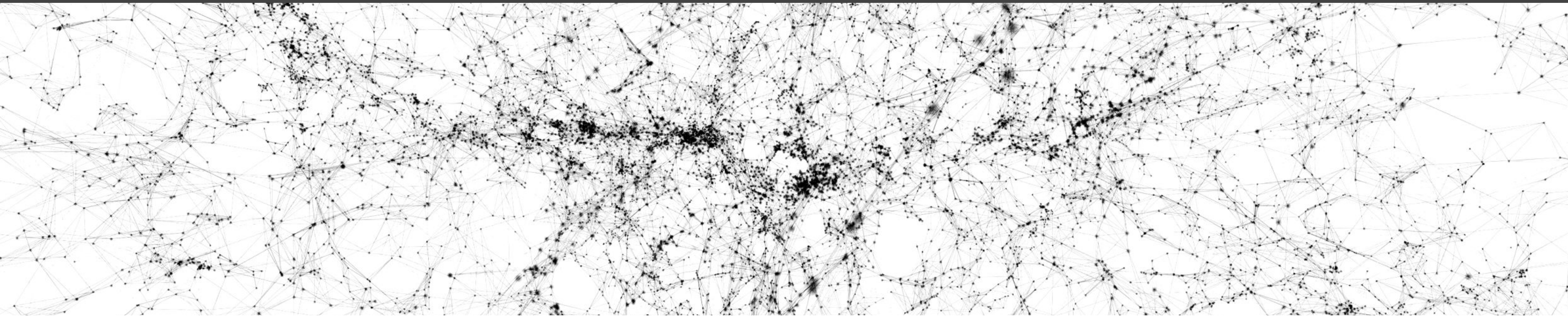
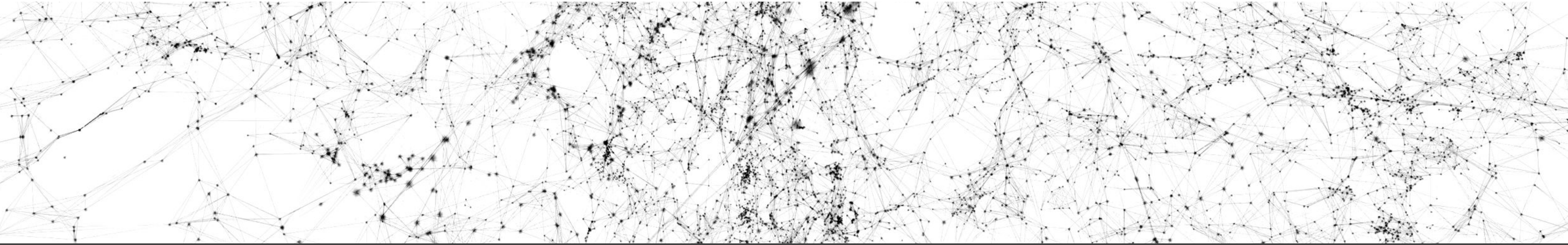


Link Prediction

Analysis of complex interconnected data



Quick Notes

- Last assignment is out and is due on Oct 18th
  - http://www.reirab.com/Teaching/NS20/Assignment_3.pdf
  - Submit 2 files (report.pdf, code.zip) as a Group (pairs or two or individual) in Mycourses
- Please select your seminars
  - Due date for selection: Tuesday night (let me know if there are any issues)
  - Please put your name for **two** slots, do not change the entries that are already booked
  - Find the link to editable spreadsheet in slack or Mycourses
- Any questions?

Deadlines

- assignment 1 due on Sep. 20th
- assignment 2 due on Oct. 4th
- assignment 3 due on Oct. 18th
- project proposal slides due on Oct. 25th
- project proposal due on Nov. 1th
- Reviews (first round) due on Nov. 8th
- project progress report due on Nov. 22nd
- Reviews (second round) due on Nov. 29th
- project final report slides due on Dec. 1st
- project final report due on Dec. 6th
- Reviews (third round) due on Dec. 13th
- project revised report and rebuttal due on Dec. 20th
- note: dates are tentative, please check them for the updated deadlines

Dynamics- Quick recap

- Graphs & Time: diffusion on graph, cascade as the graph, dynamic graph, streaming graph
- Diffusion on Graphs
  - An entity that spreads/flows over the graph: disease, meme & news (social media), etc.
  - Epidemic modelling with contact graphs & between population dynamics
  - Classic compartment based models
    - Differential equations of compartment size changes (S, I, E, R)
    - Total outbreak size (asymptotic value of R) relates to the size of giant component in ER graph
      - We have an outbreak with the similar condition as having a giant component
    - Assume full mixing (= ER contact graph)
  - Contact graph based models
    - Simulate (each node has a state, simple but powerful)
      - some measures can be derived as well, e.g. an individual's probability of infection at early times is proportional to eigenvector centrality & outbreak sizes connects to percolation
- Dynamic Graphs
  - Dynamic network analysis: all statics extended, Patten, Measure and Module examples

Common prediction tasks

- Link Prediction
- Node Classification
- Graph Classification

Examples:

https://paperswithcode.com/task/link-prediction

https://paperswithcode.com/task/node-classification

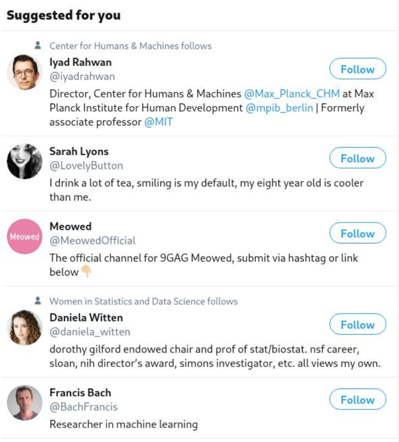
https://paperswithcode.com/task/graph-classification

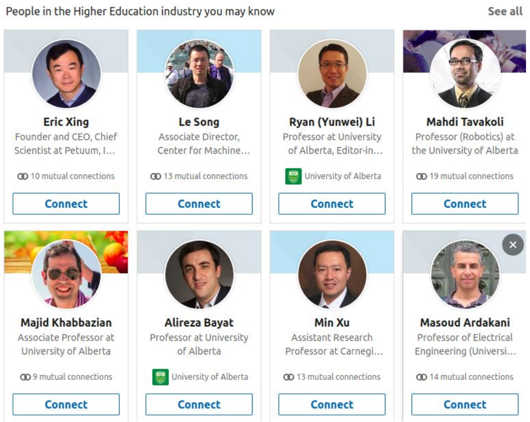
What is unsupervised node classification?

Link Prediction

Given a graph G(V,E) predict future/missing links between nodes

- Modeling of network evolution
- Predict likely interactions, not explicitly observed (e.g. terrorist network monitoring)
- Link recommendation: “friend” suggestion in social networks

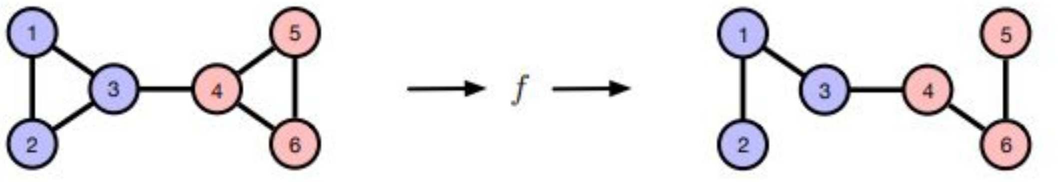




Predicting missing links

Only a subset of edges are observed

Sparse ⇒ searching for O(n) needles in a $\Theta(n^2)$ haystack



actual $G = (V, E)$ observed $G_\circ = (V, E_\circ)$

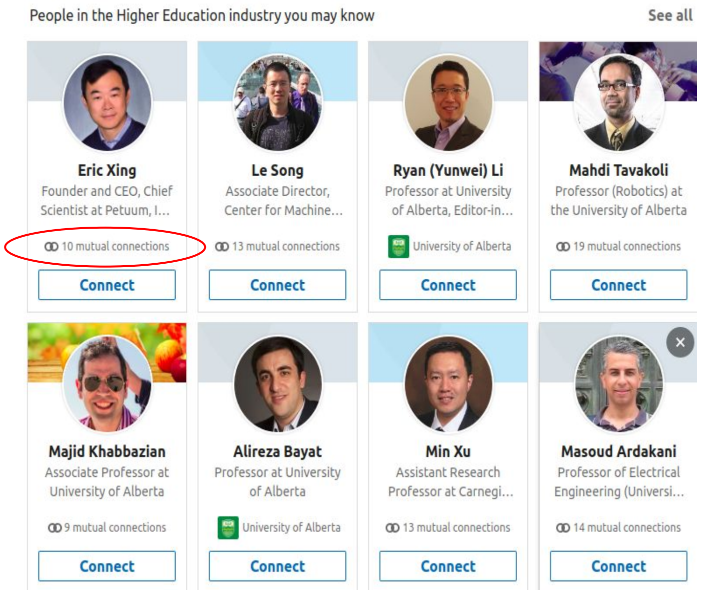
[From Clauset's Slides]

Link prediction

Score(i , j)

local topological predictors

- Number of common neighbors
- Number of shortest paths
- Product of degree
- Same cluster
- etc.



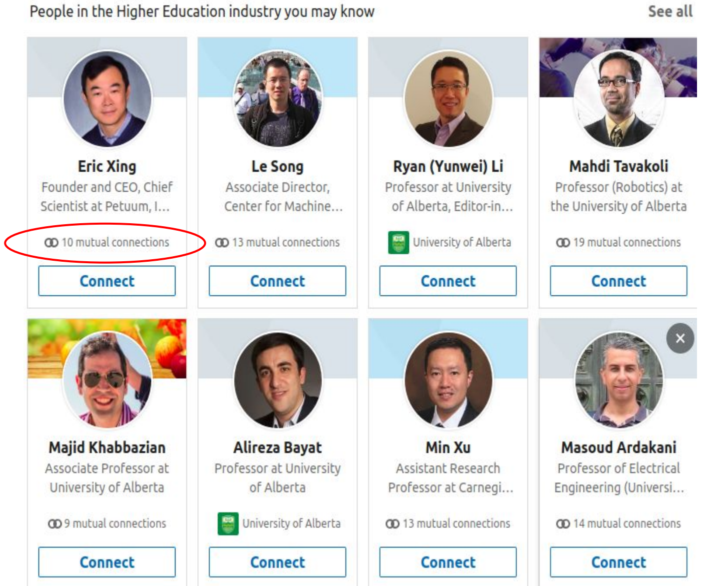
[From Clauset's Slides]

Link prediction

Score(i , j)

local topological predictors

- **Number of common neighbors**
- Number of shortest paths
- Product of degree
- Same cluster
- etc.



From Clauset's Slides

Link prediction

Jaccard coefficient

$$\text{Jaccard}(i, j) = \frac{|\nu(i) \cap \nu(j)|}{|\nu(i) \cup \nu(j)|}$$

score(i, j) = Jaccard(i, j) + Uniform(0, ε)

What happens to the network if we add edges based on this?

From Clauset's Slides

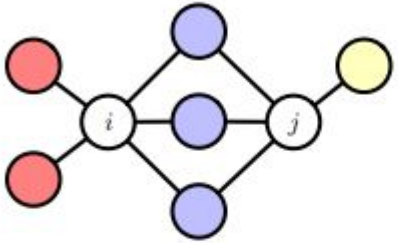
Link prediction

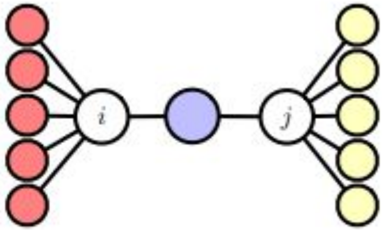
Jaccard coefficient

$$\text{Jaccard}(i, j) = \frac{|\nu(i) \cap \nu(j)|}{|\nu(i) \cup \nu(j)|}$$

score(i, j) = Jaccard(i, j) + Uniform(0, **ε**)

What happens to the network if we add edges based on this? Closes triangles





Example: Jaccard(i, j), what is it for this example ?

[From Clauset's Slides]

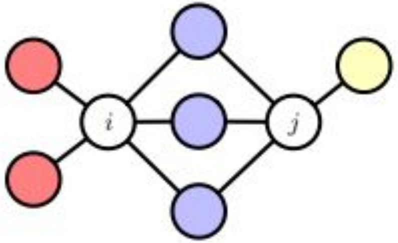
Link prediction

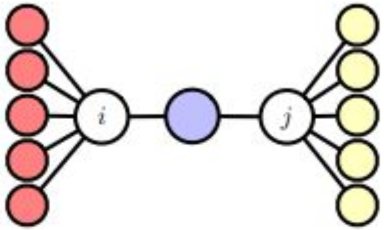
Jaccard coefficient

$$\text{Jaccard}(i, j) = \frac{|\nu(i) \cap \nu(j)|}{|\nu(i) \cup \nu(j)|}$$

score(i, j) = Jaccard(i, j) + Uniform(0, **ε**)

What happens to the network if we add edges based on this? Closes triangles





Example: Jaccard(i, j) of **0.50** (3/6) vs **0.091** (1/11)

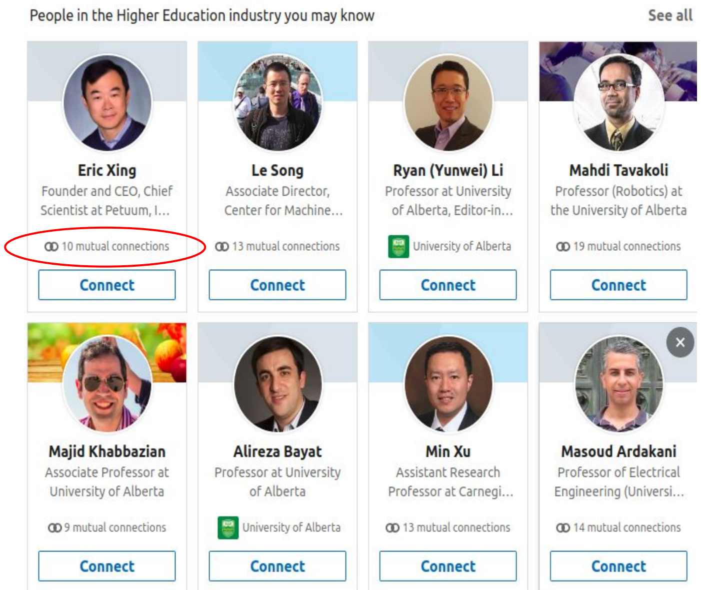
[From Clauset's Slides]

Link prediction

Score(i , j)

local topological predictors

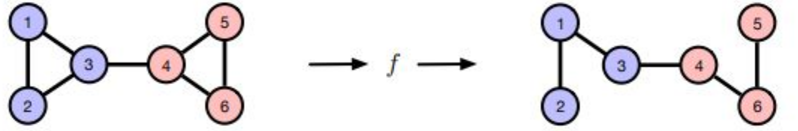
- Number of common neighbors
- Number of shortest paths
- **Product of degree**
    - nodes with high degrees are likely themselves to be connected
- Same cluster
- etc.



From Clauset's Slides

Link prediction

degree product: score(i, j) = $d_i \, d_j$ + Uniform(0, **ε**)



actual $G = (V, E)$ → f → observed $G_\circ = (V, E_\circ)$

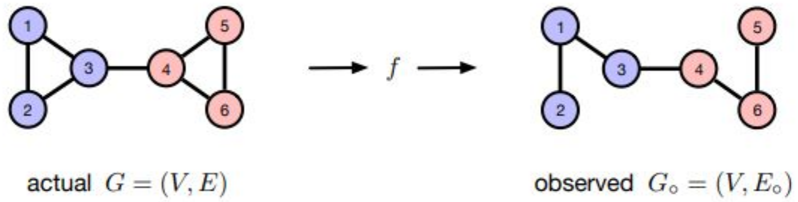
i	j	Jaccard score(i,j)
4	**5**	$1/2 + r$
2	**3**	$1/2 + r$
3	6	$1/3 + r$
1	4	$1/3 + r$
1	5	r
1	6	r
2	6	r
2	4	r
2	5	r
3	5	r

i	j	degree product score(i,j)
1	4	$4 + r$
1	6	$4 + r$
3	6	$4 + r$
1	5	$2 + r$
2	**3**	$2 + r$
2	6	$2 + r$
2	4	$2 + r$
3	5	$2 + r$
4	**5**	$2 + r$
2	5	$1 + r$

From Clauset's Slides

Link prediction

degree product: score(i, j) = $d_i\ d_j$ + Uniform(0, **ε**)



i	j	Jaccard score(i, j)
4	**5**	$1/2 + r$
2	**3**	$1/2 + r$
3	6	$1/3 + r$
1	4	$1/3 + r$
1	5	r
1	6	r
2	6	r
2	4	r
2	5	r
3	5	r

i	j	degree product score(i, j)
1	4	$4 + r$
1	6	$4 + r$
3	6	$4 + r$
1	5	$2 + r$
2	**3**	$2 + r$
2	6	$2 + r$
2	4	$2 + r$
3	5	$2 + r$
4	**5**	$2 + r$
2	5	$1 + r$

Which one is more accurate?

From Clauset's Slides

Measuring performance for ranked output

We can consider a threshold and convert it to a **binary classification**

{every i, j is either a missing link or not}

Accuracy = (TP+TN) / (P+N)
Precision = TP / RP
Recall = TP / P {also called sensitivity}
F1 score = 2. Precision x Recall / (Precision + Recall)
{Harmonic mean}

Miss rate = FN / P
Fallout = FP / N {also called false positive rate}
False discovery rate = FP / RP
Selectivity = TN / N {also called specificity}
False omission rate = FN / RN
Negative predictive value = TN / RN

	Truth		Σ
Results	TP	FP	RP
	FN	TN	RN
Σ	P	N	

i	j	Jaccard score(i,j)
4	**5**	$1/2+r$
2	**3**	$1/2+r$
3	6	$1/3+r$
1	4	$1/3+r$
1	5	r
1	6	r
2	6	r
2	4	r
2	5	r
3	5	r

Predict edge

Measuring performance

binary classification ⇒ every candidate i, j is either a missing link or not

TPR = TP/P (**recall**, sensitivity)
Links above threshold / Total Positives

FPR = FP/N (**fallout**, false alarm)
Non-links above threshold / Total Negatives

link

threshold

nonlink

i	j	Jaccard score(i,j)	i	j	degree product score(i,j)
4	**5**	$1/2+r$	1	4	$4+r$
2	**3**	$1/2+r$	1	6	$4+r$
3	6	$1/3+r$	3	6	$4+r$
1	4	$1/3+r$	1	5	$2+r$
1	5	r	**2**	**3**	$2+r$
1	6	r	2	6	$2+r$
2	6	r	2	4	$2+r$
2	4	r	3	5	$2+r$
2	5	r	**4**	**5**	$2+r$
3	5	r	2	5	$1+r$

TPR = ?, FPR = ?

	Truth		Σ
results	**TP = 2**	**FP = 2**	**RP = 4**
	FN = 0	**TN = 6**	**RN = 6**
Σ	**P = 2**	**N = 8**	

Jaccard

TPR = ?, FPR = ?

	Truth		Σ
results	**TP = 0**	**FP = 4**	**RP = 4**
	FN = 2	**TN= 4**	**RN = 6**
Σ	**P = 2**	**N = 8**	

degree product

Measuring performance

binary classification ⇒ every candidate i, j is either a missing link or not

TPR = TP/P (**recall**, sensitivity)
Links above threshold / Total Positives

FPR = FP/N (**fallout**, false alarm)
Non-links above threshold / Total Negatives

link

threshold

nonlink

i	j	Jaccard score(i,j)	i	j	degree product score(i,j)
4	**5**	$1/2+r$	1	4	$4+r$
2	**3**	$1/2+r$	1	6	$4+r$
3	6	$1/3+r$	3	6	$4+r$
1	4	$1/3+r$	1	5	$2+r$
1	5	r	**2**	**3**	$2+r$
1	6	r	2	6	$2+r$
2	6	r	2	4	$2+r$
2	4	r	3	5	$2+r$
2	5	r	**4**	**5**	$2+r$
3	5	r	2	5	$1+r$

TPR = 2/2 = 1, FPR = 2/8=0.25

	Truth		Σ
results	TP = 2	FP = 2	RP = 4
	FN = 0	TN = 6	RN = 6
Σ	P = 2	N = 8	

Jaccard

TPR = 0/2 = 0, FPR = 4/8=0.5

	Truth		Σ
results	TP = 0	FP = 4	RP = 4
	FN = 2	TN= 4	RN = 6
Σ	P = 2	N = 8	

degree product

Measuring performance for ranked output

We can consider a threshold and convert it to a **binary classification**

{every i, j is either a missing link or not}

	Truth		Σ
Results	TP	FP	RP
	FN	TN	RN
Σ	P	N	

Accuracy = (TP+TN) / (P+N)
Precision = TP / RP
Recall = TP / P {also called sensitivity}
F1 score = 2. Precision x Recall / (Precision + Recall) {Harmonic mean}

Miss rate = FN / P
Fallout = FP / N {also called false positive rate}
False discovery rate = FP / RP
Selectivity = TN / N {also called specificity}
False omission rate = FN / RN
Negative predictive value = TN / RN

Measures depend on the threshold

The tradeoff between precision and recall

no false positive
also no true positive

i	j	Jaccard score(i, j)
4	**5**	$1/2 + r$
2	**3**	$1/2 + r$
3	6	$1/3 + r$
1	4	$1/3 + r$
1	5	r
1	6	r
2	6	r
2	4	r
2	5	r
3	5	r

no false negative
also no true negative

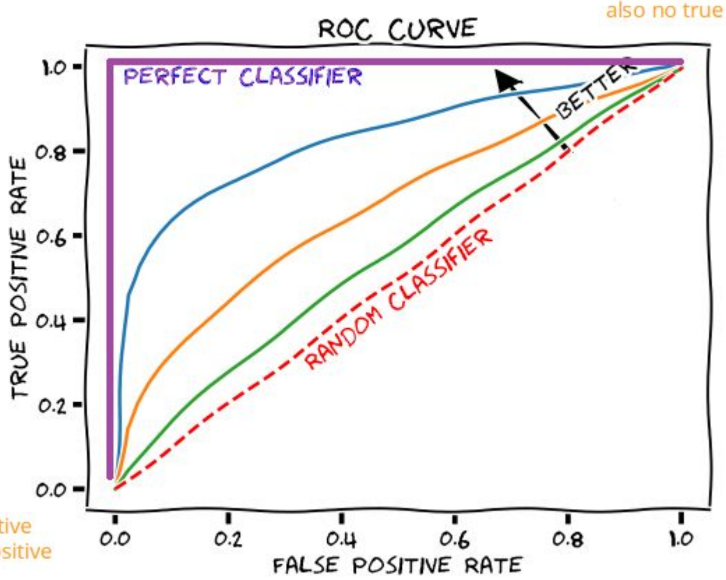
Threshold invariant: ROC & AUC

Receiver Operating Characteristic (ROC) as a function of prediction threshold

TPR(t) = TP(t)/P (recall, sensitivity at t)
FPR(t) = FP(t)/N (fallout, false alarm at t)

Area Under the Curve (AUC) of ROC
gives the probability of ranking a random positive edge higher than a random negative edge

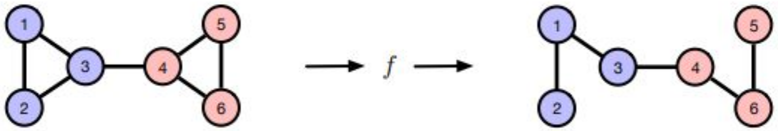
no false negative
also no true negative



no false positive
also no true positive

Threshold invariant: ROC & AUC, example

binary classification ⇒ every candidate i, j is either a missing link or not



actual $G = (V, E)$ observed $G_\circ = (V, E_\circ)$

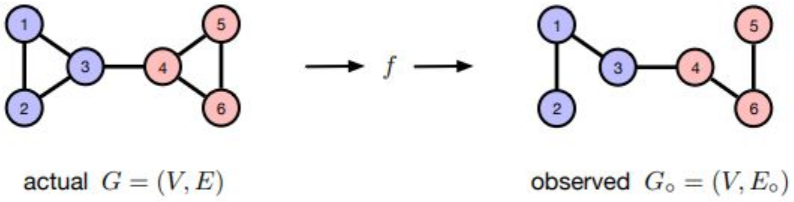
TPR = TP/P (**recall**, sensitivity)

FPR = FP/N (**fallout**, false alarm)

	i	j	Jaccard score(i,j)	i	j	degree product score(i,j)
link	**4**	**5**	$1/2 + r$	1	4	$4 + r$
link	**2**	**3**	$1/2 + r$	1	6	$4 + r$
link	3	6	$1/3 + r$	3	6	$4 + r$
link	1	4	$1/3 + r$	1	5	$2 + r$
threshold						
nonlink	1	5	r	**2**	**3**	$2 + r$
nonlink	1	6	r	2	6	$2 + r$
nonlink	2	6	r	2	4	$2 + r$
nonlink	2	4	r	3	5	$2 + r$
nonlink	2	5	r	**4**	**5**	$2 + r$
nonlink	3	5	r	2	5	$1 + r$

Threshold invariant: ROC & AUC, example

binary classification ⇒ every candidate i, j is either a missing link or not



threshold

i	j	Jaccard score(i,j)
4	**5**	$1/2 + r$
2	**3**	$1/2 + r$
3	6	$1/3 + r$
1	4	$1/3 + r$
1	5	r
1	6	r
2	6	r
2	4	r
2	5	r
3	5	r

i	j	degree product score(i,j)
1	4	$4 + r$
1	6	$4 + r$
3	6	$4 + r$
1	5	$2 + r$
2	**3**	$2 + r$
2	6	$2 + r$
2	4	$2 + r$
3	5	$2 + r$
4	**5**	$2 + r$
2	5	$1 + r$

TPR = fraction of links above threshold

FPR = fraction of non-links above threshold

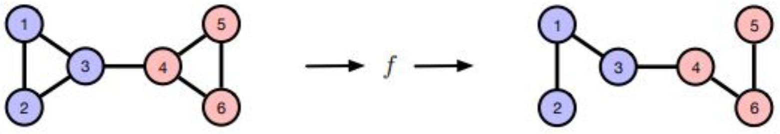
AUC = Σ_t TPR(t) (FPR (t)- FPR (t-1))

box-rule approximation

From Clauset's Slides

Threshold invariant: ROC & AUC, example

binary classification ⇒ every candidate i, j is either a missing link or not

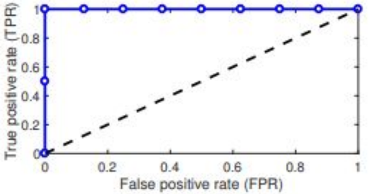


actual $G = (V, E)$ observed $G_\circ = (V, E_\circ)$

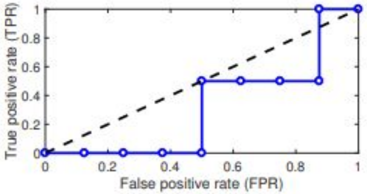
threshold

i	j	Jaccard score(i,j)
4	**5**	$1/2 + r$
2	**3**	$1/2 + r$
3	6	$1/3 + r$
1	4	$1/3 + r$
1	5	r
1	6	r
2	6	r
2	4	r
2	5	r
3	5	r

i	j	degree product score(i,j)
1	4	$4 + r$
1	6	$4 + r$
3	6	$4 + r$
1	5	$2 + r$
2	**3**	$2 + r$
2	6	$2 + r$
2	4	$2 + r$
3	5	$2 + r$
4	**5**	$2 + r$
2	5	$1 + r$



Jaccard coefficient, AUC = 1.00



degree product, AUC = 0.31

From Clauset's Slides

Topological Link Predictors

CN	common neighbors of i, j
SP	shortest path between i, j
LHN	Leicht-Holme-Newman index of neighbor sets of i, j
PPR	j-th entry of the personalized page rank of node i
PA	preferential attachment (degree product) of i, j
JC	Jaccard's coefficient of neighbor sets of i, j
AA	Adamic/Adar index of i, j
RA	resource allocation index of i, j
LRA	entry i, j in low rank approximation (LRA) via singular value decomposition (SVD)
dLRA	dot product of columns i and j in LRA via SVD for each pair of nodes i, j
mLRA	average of entries i and j's neighbors in low rank approximation
LRA-approx	an approximation of LRA
dLRA-approx	an approximation of dLRA
mLRA-approx	an approximation of mLRA
$\text{LCC}_i, \text{LCC}_j$	local clustering coefficients for i and j
$\text{AND}_i, \text{AND}_j$	average neighbor degrees for i and j
$\text{SPBC}_i, \text{SPBC}_j$	shortest-path betweenness centralities for i and j
CC_i, CC_j	closeness centralities for i and j
DC_i, DC_j	degree centralities for i and j
EC_i, EC_j	eigenvector centralities for i and j
KC_i, KC_j	Katz centralities for i and j
$\text{LNT}_i, \text{LNT}_j$	local number of triangles for i and j
PR_i, PR_j	Page rank values for i and j
LC_i, LC_j	load centralities for i and j

There are many **alternatives** to give a score to a given pair of nodes (i,j)

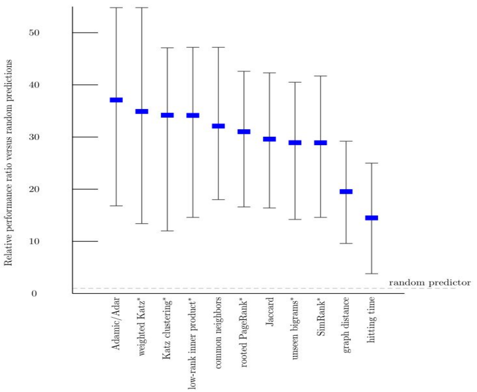
Many also used as similarity measures since homophily is a strong force in link creation

Ghasemian A, Hosseinmardi H, Galstyan A, Airoldi EM, Clauset A. Stacking Models for Nearly Optimal Link Prediction in Complex Networks. PNAS 2020.

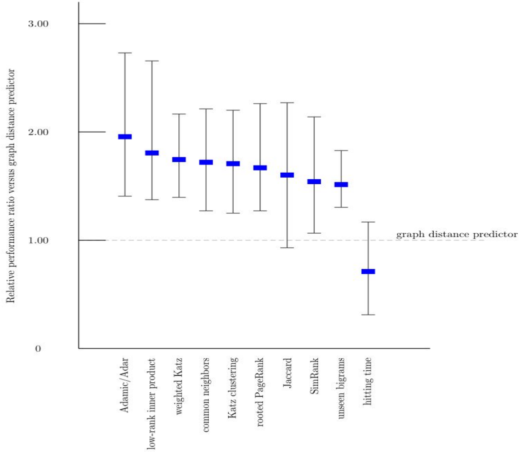
See also A Survey of Link Prediction in Complex Networks, 2015 & Link prediction in complex networks: A survey, 2011

Common neighbour is a decent predictor

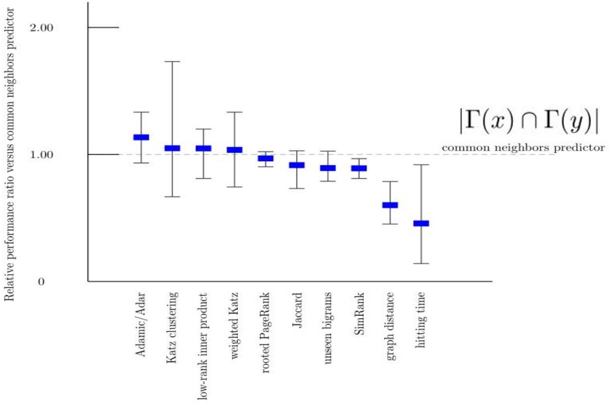
Random



Graph distance



Common neighbor



Adamic/Adar: a notable measure

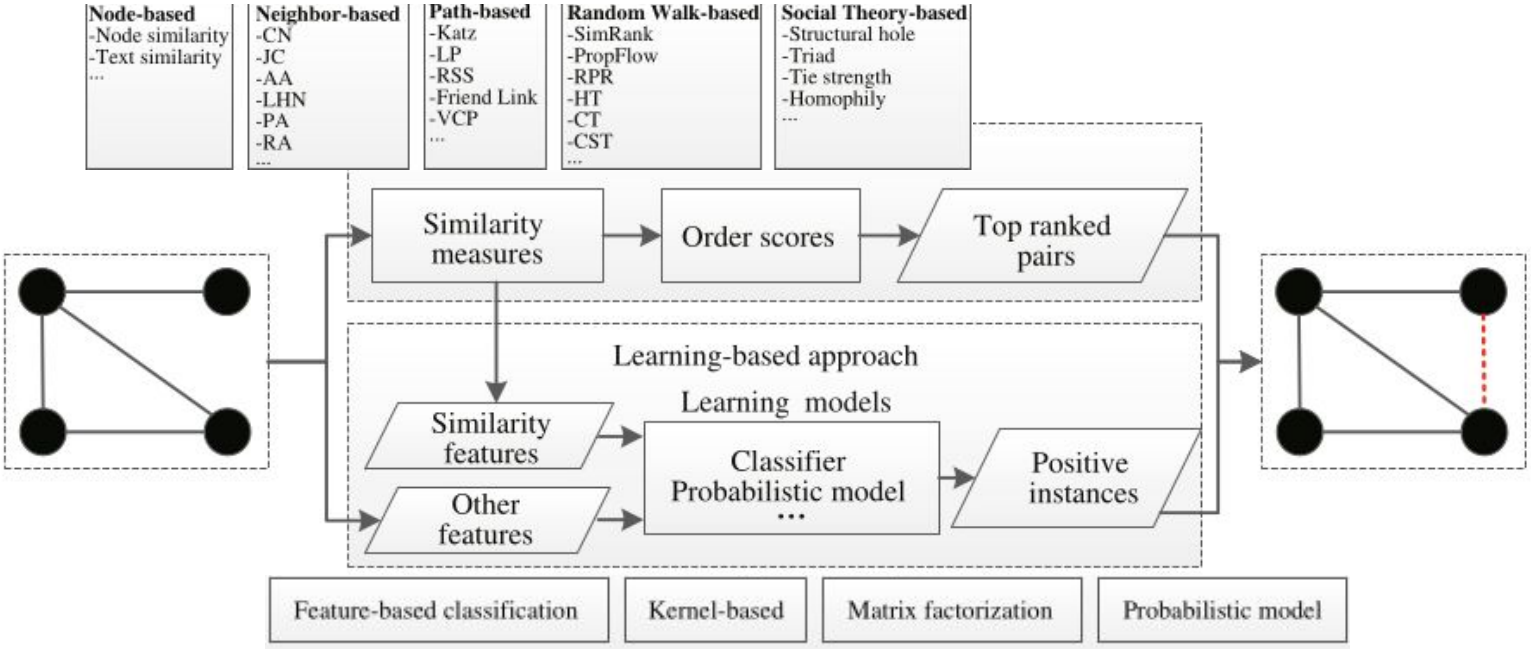
Sums over size inverse of log of degree of common neighbours

$$\sum_{z\in\Gamma(x)\cap\Gamma(y)} \frac{1}{\log|\Gamma(z)|}$$

Liben-Nowell D, Kleinberg J. The link-prediction problem for social networks. Journal of the American society for information science and technology. 2007 May;58(7):1019-31.

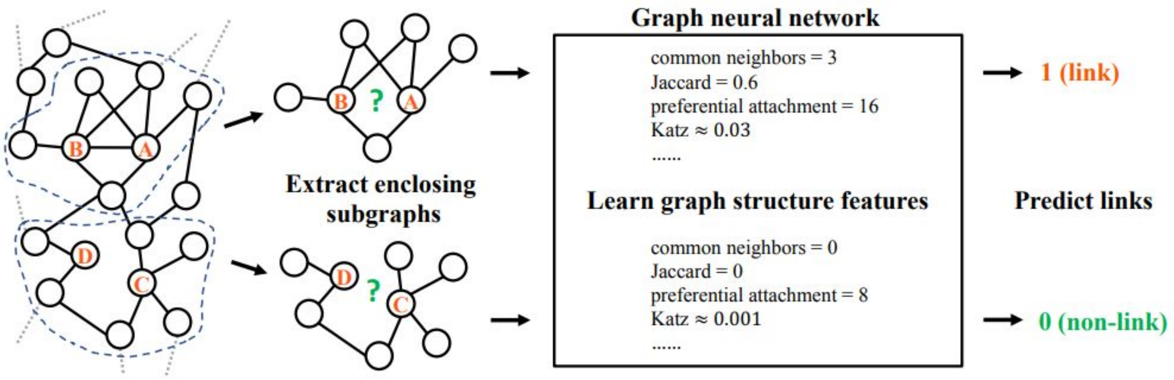
We can learn to link

Wang P, Xu B, Wu Y, Zhou X. Link prediction in social networks: the state-of-the-art. Science China Information Sciences. 2015 Jan 1;58(1):1-38.



Learn the features as well

Instead of explicit features, automatically learn a “heuristic” that suits the current network e.g. by extracting a local enclosing subgraph around it, and uses a GNN to learn general graph structure features for link prediction



Zhang M, Chen Y. Link prediction based on graph neural networks. NeurIPS 2018

Learn the features as well

Instead of explicit features, automatically learn a "heuristic" that suits the current network e.g. by extracting a local enclosing subgraph around it, and uses a GNN to learn general graph structure features for link prediction

Table 1: Comparison with heuristic methods (AUC).

Data	CN	Jaccard	PA	AA	RA	Katz	PR	SR	ENS	WLK	WLNM	SEAL
USAir	93.80±1.22	89.79±1.61	88.84±1.45	95.06±1.03	95.77±0.92	92.88±1.42	94.67±1.08	78.89±2.31	88.96±1.44	**96.63**±0.73	95.95±1.10	**96.62**±0.72
NS	94.42±0.95	94.43±0.93	68.65±2.03	94.45±0.93	94.45±0.93	94.85±1.10	94.89±1.08	94.79±1.08	97.64±0.25	98.57±0.51	98.61±0.49	**98.85**±0.47
PB	92.04±0.35	87.41±0.39	90.14±0.45	92.36±0.34	92.46±0.37	92.92±0.35	93.54±0.41	77.08±0.80	90.15±0.45	93.83±0.59	93.49±0.47	**94.72**±0.46
Yeast	89.37±0.61	89.32±0.60	82.20±1.02	89.43±0.62	89.45±0.62	92.24±0.61	92.76±0.55	91.49±0.57	82.36±1.02	95.86±0.54	95.62±0.52	**97.91**±0.52
C.ele	85.13±1.61	80.19±1.64	74.79±2.04	86.95±1.40	87.49±1.41	86.34±1.89	**90.32**±1.49	77.07±2.00	74.94±2.04	89.72±1.67	86.18±1.72	**90.30**±1.35
Power	58.80±0.88	58.79±0.88	44.33±1.02	58.79±0.88	58.79±0.88	65.39±1.59	66.00±1.59	76.15±1.06	79.52±1.78	82.41±3.43	84.76±0.98	**87.61**±1.57
Router	56.43±0.52	56.40±0.52	47.58±1.47	56.43±0.51	56.43±0.51	38.62±1.35	38.76±1.39	37.40±1.27	47.58±1.48	87.42±2.08	94.41±0.88	**96.38**±1.45
E.coli	93.71±0.39	81.31±0.61	91.82±0.58	95.36±0.34	95.95±0.35	93.50±0.44	95.57±0.44	62.49±1.43	91.89±0.58	96.94±0.29	97.21±0.27	**97.64**±0.22

Table 2: Comparison with latent feature methods (AUC).

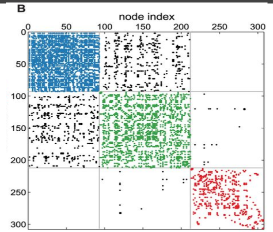
Data	MF	SBM	N2V	LINE	SPC	VGAE	SEAL
USAir	94.08±0.80	94.85±1.14	91.44±1.78	81.47±10.71	74.22±3.11	89.28±1.99	**97.09**±0.70
NS	74.55±4.34	92.30±2.26	91.52±1.28	80.63±1.90	89.94±2.39	94.04±1.64	**97.71**±0.93
PB	94.30±0.53	93.90±0.42	85.79±0.78	76.95±2.76	83.96±0.86	90.70±0.53	**95.01**±0.34
Yeast	90.28±0.69	91.41±0.60	93.67±0.46	87.45±3.33	93.25±0.40	93.88±0.21	**97.20**±0.64
C.ele	85.90±1.74	86.48±2.60	84.11±1.27	69.21±3.14	51.90±2.57	81.80±2.18	**89.54**±2.04
Power	50.63±1.10	66.57±2.05	76.22±0.92	55.63±1.47	**91.78**±0.61	71.20±1.65	84.18±1.82
Router	78.03±1.63	85.65±1.93	65.46±0.86	67.15±2.10	68.79±2.42	61.51±1.22	**95.68**±1.22
E.coli	93.76±0.56	93.82±0.41	90.82±1.49	82.38±2.19	94.92±0.32	90.81±0.63	**97.22**±0.28

Zhang M, Chen Y. Link prediction based on graph neural networks. NeurIPS 2018

Link prediction approaches

- local topological predictors
- Global predictors, learning
  - **Model-based**
    - Fit a model to data by maximizing likelihood which is defined in terms of edge probabilities ⇒ $\Pr(i \rightarrow j \mid \theta)$
      - E.g. stochastic block model
  - **Optimization-based**
    - Adding an edge increases a measure, e.g. Q modularity
  - **Embedding-based**
    - Proximity in the embedded space {put connected nodes close together}

From Clauset's Slides



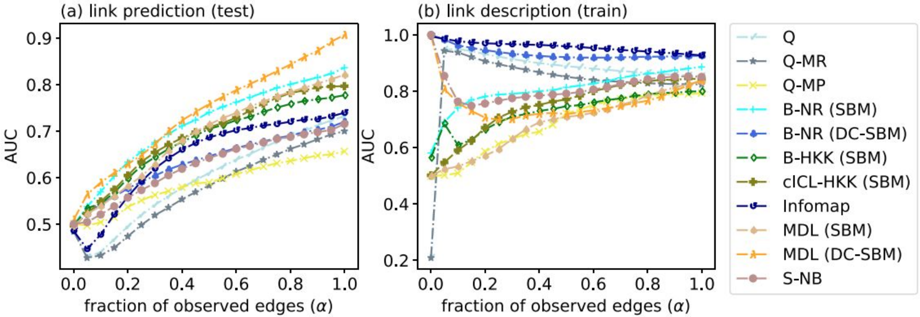
Model based link prediction

Infer Pr (i → j | θ) for each candidate pair based on maximizing likelihood of the observed graph or other optimizations

SBM variants, Q-modularity and Infomap, e.g. Number of edges between module node i and j belong to divided by maximum possible edges between those modules

Assume links are within modules

Abbreviation	Description
Q	modularity, Newman-Girvan
Q-MR	modularity, Newman's multiresolution
Q-MP	modularity, message passing
B-NR (SBM)	Bayesian stochastic block model, Newman and Reinert
B-NR (DC-SBM)	Bayesian degree-corrected stochastic block model, Newman and Reinert
B-HKK (SBM)	Bayesian stochastic block model, Hayashi, Konishi and Kawamoto
cICL-HKK (SBM)	Corrected integrated classification likelihood, stochastic block model
Infomap	Map equation
MDL (SBM)	Minimum description length, stochastic block model
MDL (DC-SBM)	Minimum description length, degree-corrected stochastic block model
S-NB	Spectral with non-backtracking matrix

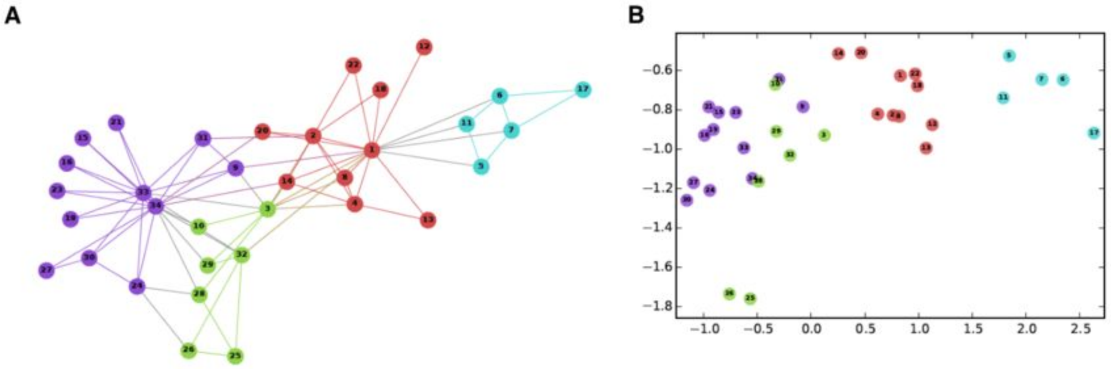


Evaluating Overfit and Underfit in Models of Network Community Structure, TKDE 2020

Embedding based link prediction

G ⟶ embed in vector space ⟶ distance in the embedded space

Node embedding methods derive a vector representation per each node in the graph so that connected nodes have similar vectors ⇒ close in the embedded space means more likely to be linked



Matrix factorization based
e.g. svd
⇒
Deep learning methods
e.g. deepwalk

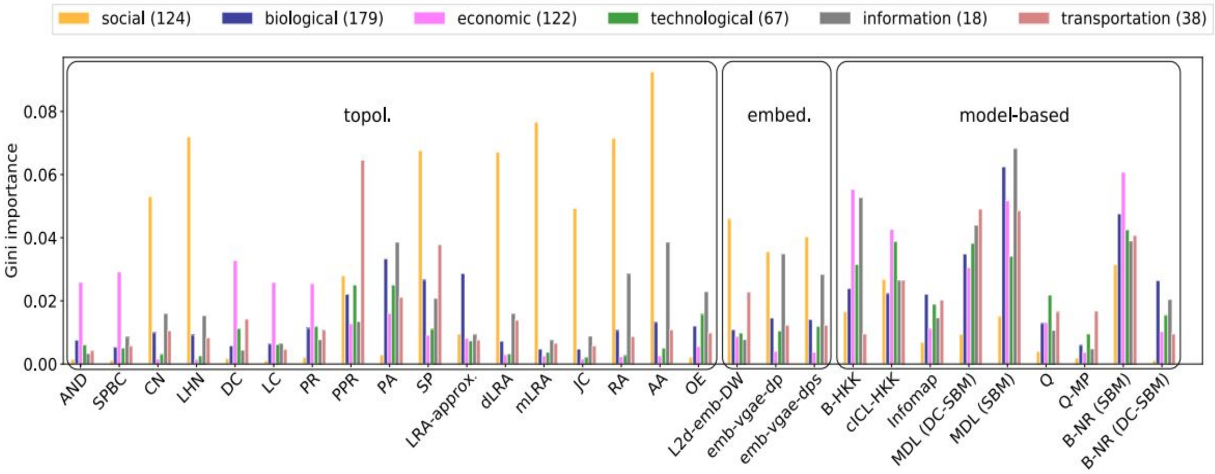
What embedding to use? [Graph Representation Learning](#)

See [A Tutorial on Network Embeddings,](#) 2018

Which one is the best?

no one predictor or family is best, or worst, across all realistic inputs

550 structurally diverse networks from six scientific domains



Ghasemian A, Hosseinmardi H, Galstyan A, Airoldi EM, Clauset A. Stacking Models for Nearly Optimal Link Prediction in Complex Networks. PNAS 2020.

Which one to choose?

Stack the models

learns to apply the best individual predictor according to the input's characteristics

algorithm	AUC	precision	recall
Q	0.7 ± 0.14	0.14 ± 0.17	0.67 ± 0.15
Q-MR	0.67 ± 0.15	0.12 ± 0.17	0.63 ± 0.13
Q-MP	0.64 ± 0.15	0.09 ± 0.11	0.59 ± 0.17
B-NR (SBM)	0.81 ± 0.13	0.13 ± 0.12	0.65 ± 0.22
B-NR (DC-SBM)	0.7 ± 0.2	0.12 ± 0.12	0.61 ± 0.24
cICL-HKK	0.79 ± 0.13	0.14 ± 0.14	0.58 ± 0.25
B-HKK	0.77 ± 0.13	0.11 ± 0.1	0.51 ± 0.26
Infomap	0.73 ± 0.14	0.12 ± 0.12	0.68 ± 0.13
MDL (SBM)	0.79 ± 0.15	0.14 ± 0.13	0.57 ± 0.3
MDL (DC-SBM)	0.84 ± 0.1	0.13 ± 0.11	0.78 ± 0.12
S-NB	0.71 ± 0.19	0.12 ± 0.13	0.66 ± 0.17
mean model-based	0.74 ± 0.16	0.12 ± 0.13	0.63 ± 0.21
mean indiv. topol.	0.6 ± 0.13	0.09 ± 0.16	0.53 ± 0.35
mean indiv. topol. & model	0.63 ± 0.15	0.09 ± 0.16	0.55 ± 0.33
emb-DW	0.63 ± 0.23	0.17 ± 0.19	0.42 ± 0.35
emb-vgae	0.69 ± 0.19	0.05 ± 0.05	0.69 ± 0.21
all topol.	0.86 ± 0.11	0.42 ± 0.33	0.44 ± 0.32
all model-based	0.83 ± 0.12	0.39 ± 0.34	0.3 ± 0.29
all embed.	0.77 ± 0.16	0.32 ± 0.32	0.32 ± 0.31
all topol. & model	0.87 ± 0.1	0.48 ± 0.36	0.35 ± 0.35
all topol. & embed.	0.84 ± 0.13	0.4 ± 0.34	0.39 ± 0.33
all model & embed.	0.84 ± 0.13	0.36 ± 0.32	0.36 ± 0.31
all topol., model & embed.	0.85 ± 0.14	0.42 ± 0.34	0.39 ± 0.33

550 structurally diverse networks from six scientific domains

Ghasemian A, Hosseinmardi H, Galstyan A, Airoldi EM, Clauset A. Stacking Models for Nearly Optimal Link Prediction in Complex Networks. arXiv preprint arXiv:1909.07578. 2019 Sep 17.

Which one to choose?

Stack the models

learns to apply the best individual predictor according to the input's characteristics

Near perfect in social networks

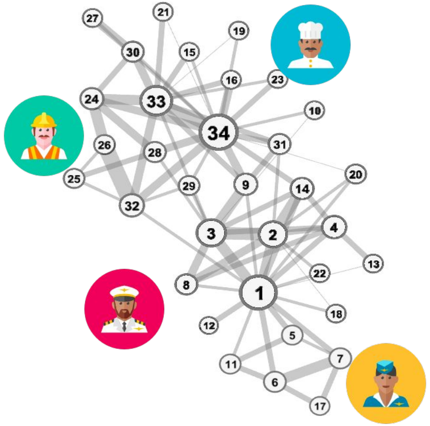
Algorithm	AUC	Precision	Recall
Q	0.89 ± 0.07	0.42 ± 0.13	0.85 ± 0.08
Q-MR	0.87 ± 0.07	0.38 ± 0.16	0.78 ± 0.07
Q-MP	0.86 ± 0.08	0.25 ± 0.07	0.83 ± 0.09
B-NR (SBM)	0.93 ± 0.06	0.3 ± 0.08	0.85 ± 0.12
B-NR (DC-SBM)	0.93 ± 0.07	0.28 ± 0.08	0.88 ± 0.08
cICL-HKK	0.93 ± 0.08	0.34 ± 0.1	0.85 ± 0.14
B-HKK	0.88 ± 0.07	0.17 ± 0.05	0.79 ± 0.17
Infomap	0.91 ± 0.04	0.29 ± 0.08	0.83 ± 0.05
MDL (SBM)	0.94 ± 0.07	0.31 ± 0.09	0.87 ± 0.16
MDL (DC-SBM)	0.93 ± 0.09	0.26 ± 0.09	0.89 ± 0.11
S-NB	0.94 ± 0.07	0.3 ± 0.1	0.87 ± 0.08
mean model-based	0.91 ± 0.08	0.3 ± 0.12	0.84 ± 0.12
mean indiv. topol.	0.64 ± 0.19	0.2 ± 0.27	0.56 ± 0.33
mean indiv. topol. & model	0.7 ± 0.21	0.22 ± 0.25	0.62 ± 0.32
emd-DW	0.95 ± 0.1	0.45 ± 0.16	0.92 ± 0.13
emb-vgae	0.95 ± 0.08	0.09 ± 0.02	0.96 ± 0.09
all topol.	0.97 ± 0.08	0.89 ± 0.21	0.88 ± 0.2
all model-based	0.95 ± 0.07	0.76 ± 0.2	0.68 ± 0.17
all embed.	0.95 ± 0.11	0.75 ± 0.23	0.74 ± 0.23
all topol. & model	0.98 ± 0.06	0.89 ± 0.22	0.88 ± 0.19
all topol. & embed.	0.96 ± 0.1	0.86 ± 0.22	0.83 ± 0.25
all model & embed.	0.96 ± 0.09	0.78 ± 0.21	0.74 ± 0.22
all topol., model & embed.	0.97 ± 0.09	0.86 ± 0.23	0.84 ± 0.23

Ghasemian A, Hosseinmardi H, Galstyan A, Airoldi EM, Clauset A. Stacking Models for Nearly Optimal Link Prediction in Complex Networks. arXiv preprint arXiv:1909.07578. 2019 Sep 17.

Link Prediction in Attributed Graphs

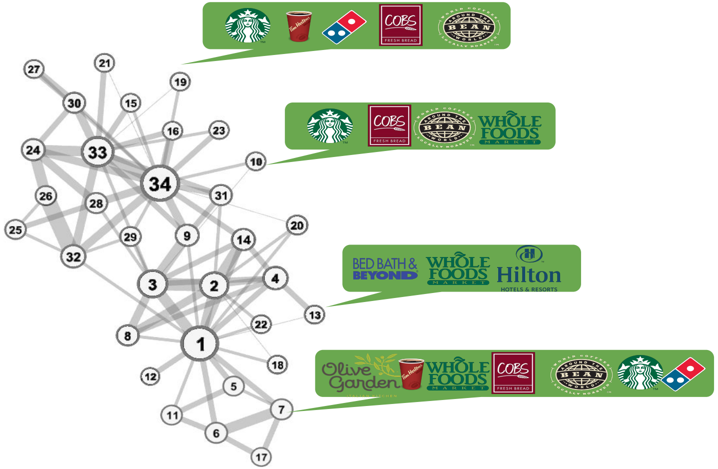
Individual characteristics (attributes) & relations (graph)

Annotated networks, **metadata** on nodes, **side** information



characteristics

age, occupation, salary, sex, etc.



activity & interest

check-ins, page-likes, group memberships, movies

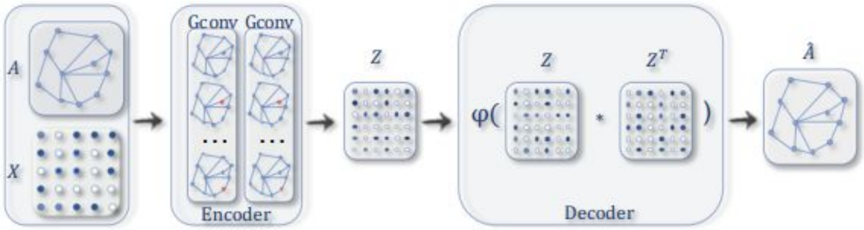
Link Prediction in Attributed Graphs

Interplay between attributes and relations

- Social **selection**: similarity of individuals' characteristics motivates them to form relations
- Social **influence**: Characteristics of individuals may be affected by the characteristics of their relations

Link Prediction in Attributed Graphs

Graph Neural Networks get attributed graphs as the input and can be used for many tasks including link prediction



Approach	Category	Inputs	Pooling	Readout	Time Complexity
GNN* (2009) [15]	RecGNN	A, X, X^e	-	a dummy super node	-
GraphESN (2010) [16]	RecGNN	A, X	-	mean	-
GGNN (2015) [17]	RecGNN	A, X	-	attention sum	-
SSE (2018) [18]	RecGNN	A, X	-	-	-
Spectral CNN (2014) [19]	Spectral-based ConvGNN	A, X	spectral clustering+max pooling	max	$O(n^3)$
Henaff et al. (2015) [20]	Spectral-based ConvGNN	A, X	spectral clustering+max pooling		$O(n^3)$
ChebNet (2016) [21]	Spectral-based ConvGNN	A, X	efficient pooling	sum	$O(m)$
GCN (2017) [22]	Spectral-based ConvGNN	A, X	-	-	$O(m)$
CayleyNet (2017) [23]	Spectral-based ConvGNN	A, X	mean/graclus pooling	-	$O(m)$
AGCN (2018) [40]	Spectral-based ConvGNN	A, X	max pooling	sum	$O(n^2)$
DualGCN (2018) [41]	Spectral-based ConvGNN	A, X	-	-	$O(m)$
NN4G (2009) [24]	Spatial-based ConvGNN	A, X	-	sum/mean	$O(m)$
DCNN (2016) [25]	Spatial-based ConvGNN	A, X	-	mean	$O(n^2)$
PATCHY-SAN (2016) [26]	Spatial-based ConvGNN	A, X, X^e	-	concat	-
MPNN (2017) [27]	Spatial-based ConvGNN	A, X, X^e	-	attention sum/ set2set	$O(m)$
GraphSage (2017) [42]	Spatial-based ConvGNN	A, X	-	-	-
GAT (2017) [43]	Spatial-based ConvGNN	A, X	-	-	$O(m)$
MoNet (2017) [44]	Spatial-based ConvGNN	A, X	-	-	$O(m)$
PGC-DGCNN (2018) [46]	Spatial-based ConvGNN	A, X	sort pooling	attention sum	$O(n^3)$
CGMM (2018) [47]	Spatial-based ConvGNN	A, X	-	concat	-
LGCN (2018) [45]	Spatial-based ConvGNN	A, X	-	-	-
GAAN (2018) [48]	Spatial-based ConvGNN	A, X	-	-	$O(m)$
FastGCN (2018) [49]	Spatial-based ConvGNN	A, X	-	-	-
StoGCN (2018) [50]	Spatial-based ConvGNN	A, X	-	-	-
Huang et al. (2018) [51]	Spatial-based ConvGNN	A, X	-	-	-
DGCNN (2018) [52]	Spatial-based ConvGNN	A, X	sort pooling	-	$O(m)$
DiffPool (2018) [54]	Spatial-based ConvGNN	A, X	differential pooling	mean	$O(n^2)$
GeniePath (2019) [55]	Spatial-based ConvGNN	A, X	-	-	$O(m)$
DGI (2019) [56]	Spatial-based ConvGNN	A, X	-	-	$O(m)$
GIN (2019) [57]	Spatial-based ConvGNN	A, X	-	concat+sum	$O(m)$
ClusterGCN (2019) [58]	Spatial-based ConvGNN	A, X	-	-	-

numerous methods, multiple surveys, e.g. this one (2019),
two of the notable works: GCN (2016), GAT (2018),
an excellent course last term on this & a new book!