graphs, $\kappa(\theta, \mathcal{Y})$ can be enormous, so closed-form solutions are unfeasible. The number of labeled, undirected graphs of n vertices is $2^{n(n-1)/2}$, which can get big fast. For example, for a network of n > 7, there are over two million undirected graphs, which means that you would need to calculate the likelihood for each one of these in order to compute κ . This is generally not practical.

ERGM Model

Some Definitions and Notation

- y_{ij} denotes the ij th dyad in graph $y_{. If} y_{ij} = 1$, then i and j are connected by an edge, if $y_{ij} = 0$, they are not.
- y_{ij}^c is the status of all other pairs of vertices in y other than (i, j).
- y_{ij}^+ is the same network as $y_{\text{except that}} y_{ij} = 1$.
- y_{ij}^- is the same network as $y_{ ext{except that}} y_{ij} = 0$
- $\delta(y_{ij})_{is the change statistic.} \delta(y_{ij}) = g(y_{ij}^+) g(y_{ij}^-)_{is is a measure of how the graph statistic <math>g(y)_{is the ij}$ changes if the ij_{th} vertex is toggled on or off.

The ergm equation can be re-written in terms of change statistics. The log-odds of a tie y_{ij} is:

$$logit(Y_{ij} = 1 | y_{ij}^c) = \theta^T \delta(y_{ij})$$

Example of ERGM

How reciprocal edges and number of edge influence guarantee network in financial crisis and stimulus program?



Fig. 4 Dynamic changes of coefficients in ERGM. Source data are provided as a Source Data file.

JOHNS HOPKINS WHITING SCHOOL of ENGINEERING Wang, Y., Zhang, Q., & Yang, X. (2020). Evolution of the Chinese guarantee network under financial crisis and stimulus program. Nature Communications, 11(1), 2693.

Extended ERGM family and other Relevant Inference models

- Social selection: predict ties
- Social influence: predict attributes of nodes

Choosing the Right Network Model Framework



Problem of ERGM family

- Not practical for a large graph (typically within 3k-5k nodes)
- One solution is **network sampling**, sample a small graph from the large graph (another solution is Graph Neural Network)

			St	atic gra	Temporal graph patterns								
	in-deg	$\operatorname{out-deg}$	wcc	SCC	hops	sng-val	sng-vec	clust	diam	cc-sz	sng-val	clust	AVG
RN	0.084	0.145	0.814	0.193	0.231	0.079	0.112	0.327	0.074	0.570	0.263	0.371	0.272
RPN	0.062	0.097	0.792	0.194	0.200	0.048	0.081	0.243	0.051	0.475	0.162	0.249	0.221
RDN	0.110	0.128	0.818	0.193	0.238	0.041	0.048	0.256	0.052	0.440	0.097	0.242	0.222
RE	0.216	0.305	0.367	0.206	0.509	0.169	0.192	0.525	0.164	0.659	0.355	0.729	0.366
RNE	0.277	0.404	0.390	0.224	0.702	0.255	0.273	0.709	0.370	0.771	0.215	0.733	0.444
HYB	0.273	0.394	0.386	0.224	0.683	0.240	0.251	0.670	0.331	0.748	0.256	0.765	0.435
RNN	0.179	0.014	0.581	0.206	0.252	0.060	0.255	0.398	0.058	0.463	0.200	0.433	0.258
RJ	0.132	0.151	0.771	0.215	0.264	0.076	0.143	0.235	0.122	0.492	0.161	0.214	0.248
$\mathbf{R}\mathbf{W}$	0.082	0.131	0.685	0.194	0.243	0.049	0.033	0.243	0.036	0.423	0.086	0.224	0.202
\mathbf{FF}	0.082	0.105	0.664	0.194	0.203	0.038	0.092	0.244	0.053	0.434	0.140	0.211	0.205

Table 1: Scale-down sampling criteria. On average RW and FF perform best.



Leskovec, J., & Faloutsos, C. (2006, August). Sampling from large graphs. In Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 631-636).



- Causal inference (Feb 14)
- How to conduct causal inference in network analysis?

How can we measure ATE without this problem?

- Randomized control trial (RCT)
- More realistic scenario:
 - We'll probably study effects of medicine on someone who is sick
 - If we survey people, there still might be differences: lower income person may not be able to afford medicine and may also have worse nutrition that leads to more severe illness: income is a confounder (X)
- Instead of surveying people, we take a group of people and randomly assign them to "treatment" or "control" group



Example 1: Simulation + Matching

Remove matched nodes and see what happens

Malfeasance and the Foundations for Global Trade: The Structure of English Trade in the East Indies, 1601–1833¹

Emily Erikson University of Massachusetts, Amherst

Peter Bearman Columbia University





Total Trade Network



Erikson, E., & Bearman, P. (2006). Malfeasance and the foundations for global trade: The structure of English trade in the East Indies, 1601–1833. American Journal of Sociology, 112(1), 195-230., J. C. (2011). Logistic regression: a brief primer. Academic emergency medicine, 18(10), 1099-1104.

Private Trade Removed

FIG. 8.—Simulations of data presented in fig. 6

FIG. 4.-Network visualizations of the EIC's Eastern trade

Example 2: Experiment

Recruit people and allocate them into different networks.

Experimental evidence for tipping points in social convention



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Centola, D., Becker, J., Brackbill, D., & Baronchelli, A. (2018). Experimental evidence for tipping points in social convention. *Science*, *360*(6393), 1116-1119.





Graph Neural Network

Call back: Large Graph Issue for ERGM

- Solution 1: **Network sampling**.
- Solution 2: Transform graph information to other data structures (e.g., node embedding).
- Solution 3: Analyzing the graph at the local neural level and then aggregating the neurons together (e.g., Graph Neural Network).
- These 3 solutions are actually intertwined in practice:

You can use network sampling methods (e.g., random walk) to calculate node embeddings;

You can also use node embedding results as input for Graph Neural Networks (GNN).



Node Embedding

- Logic of Node Embedding
- 1. Define a function that maps node u, v to vectors z_u , z_v
- 2. Define a node similarity function for u, v
- 3. Optimize parameters so that:

similarity(u, v) $\approx z_v^T z_u$







Example: similarity based on random walks

- Given a random node u, predict its neighbor NR(u), equivalently minimizing L.
- Intuition: Optimize embedding zu to max the likelihood of random walk co-occurrences.



- 1. Simulate many short random walks starting from each node using a strategy *R*
- 2. For each node u, get $N_R(u)$ as a sequence of nodes visited by random walks starting at u
- 3. For each node u, learn its embedding by predicting which nodes are in $N_R(u)$:

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

Can efficiently approximate using negative sampling

Example: similarity based on random walks

- Given a random node u, predict its neighbor NR(u), equivalently minimizing L.
- Intuition: Optimize embedding zu to max the likelihood of random walk co-occurrences.
- Use softmax to parameterize P(v | z_u) (make v to be most similar to u).



Random walk embeddings = z_u minimizing **L**

Recall negative sampling in word2vec

- Calculating L is expensive: pick random negative samples to normalize
- Negative sampling (Jan 31)



Random walk embeddings = z_u minimizing **L**



Recall negative sampling in word2vec

- Calculating L is expensive: pick random negative samples to normalize
- Negative sampling (Jan 31): Sample k negative nodes each with prob. proportional to its degree (k=5~20)
- Gradient Descent to minimize L

Skip-gram: Negative sampling $\underbrace{exp(u_o^T v_c)}_{\overline{\Sigma}_{i=1}^V exp(u_i^T v_c)} \xrightarrow{Encourage center word and all other words to have different vectors} \xrightarrow{Encourage center word and all other words to have different vectors} \xrightarrow{Co} \sum_{n \in V} e^{n} \xrightarrow{Co} \sum_{n \in V} e^{n}$

Solution: Negative sampling (Mikolov et al., 2013)

$$\log\left(\frac{\exp(\mathbf{z}_{u}^{\top}\mathbf{z}_{v})}{\sum_{n\in V}\exp(\mathbf{z}_{u}^{\top}\mathbf{z}_{n})}\right)$$

$$\approx \log(\sigma(\mathbf{z}_{u}^{\top}\mathbf{z}_{v})) - \sum_{i=1}^{k}\log(\sigma(\mathbf{z}_{u}^{\top}\mathbf{z}_{n_{i}})), n_{i} \sim P_{V}$$
sigmoid function
random distribution
over all nodes

i.e., instead of normalizing w.r.t. all nodes, just normalize against ${\bf k}$ random negative samples

Call back Neural Network (Feb 14)

 Can we directly apply neural network to graph, taking adjacency matrix and network metrics as input?



Issues with naïve neural network

Node order; Graph size change...



Two-layer Neural Network with scalar output



Graph Neural Network

- Logic of GNN
- 1) Network neighborhood defines a computation graph
- 2) Generate **node embeddings/link messages** based on local network neighborhoods
- 3) Aggregate information across layers
- 4) Train the neural network





Graph Neural Network Training

Supervised Training

Directly train the model for a supervised task (e.g., node classification)



Unsupervised Training

- Train in an unsupervised manner:
 - Use only the graph structure
 - "Similar" nodes have similar embeddings
- Unsupervised loss function can be anything from the last section, e.g., a loss based on
 - Random walks (node2vec, DeepWalk, struc2vec)
 - Graph factorization
 - Node proximity in the graph

Example 1: Predict Twitter (X) Interaction

Dynamic GNN

TEMPORAL GRAPH NETWORKS FOR DEEP LEARNING ON DYNAMIC GRAPHS

Emanuele Rossi* Twitter

Ben Chamberlain Twitter

Fabrizio Frasca Twitter

Michael Bronstein

Twitter

Davide Eynard Twitter

Federico Monti

Twitter



Figure 1: Computations performed by TGN on a batch of time-stamped interactions. Top: embeddings are produced by the embedding module using the temporal graph and the node's memory (1). The embeddings are then used to predict the batch interactions and compute the loss (2, 3). Bottom: these same interactions are used to update the memory (4, 5, 6). This is a simplified flow of operations which would prevent the training of all the modules in the bottom as they would not receiving a gradient. Section 3.2 explains how to change the flow of operations to solve this problem and figure 2 shows the complete diagram.



Rossi, E., Chamberlain, B., Frasca, F., Eynard, D., Monti, F., & Bronstein, M. (2020). Temporal graph networks for deep learning on dynamic graphs. arXiv preprint arXiv:2006.10637.

Example 2: GraphSAGE

Heterogeneous Nodes and Edges

Inductive Representation Learning on Large Graphs

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Figure 1: Visual illustration of the GraphSAGE sample and aggregate approach.



Hamilton, W., Ying, Z., & Leskovec, J. (2017). Inductive representation learning on large graphs. *Advances in neural information processing systems*, *30*.

Issues with GNN

- Lost global information (Complex system studies are good at dealing with global info)
- Interpretability (Ongoing research)



Fig. 1. An overview of our proposed taxonomy. We categorize existing GNN explanation approaches into two branches: instance-level methods and model-level methods. For the instance-level methods, the gradients/features-based methods include SA [54], Guided BP [54], CAM [55], and Grad-CAM [55]; the perturbation-based methods are GNNExplainer [46], PGExplainer [47], ZORRO [56], GraphMask [57], Causal Screening [58], and SubgraphX [48]; the decomposition methods contains LRP [54], [59], Excitation BP [55] and GNN-LRP [60]; the surrogate methods include GraphLime [61], RelEx [62], and PGM-Explainer [63]. For the model-level methods, the only existing approach is XGNN [45].

JOHNS HOPKINS WHITING SCHOOL of ENGINEERING Yuan, H., Yu, H., Gui, S., & Ji, S. (2022). Explainability in graph neural networks: A taxonomic survey. IEEE transactions **50** on pattern analysis and machine intelligence, 45(5), 5782-5799.

Examples of complex system network studies

- Watts, D. J., & Strogatz, S. H. (1998). Collective dynamics of 'small-world'networks. nature, 393(6684), 440-442.
- Barabási, A. L., & Albert, R. (1999). Emergence of scaling in random networks. science, 286(5439), 509-512.
- Muscoloni, A., Thomas, J. M., Ciucci, S., Bianconi, G., & Cannistraci, C. V. (2017). Machine learning meets complex networks via coalescent embedding in the hyperbolic space. Nature communications, 8(1), 1615.
- Wang, D., & Barabási, A. L. (2021). The science of science. Cambridge University Press.



Recommended readings

- Grover, A., & Leskovec, J. (2016, August). node2vec: Scalable feature learning for networks. In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 855-864).
- Xu, K., Hu, W., Leskovec, J., & Jegelka, S. (2018). How powerful are graph neural networks?. arXiv preprint arXiv:1810.00826.
- Yuan, H., Yu, H., Gui, S., & Ji, S. (2022). Explainability in graph neural networks: A taxonomic survey. IEEE transactions on pattern analysis and machine intelligence, 45(5), 5782-5799.

