Structure, Inference, and Optimization in Complex Networks

Tzu-Chi Yen, Dissertation Defense, June 29th, 2023

Graph 101

Input, raw

Output, processed Data

DATA → QUESTION → FRAMEWORK → REPRESENTATION

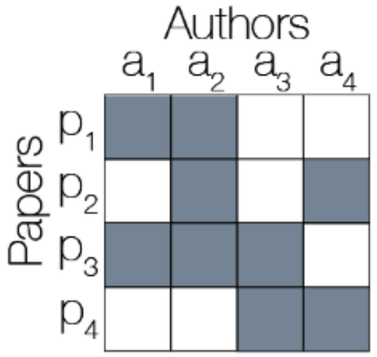
Paper : Authors

$p_1 : a_1, a_2$

$p_2 : a_2, a_4$

$p_3 : a_1, a_2, a_3$

$p_4 : a_3, a_4$



Graph 1O1

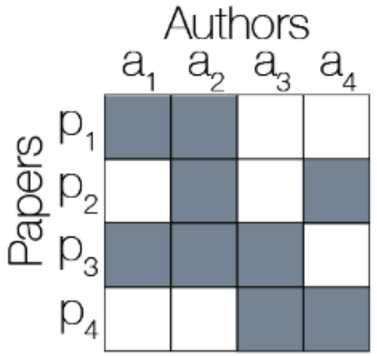
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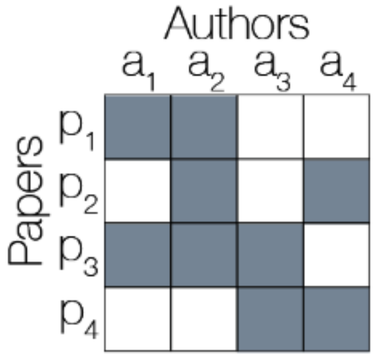
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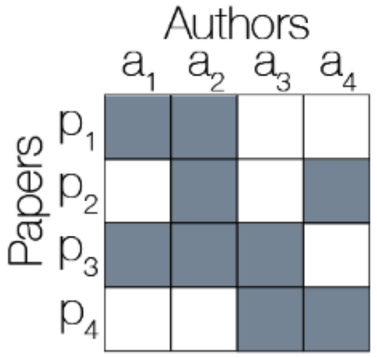
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Pick any 2 nodes as an edge



Graph 1O1

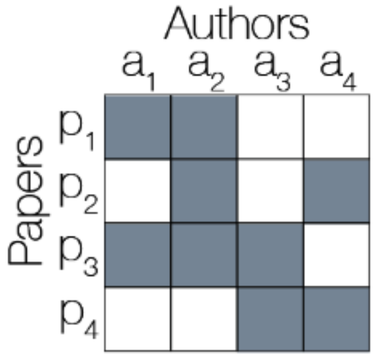
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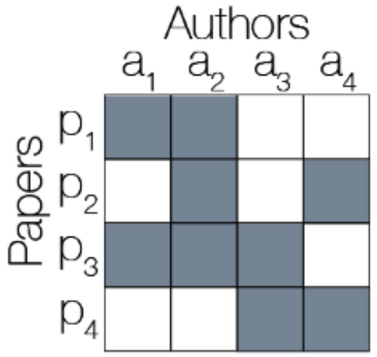
DATA

QUESTION

FRAMEWORK

REPRESENTATION

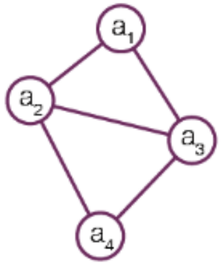
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Graph



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DATA

QUESTION

FRAMEWORK

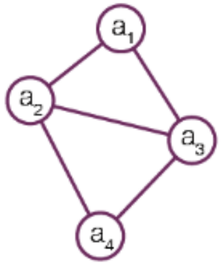
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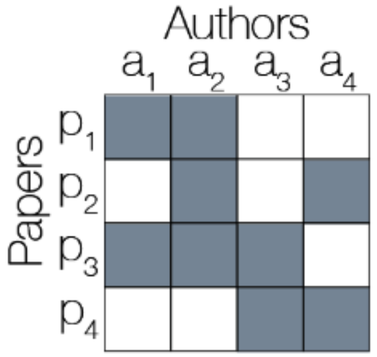
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→ *Graph* →



$G = (V, \{e\})$

$\{e\} = \{(1, 2), (2, 4), (1, 2), (1, 3), (2, 3), (3, 4)\}$



Pick any 2 nodes as an edge

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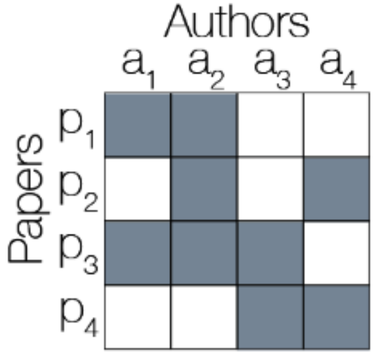
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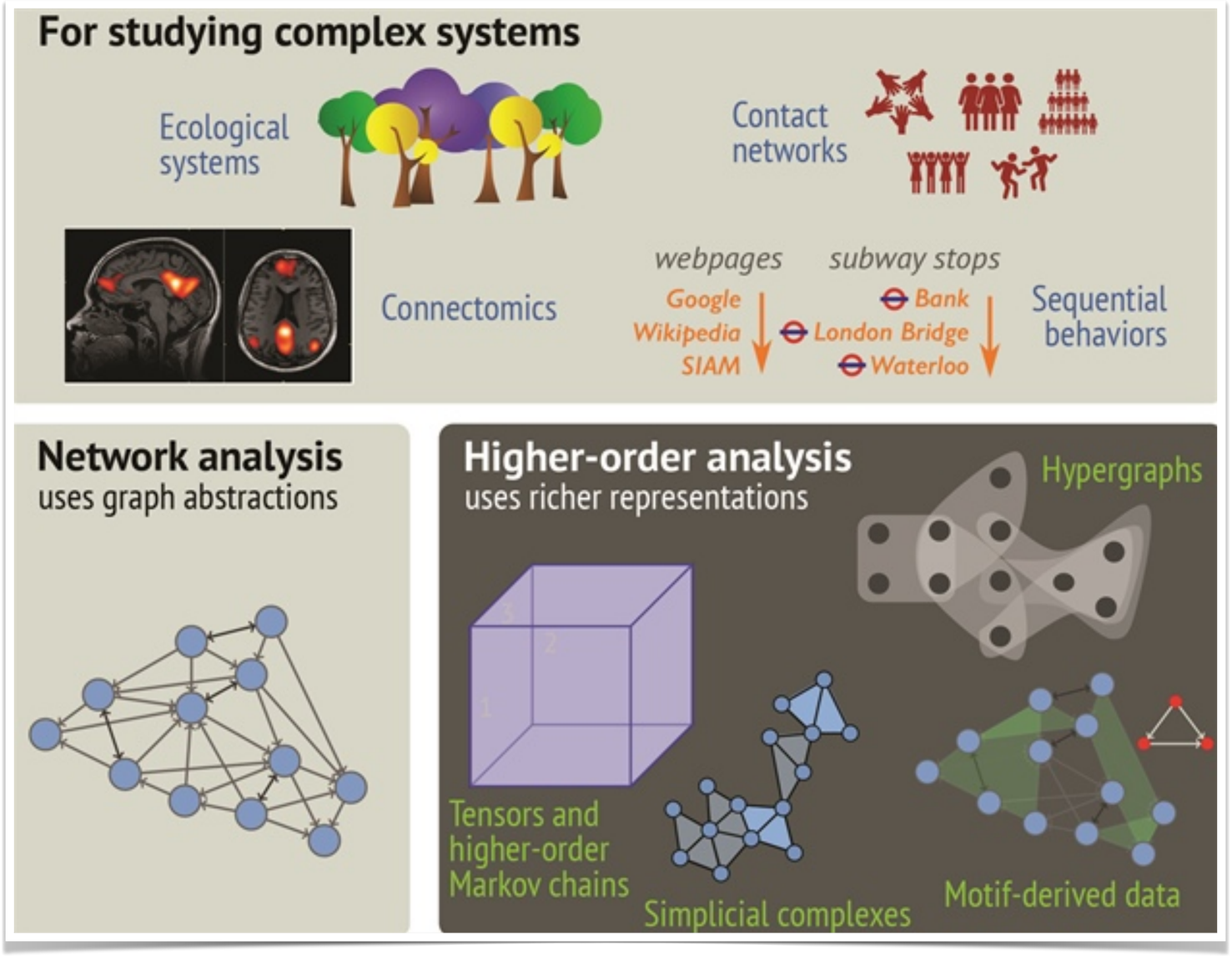
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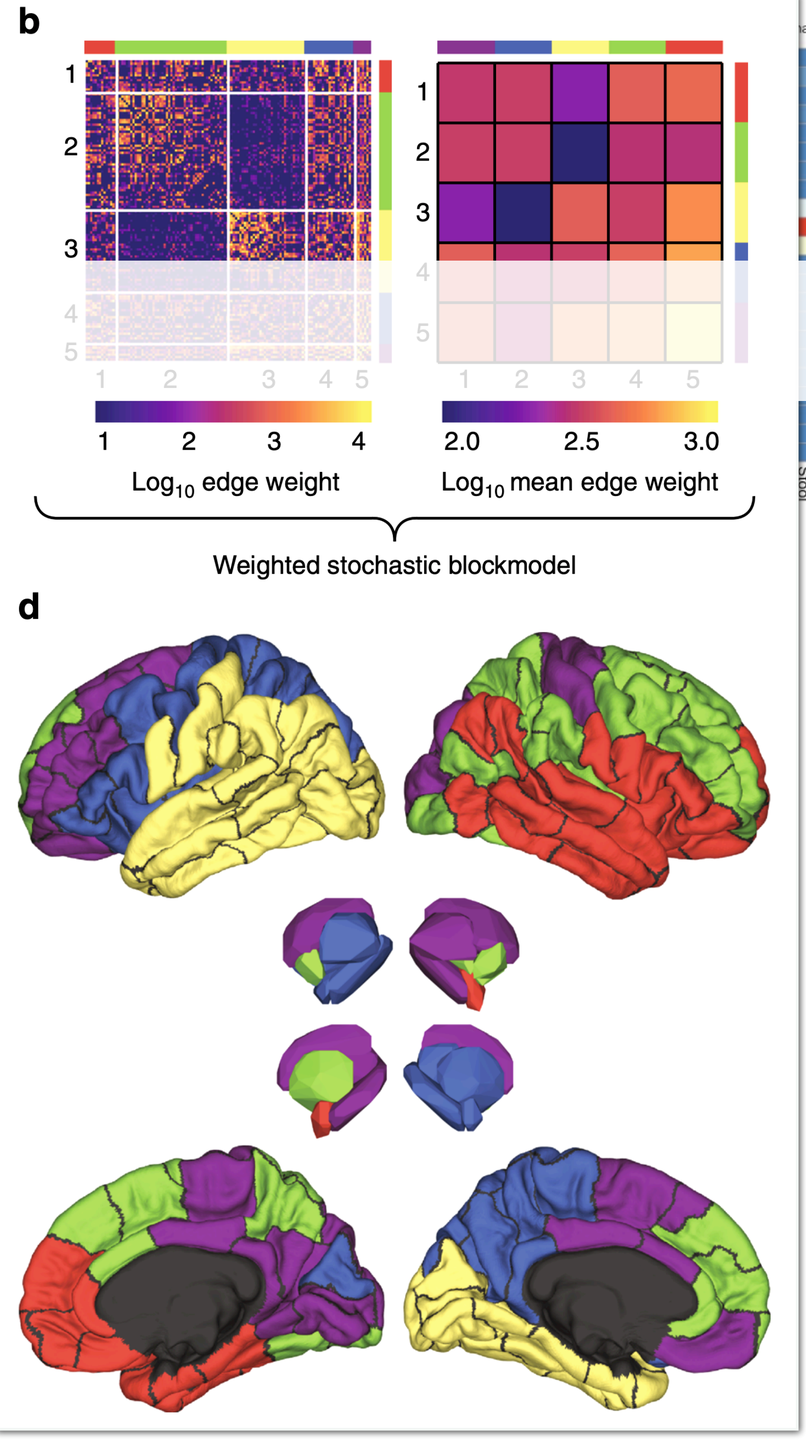


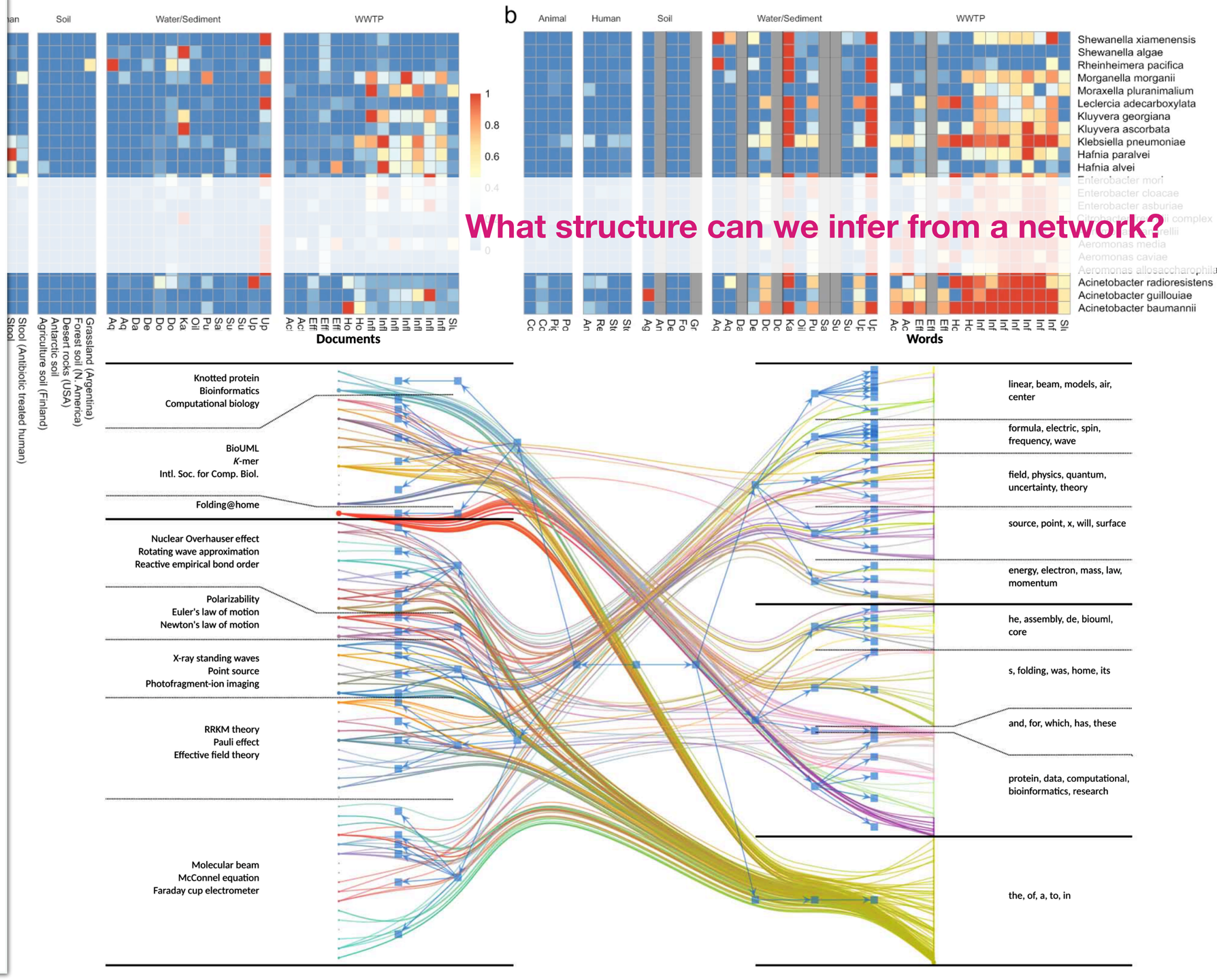


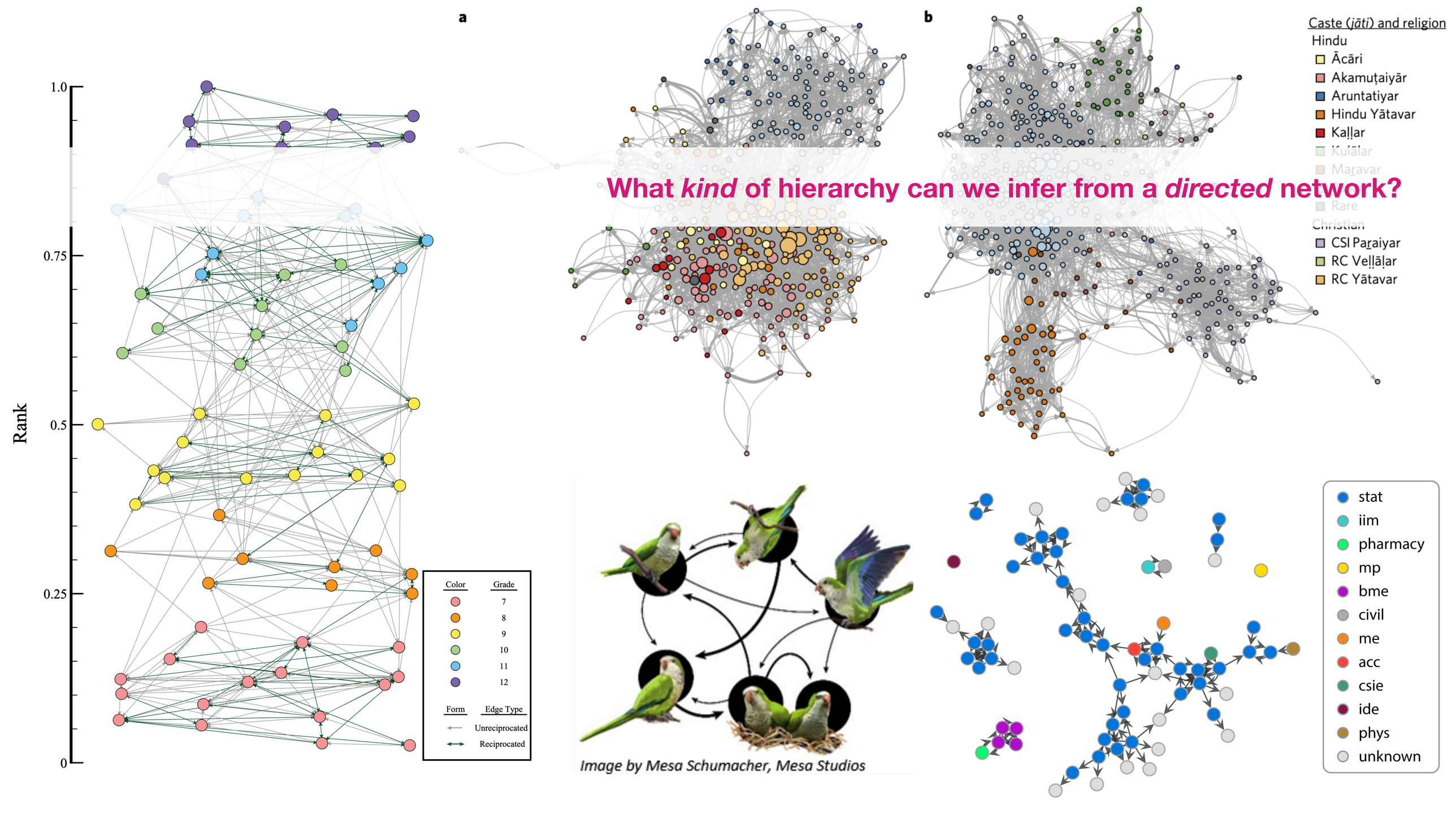
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b
1
2
3
4
5
1 2 3 4 5
1 2 3 4
Log10 edge weight
2.0 2.5 3.0
Log10 mean edge weight
Weighted stochastic blockmodel
d


Soil
Water/Sediment
WWTP
1
0.8
0.6
0.4
0
Documents
Stool (Antibiotic treated human)
Stool
Grassland (Argentina)
Forest soil (N. America)
Desert rocks (USA)
Antarctic soil
Agriculture soil (Finland)
b
Animal
Human
Soil
Water/Sediment
WWTP
Shewanella xiamenensis
Shewanella algae
Rheinheimera pacifica
Morganella morganii
Moraxella pluranimalium
Leclercia adecarboxylata
Kluyvera georgiana
Kluyvera ascorbata
Klebsiella pneumoniae
Hafnia paralvei
Hafnia alvei
Enterobacter mori
Enterobacter cloacae
Enterobacter asburiae
Aeromonas media
Aeromonas caviae
Aeromonas allosaccharophila
Acinetobacter radioresistens
Acinetobacter guillouiae
Acinetobacter baumannii
Words
What structure can we infer from a network?
Knotted protein
Bioinformatics
Computational biology
BioUML
K-mer
Intl. Soc. for Comp. Biol.
Folding@home
Nuclear Overhauser effect
Rotating wave approximation
Reactive empirical bond order
Polarizability
Euler's law of motion
Newton's law of motion
X-ray standing waves
Point source
Photofragment-ion imaging
RRKM theory
Pauli effect
Effective field theory
Molecular beam
McConnel equation
Faraday cup electrometer
linear, beam, models, air, center
formula, electric, spin, frequency, wave
field, physics, quantum, uncertainty, theory
source, point, x, will, surface
energy, electron, mass, law, momentum
he, assembly, de, biouml, core
s, folding, was, home, its
and, for, which, has, these
protein, data, computational, bioinformatics, research
the, of, a, to, in


a
b
Caste (jāti) and religion
Hindu
Ācāri
Akamuṭaiyār
Aruntatiyar
Hindu Yātavar
Kaḷḷar
Kuḷālar
Maṟavar
Rare
Christian
CSI Paṟaiyar
RC Veḷḷāḷar
RC Yātavar
What kind of hierarchy can we infer from a directed network?
Rank
1.0
0.75
0.5
0.25
0
Color
Grade
7
8
9
10
11
12
Form
Edge Type
Unreciprocated
Reciprocated
Image by Mesa Schumacher, Mesa Studios
stat
iim
pharmacy
mp
bme
civil
me
acc
csie
ide
phys
unknown

Outline

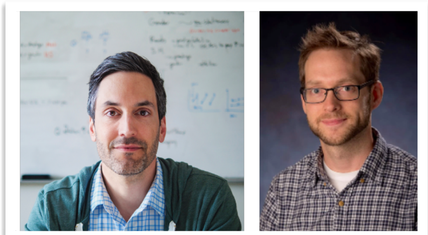
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2.  Aspiration of prestige in institutional peer selection (chapter 5)
3.  Community detection in bipartite networks (chapter 2)
4.  Regularized methods for efficient ranking (chapter 3)
5.  A detour in higher-order structures (chapter 4)
6. Conclusions & future research (chapter 6)

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SCIENCE ADVANCES | RESEARCH ARTICLE

SOCIAL SCIENCES

Aspirational pursuit of mates in online dating markets

Elizabeth E. Bruch[1,2]* and M. E. J. Newman[2,3]

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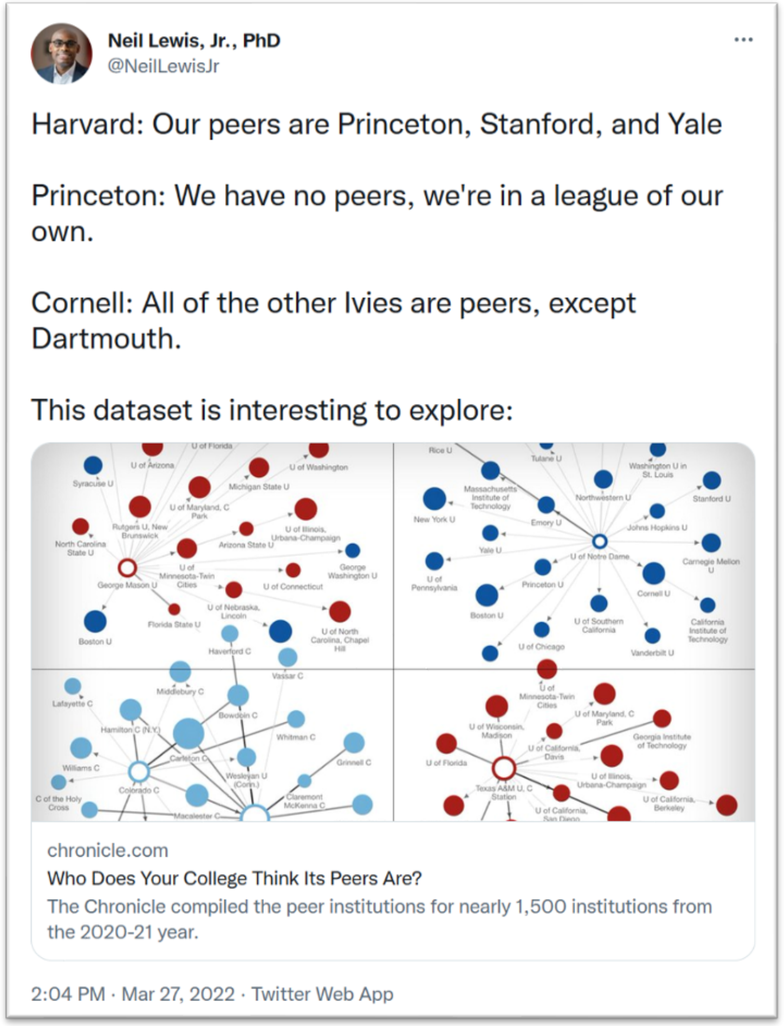
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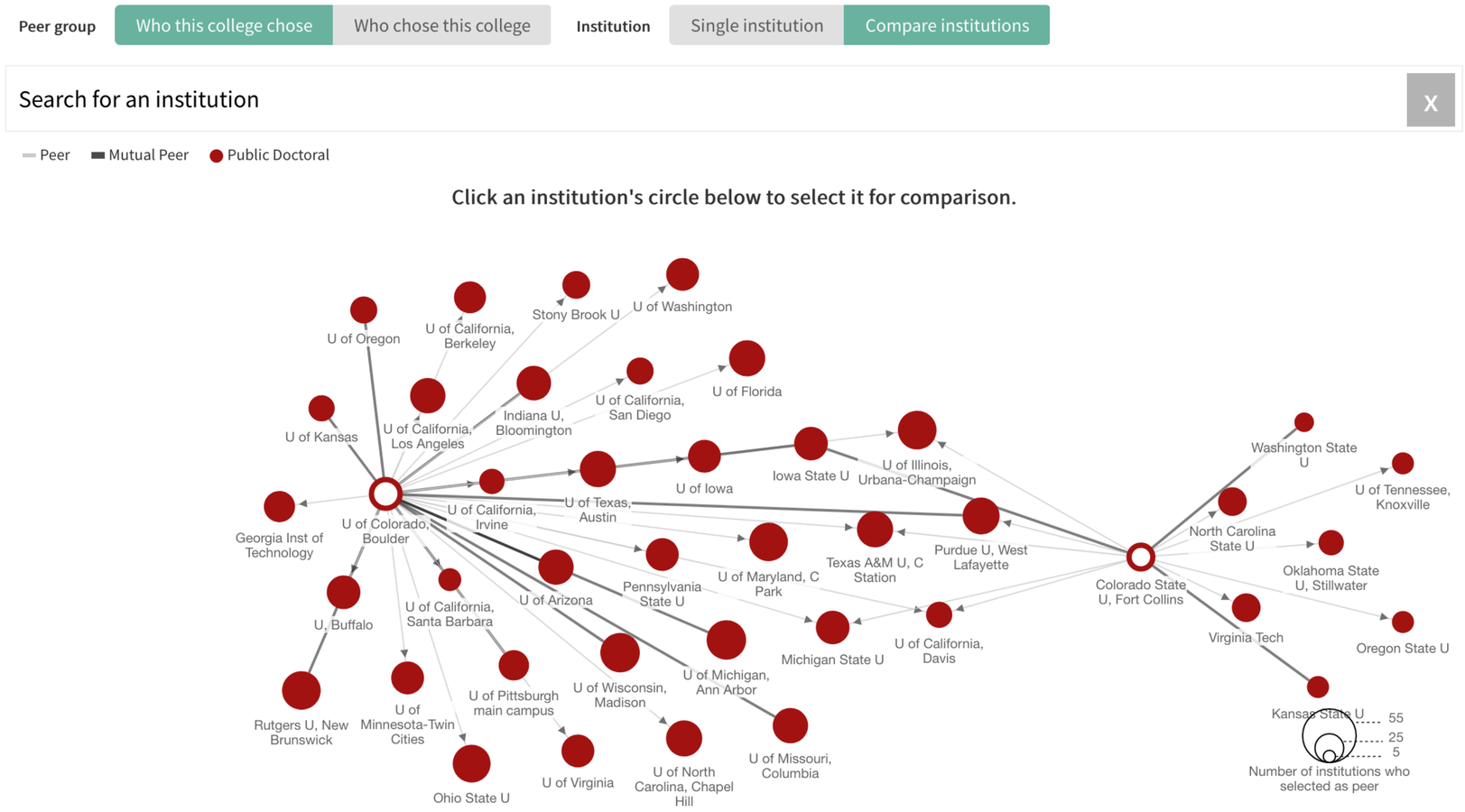
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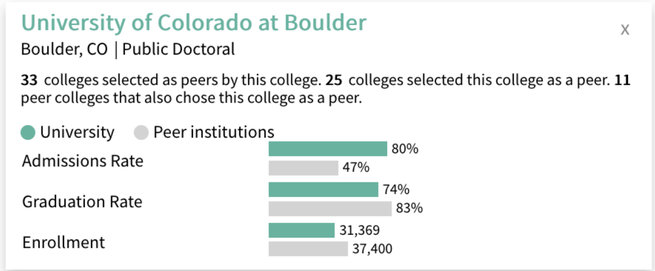
Published online by Cambridge University Press: **15 April 2013**

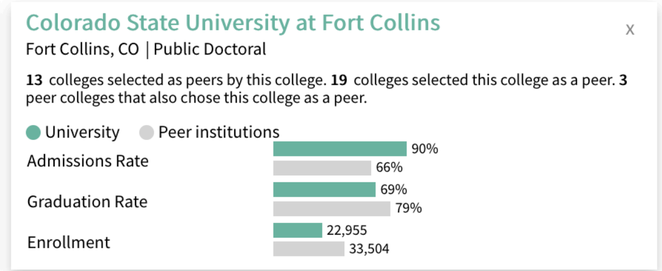
BRIAN BALL and M.E.J. NEWMAN

Peer institutions (dataset to study the *psychology* behind structure)

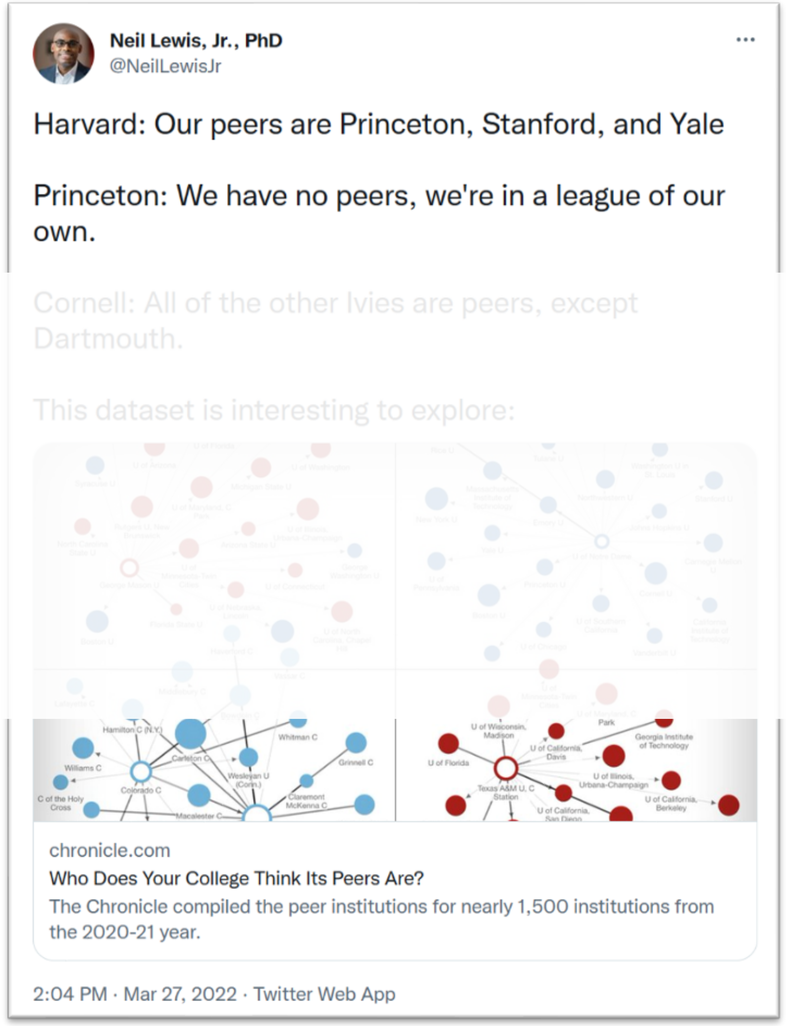


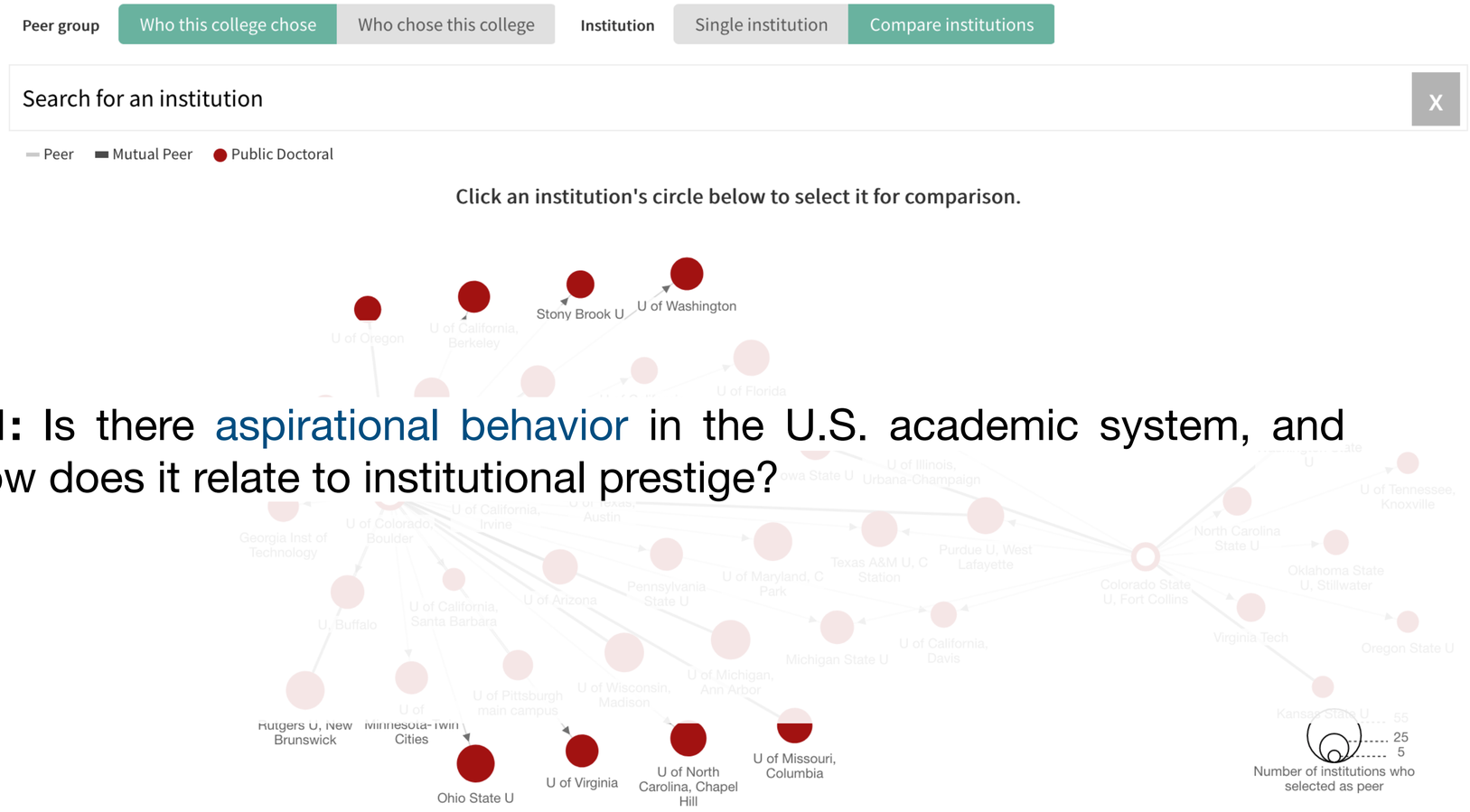




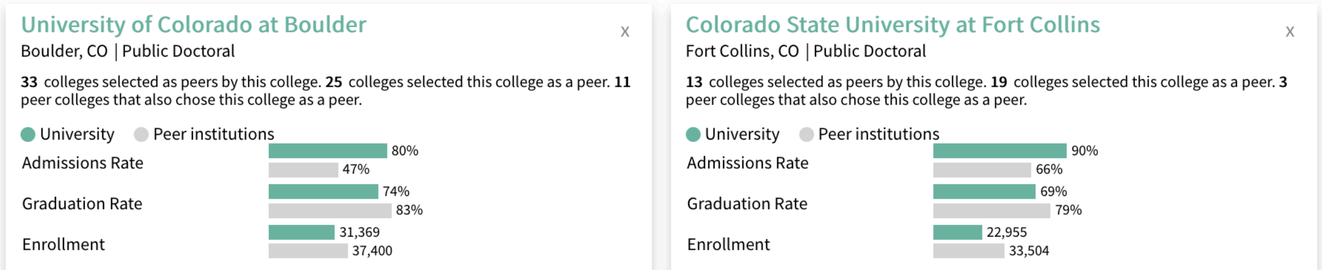


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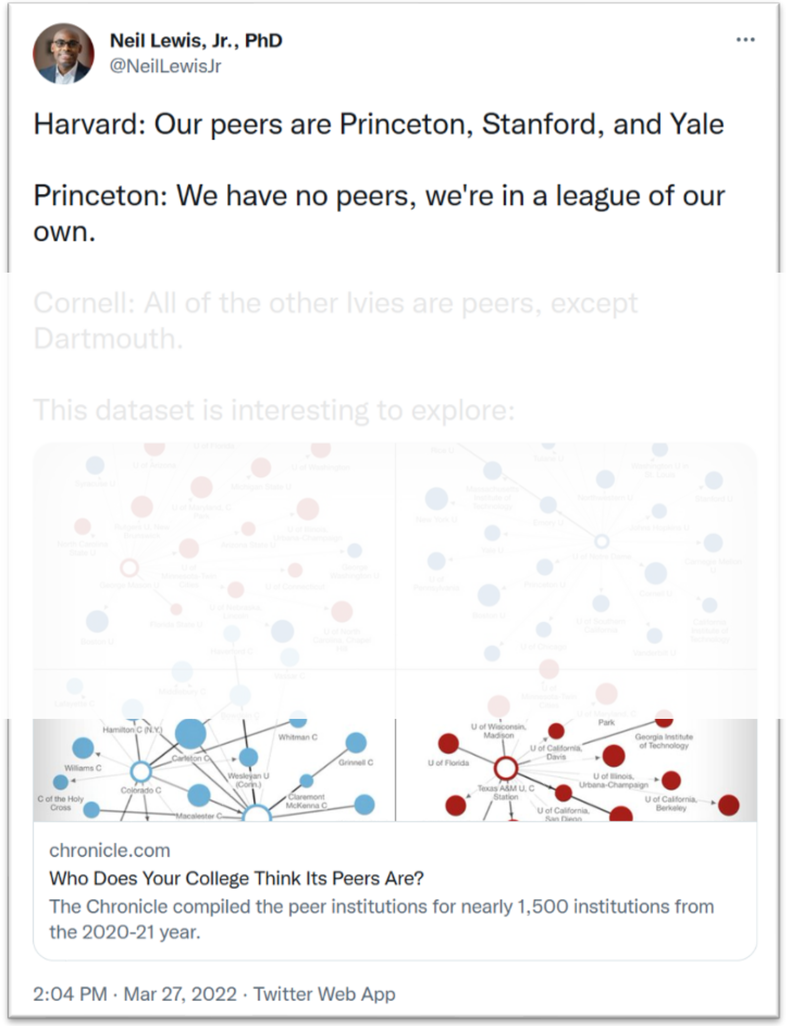


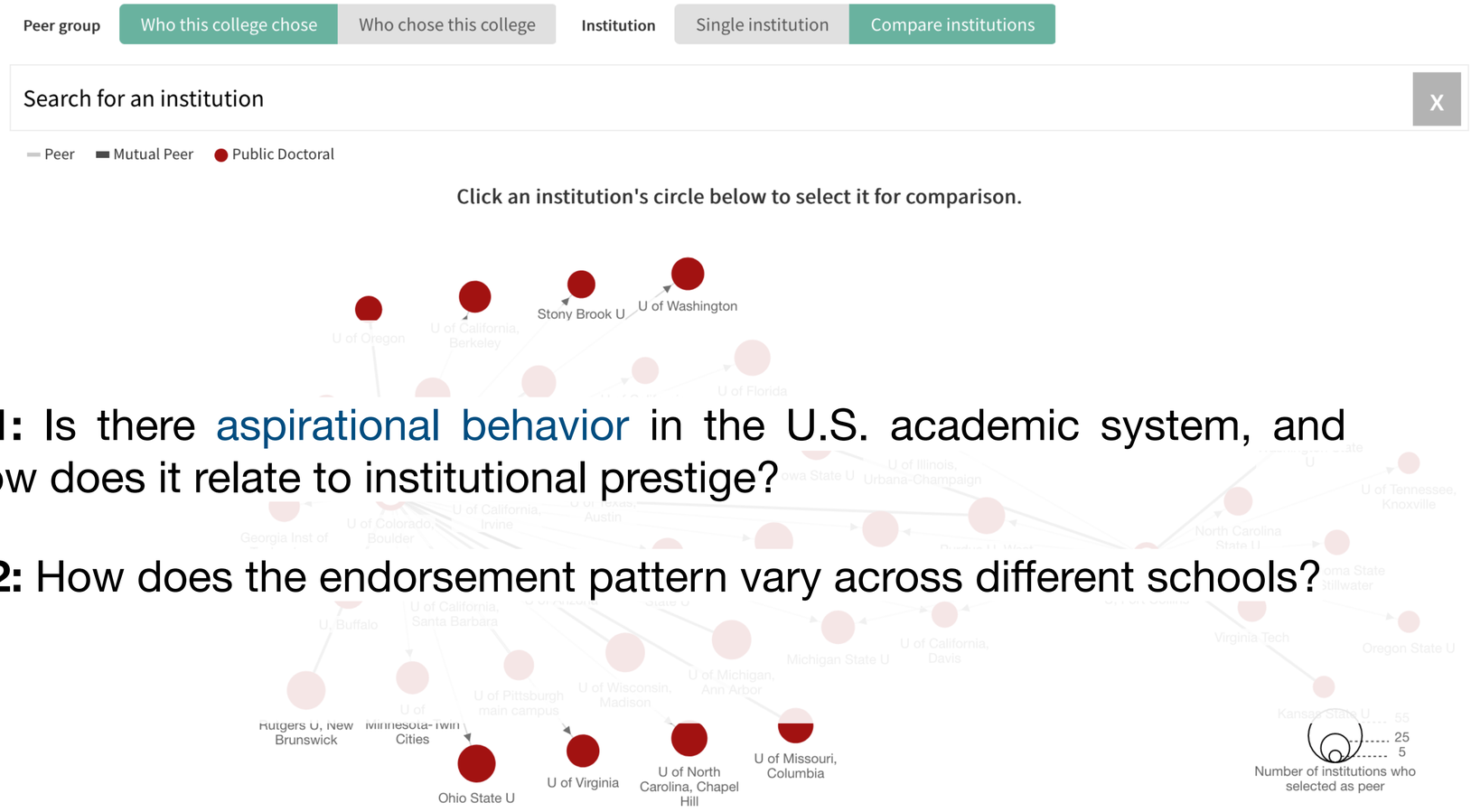


R1: Is there aspirational behavior in the U.S. academic system, and how does it relate to institutional prestige?



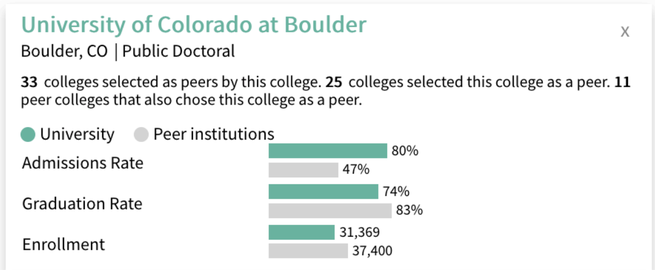
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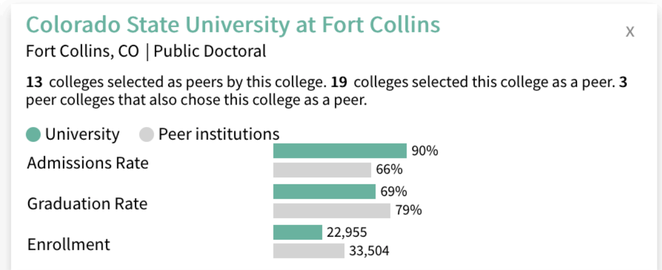




R1: Is there aspirational behavior in the U.S. academic system, and how does it relate to institutional prestige?

R2: How does the endorsement pattern vary across different schools?





Method (data collection)

Code	Type of Institutions	N
15 (R1)	Doctoral Universities: Highest Research Activity	125
16 (R2)	Doctoral Universities: Higher Research Activity	114
17 (R3)	Doctoral Universities: Moderate Research Activity	30
18 (M:Large)	Master's Colleges & Universities: Larger Programs	18
19 (M:Med)	Master's Colleges & Universities: Medium Programs	2
20 (M:Small)	Master's Colleges & Universities: Small Programs	1
21 (B:A&S)	Baccalaureate Colleges: Arts & Sciences Focus	6
26 (S:Health)	Special Focus Four-Year: Other Health Professions Schools	1
27 (S:Engineer)	Special Focus Four-Year: Engineering Schools	1
		total = 298

Aspiration: Peer institutions survey (IPEDS, 2020–21). Of the 1179 institutions and 18817 nominations collected, we matched the names with the faculty hiring dataset & restricted to Ph.D.-granting ones, resulting in 298 institutions.

Institutional prestige: Faculty hiring dataset (existing, 2011–12). Each institution is annotated by a data-driven estimate of its "prestige" within the faculty hiring system. Proxy for an institution's ability to place its graduates as faculty at other institutions.

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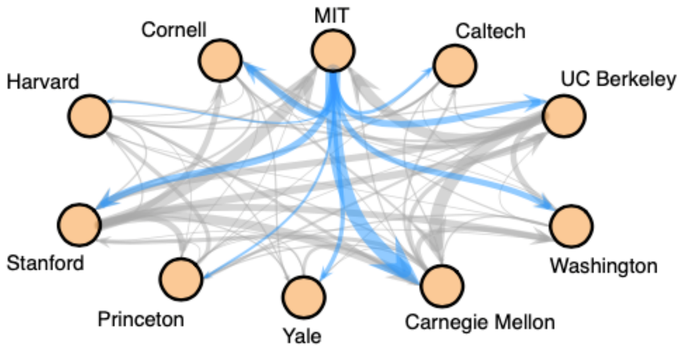
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20 (M:Small)	Master's Colleges & Universities: Small Programs	1
21 (B:A&S)	Baccalaureate Colleges: Arts & Sciences Focus	6
26 (S:Health)	Special Focus Four-Year: Other Health Professions Schools	1
27 (S:Engineer)	Special Focus Four-Year: Engineering Schools	1
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Aspiration: Peer institutions survey (IPEDS, 2020–21). Of the 1179 institutions and 18817 nominations collected, we matched the names with the faculty hiring dataset & restricted to Ph.D.-granting ones, resulting in 298 institutions.

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Method (quantifying prestige/desirability via SpringRank)

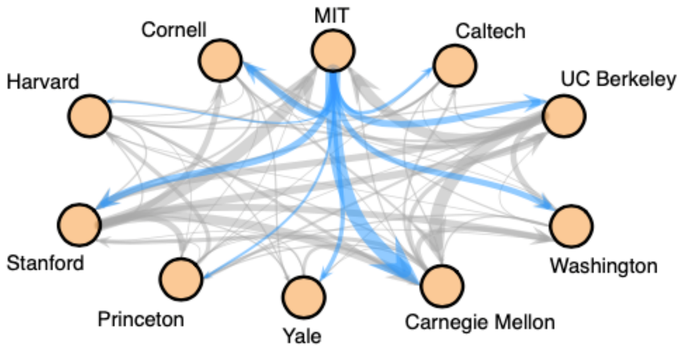
Each directed edge $u \to v$ implies
PhD from u becomes faculty at v



Computer science faculty hiring network; http://tuvalu.santafe.edu/~aaronc/facultyhiring/. See also: *Sci. Adv.* 1(1), e1400005, 2015.

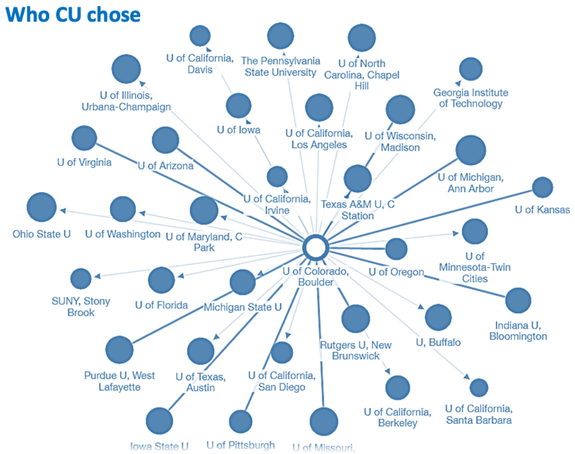
Method (quantifying prestige/desirability via SpringRank)

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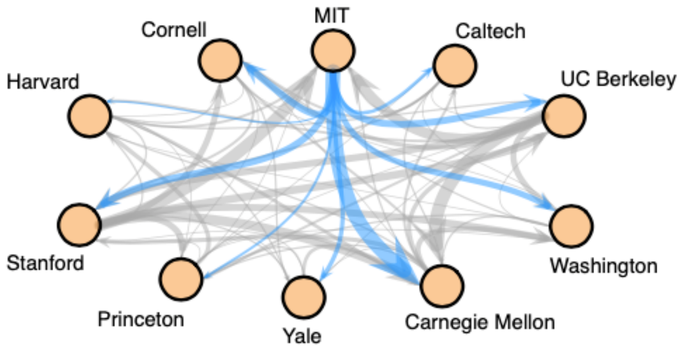
Computer science faculty hiring network; http://tuvalu.santafe.edu/~aaronc/facultyhiring/. See also: *Sci. Adv.* 1(1), e1400005, 2015.

Each directed edge $u \to v$ implies
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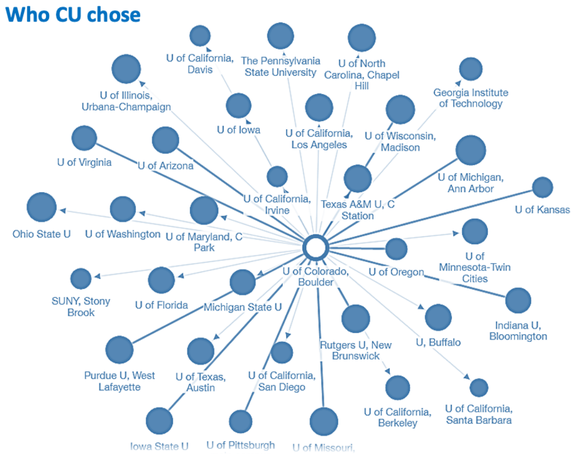
Method (quantifying prestige/desirability via SpringRank)

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Computer science faculty hiring network; http://tuvalu.santafe.edu/~aaronc/facultyhiring/. See also: *Sci. Adv.* 1(1), e1400005, 2015.

Each directed edge $u \to v$ implies institution u selects institution v

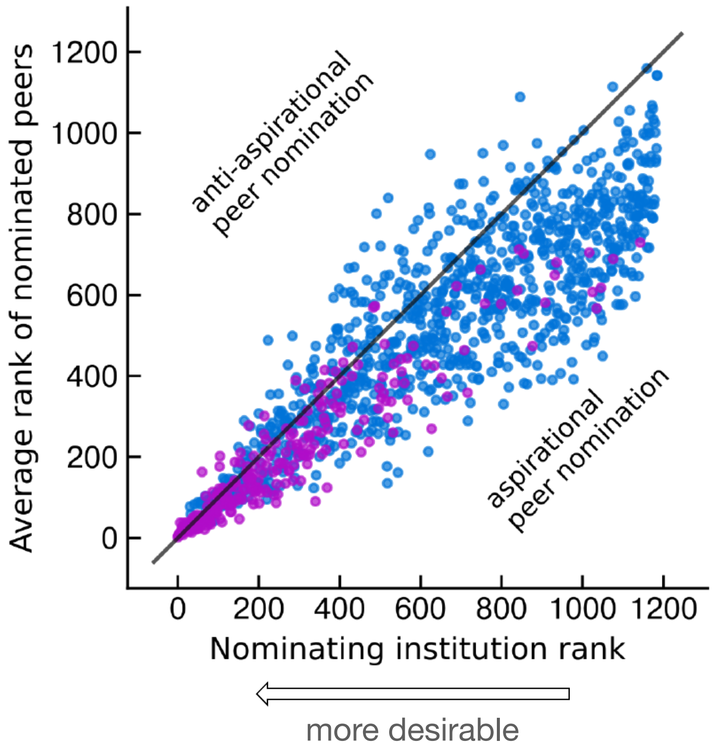


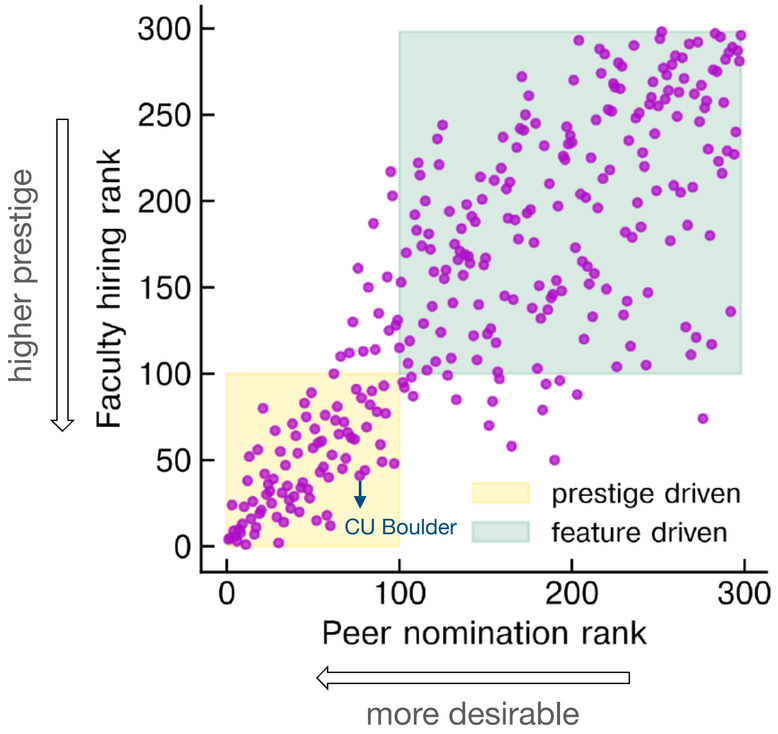
SpringRank: Let $\mathbf{A} = \{A_{ij}\}$ be the adjacency matrix of a directed multigraph.

The SpringRank Model finds the ranking $\mathbf{s}^*$ of the nodes by solving:

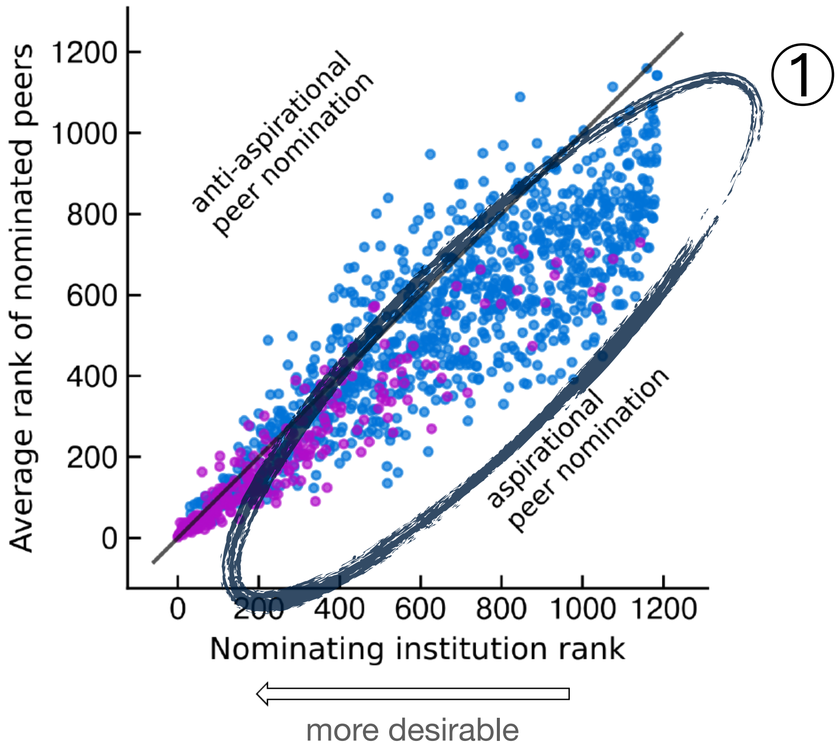
$$\underset{\boldsymbol{s}\in\mathbb{R}^N}{\text{minimize}}\ \frac{1}{2}\sum_{ij} A_{ij}(s_i - s_j - 1)^2 \ .$$

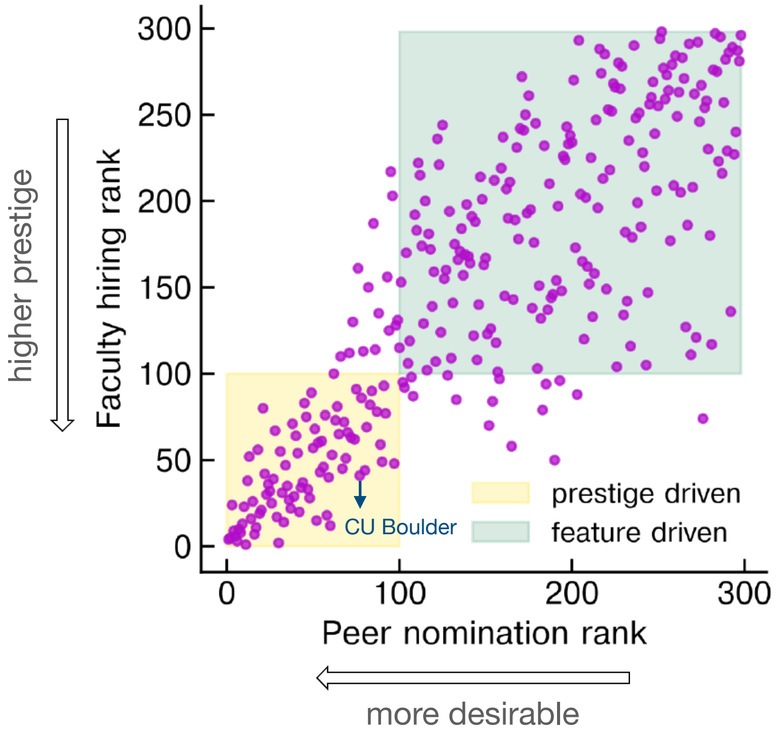
Institutions name higher prestige institutions as their peers



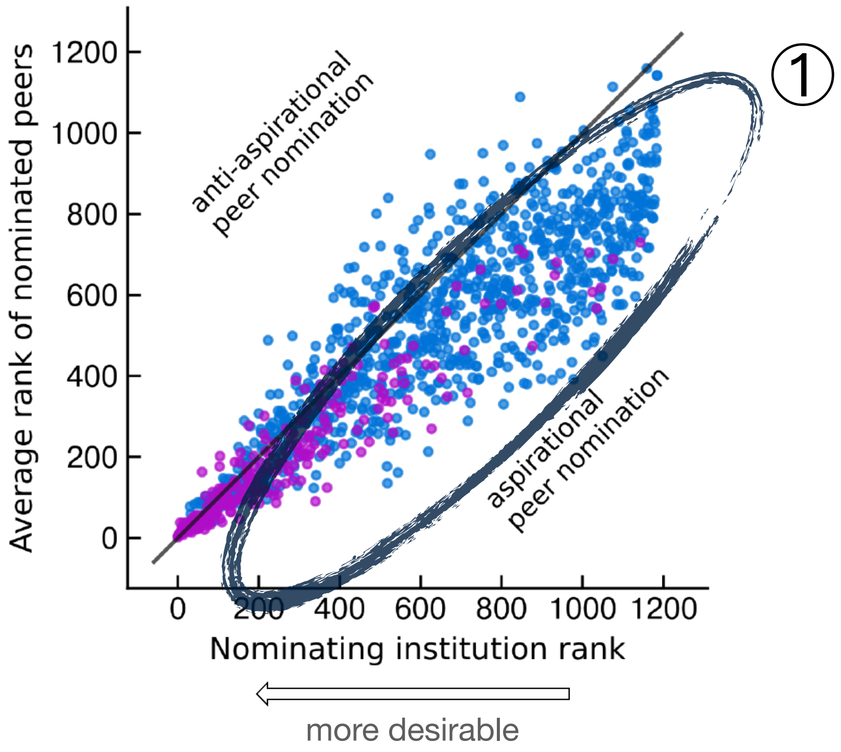


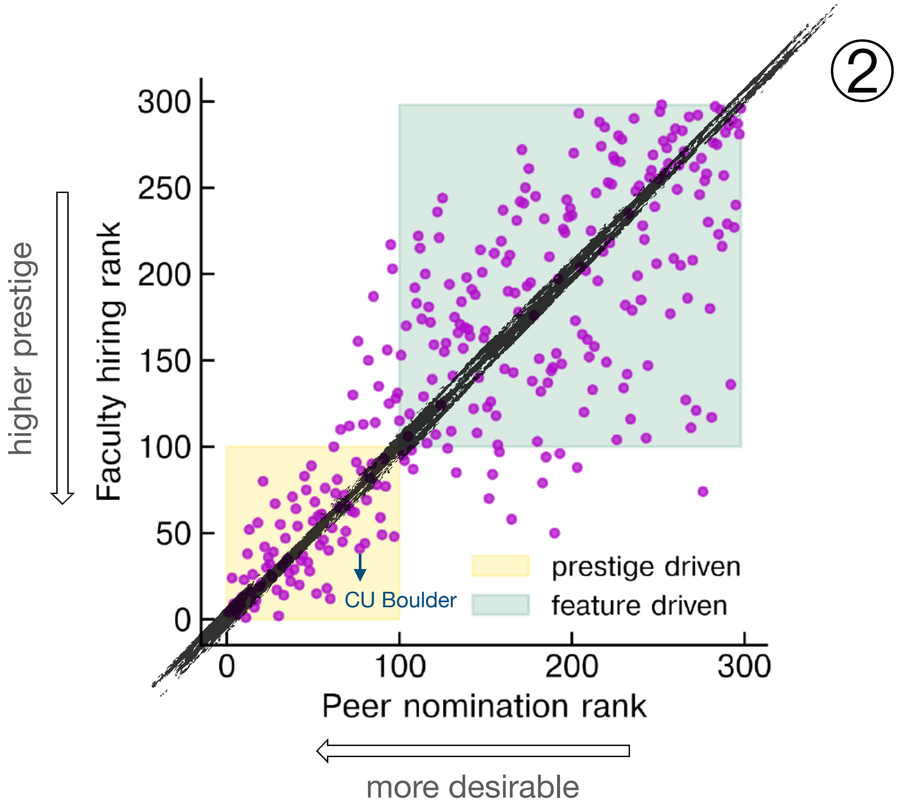
Institutions name higher prestige institutions as their peers



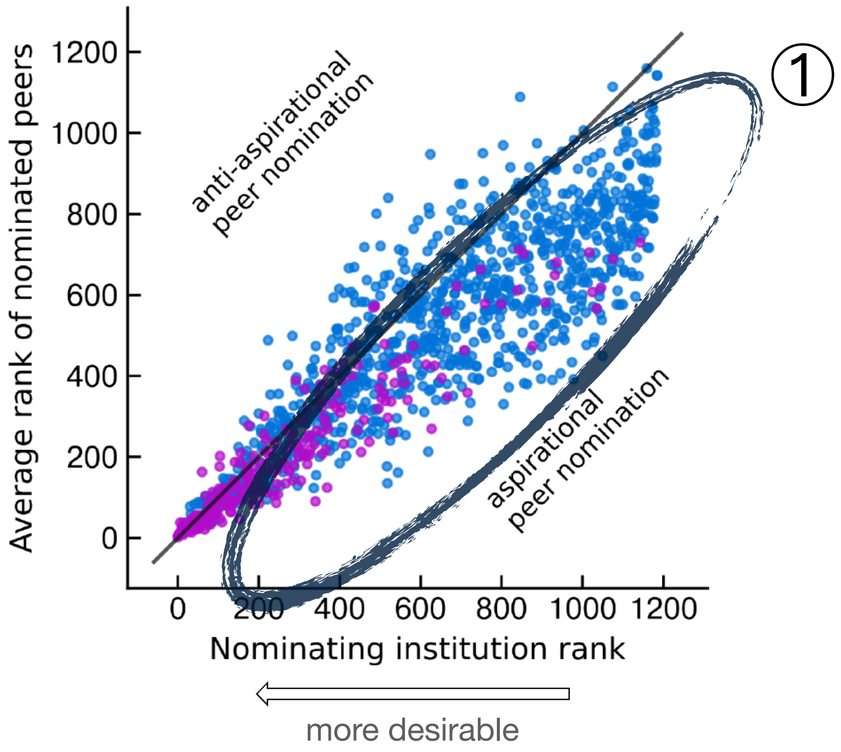


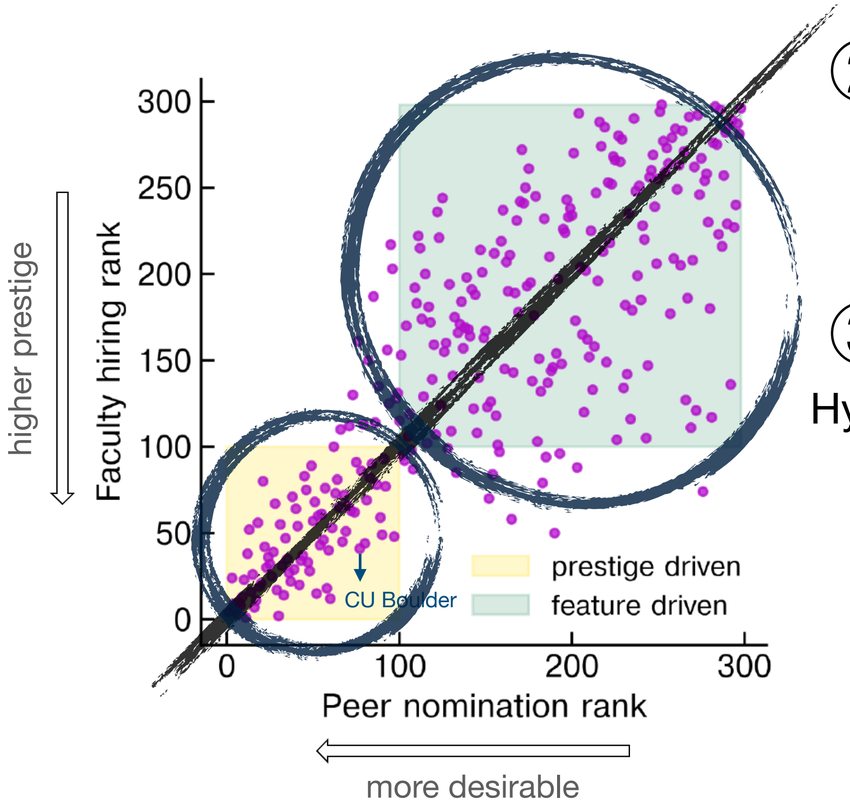
Institutions name higher prestige institutions as their peers





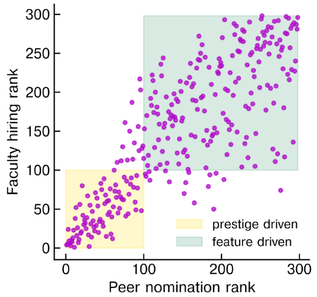
Institutions name higher prestige institutions as their peers





Hypothesized strata 🤔

Method (logistic regression with LASSO and Laplacian regularization*)



$$\underset{\boldsymbol{\beta}\in\mathbb{R}^p}{\text{minimize}}\ \ell(\boldsymbol{y}, \boldsymbol{\beta}^\mathsf{T}\boldsymbol{x}) + \lambda\|\boldsymbol{\beta}\|_1$$

LASSO ($\ell 1$ regularization)

(logistic) loss

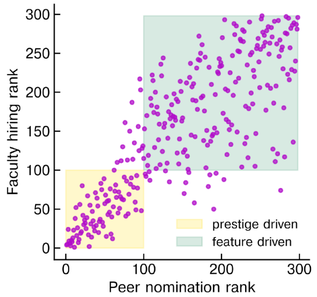
actual data

predicted data

Institutional features (nodal features)	Type	Total features	Total derived features (one for each edge)
Historically black?	binary	2	4
Sector (public or private)	categorical	2	4
Carnegie Classification	categorical	9	78
Two-letter state abbreviation	categorical	50	2494
Avg enrollment of full-time students	numeric	1	2
Graduation rates	numeric	1	2
Admission rates	numeric	1	2
Prestige rank	numeric	1	2

*Solution method: alternating direction method of multipliers (ADMM), see Tuck, Barrett, Boyd in J. Machine Learning Research 22, 1-37 (2021).

Method (logistic regression with LASSO and Laplacian regularization*)



$$\underset{\boldsymbol{\beta}\in\mathbb{R}^p}{\text{minimize}}\ \ell(\boldsymbol{y}, \boldsymbol{\beta}^\mathsf{T}\boldsymbol{x}) + \lambda\|\boldsymbol{\beta}\|_1$$

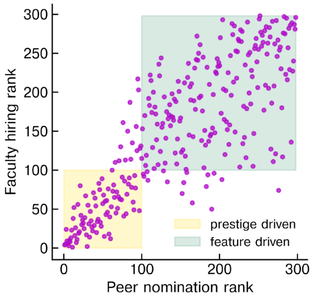
- $\ell(\boldsymbol{y}, \boldsymbol{\beta}^\mathsf{T}\boldsymbol{x})$: (logistic) loss
- $\boldsymbol{y}$: actual data
- $\boldsymbol{\beta}^\mathsf{T}\boldsymbol{x}$: predicted data
- $\lambda\|\boldsymbol{\beta}\|_1$: LASSO ($\ell 1$ regularization)

use when #features / #samples ~ 1

Institutional features (nodal features)	Type	Total features	Total derived features (one for each edge)
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$$\underset{\boldsymbol{\beta}\in\mathbb{R}^p}{\text{minimize}}\ \ell(\boldsymbol{y}, \boldsymbol{\beta}^\mathsf{T}\boldsymbol{x}) + \lambda\|\boldsymbol{\beta}\|_1$$

(logistic) loss

actual data

predicted data

LASSO ($\ell 1$ regularization)

use when #features / #samples ~ 1

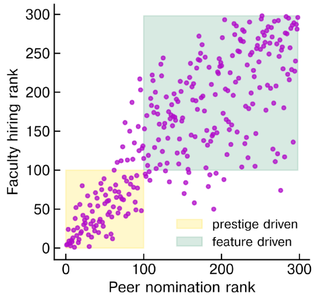
Institutional features (nodal features)	Type	Total features	Total derived features (one for each edge)
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Prestige rank	numeric	1	2

$$\begin{aligned}\underset{\boldsymbol{\beta}_{\text{high}},\boldsymbol{\beta}_{\text{low}}\in\mathbb{R}^p}{\text{minimize}}\ & \ell(\boldsymbol{y}_{\text{high}}, \boldsymbol{\beta}_{\text{high}}^\mathsf{T}\boldsymbol{x}) + \lambda\|\boldsymbol{\beta}_{\text{high}}\|_1 \\ & + \ell(\boldsymbol{y}_{\text{low}}, \boldsymbol{\beta}_{\text{low}}^\mathsf{T}\boldsymbol{x}) + \lambda\|\boldsymbol{\beta}_{\text{low}}\|_1 \\ & + \lambda_L\|\boldsymbol{\beta}_{\text{high}} - \boldsymbol{\beta}_{\text{low}}\|_2^2\end{aligned}$$

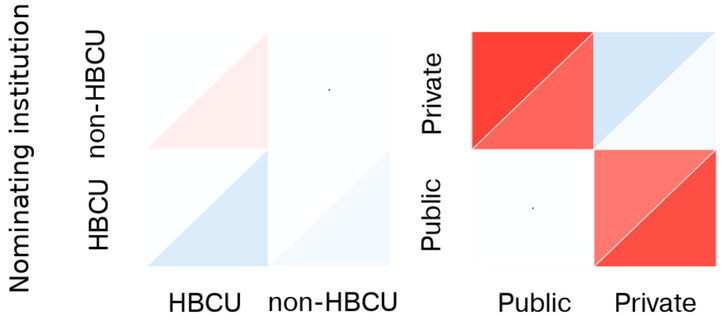
Idea: Parameters in adjacent strata should be similar. Plus, parameters are encouraged to be zero (not used).

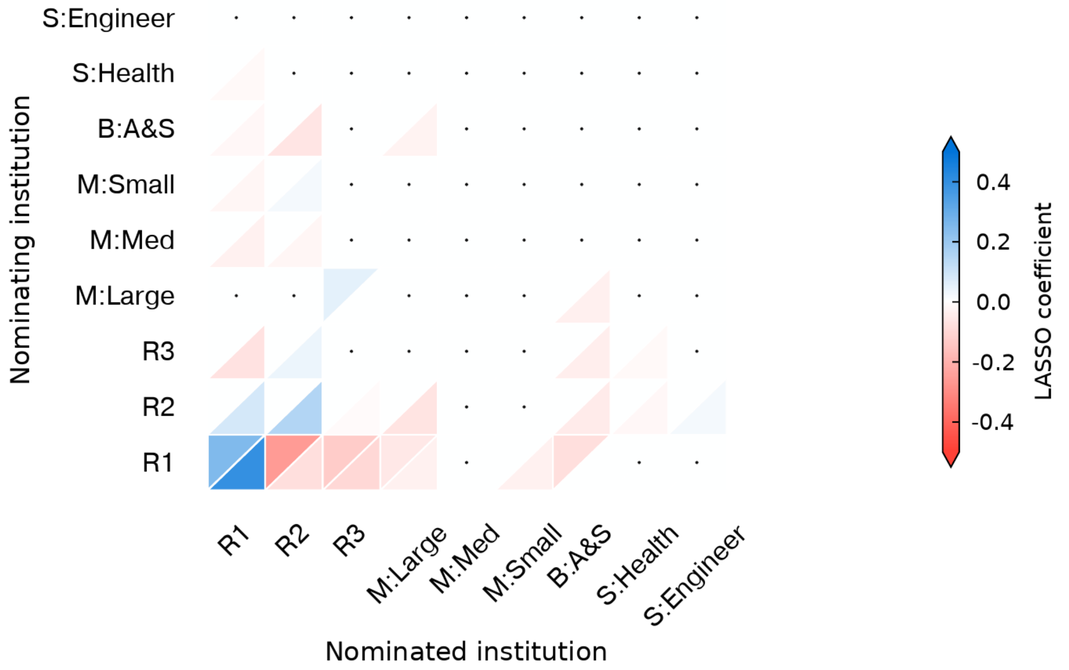
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Rich peer decision patterns (categorical features)



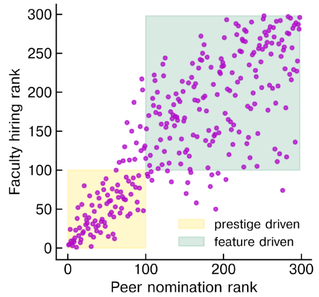
◸ : higher prestige
◿ : lower prestige



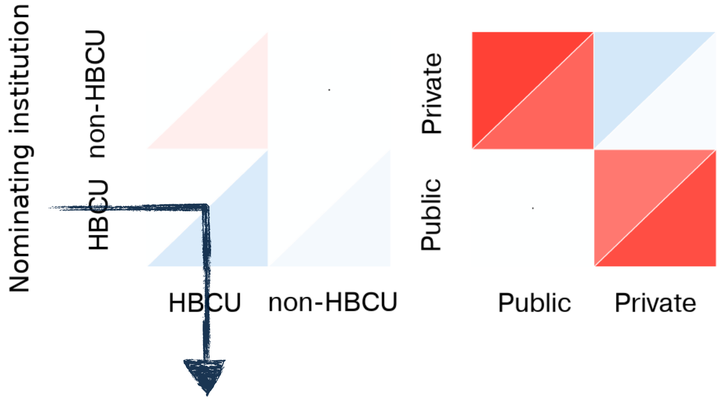


*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

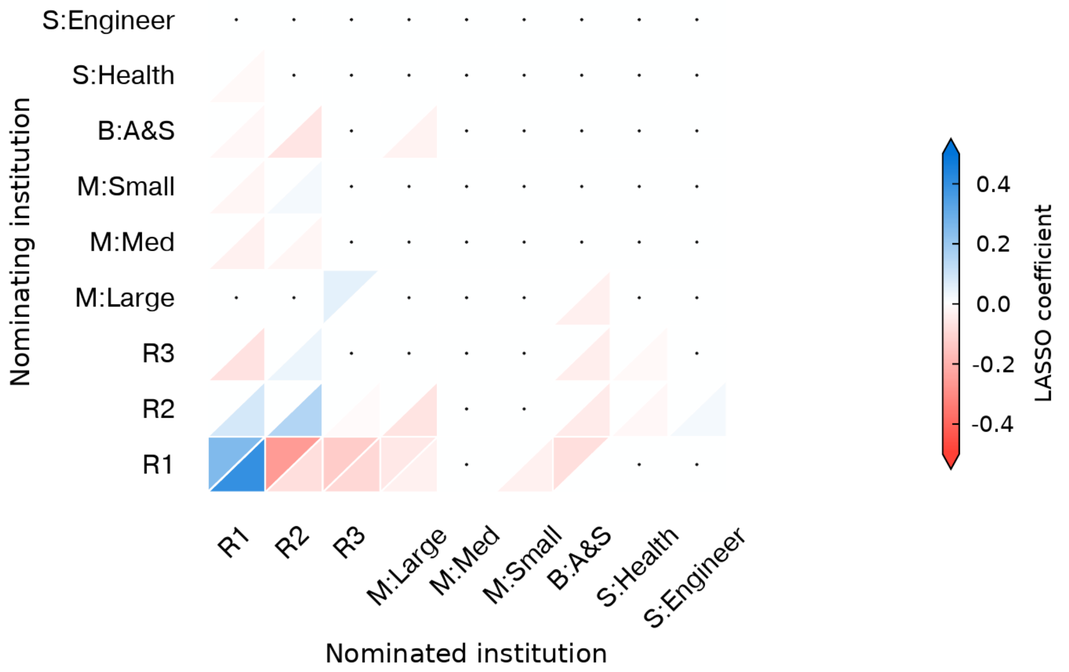
Rich peer decision patterns (categorical features)



◸ : higher prestige
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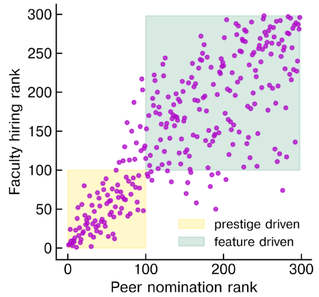


HBCU tends (slightly) to choose other HBCUs.

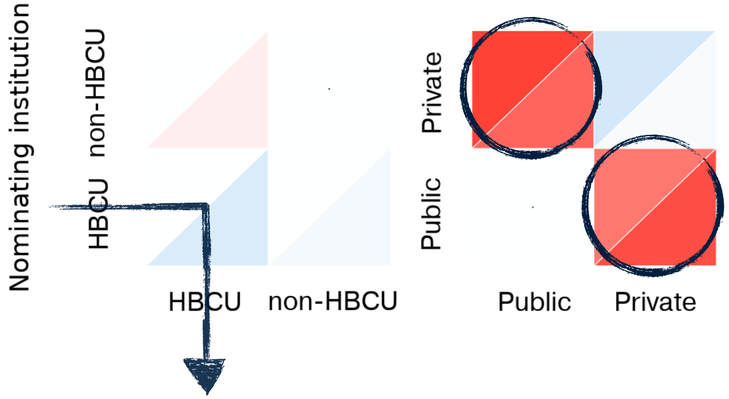


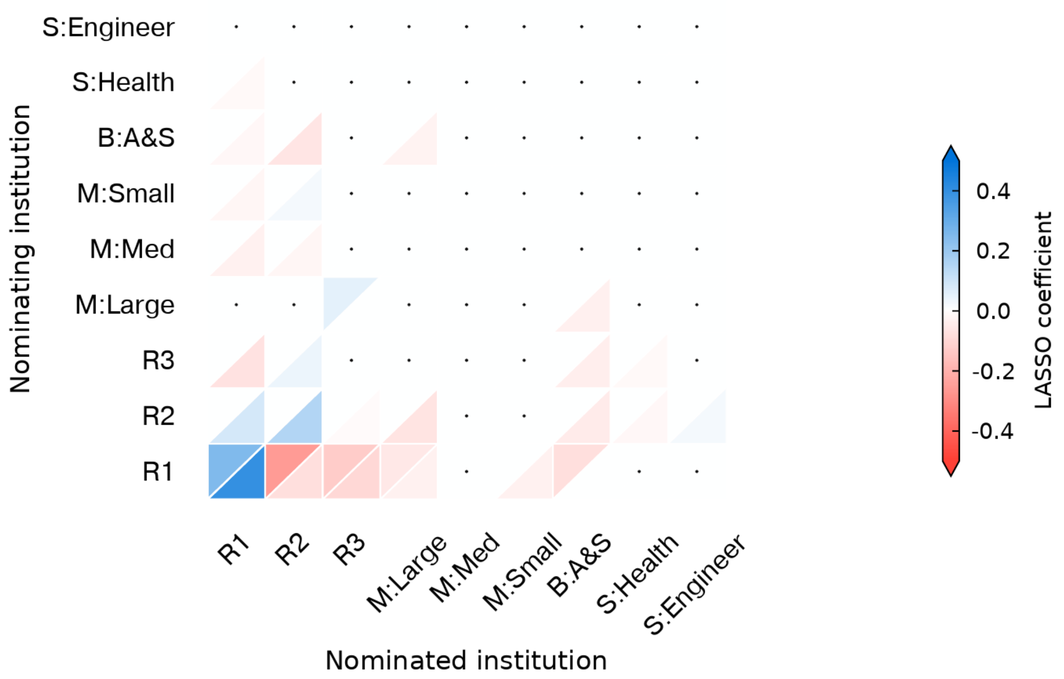
*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

Rich peer decision patterns (categorical features)



◸ : higher prestige
◿ : lower prestige



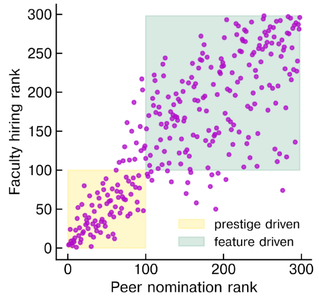


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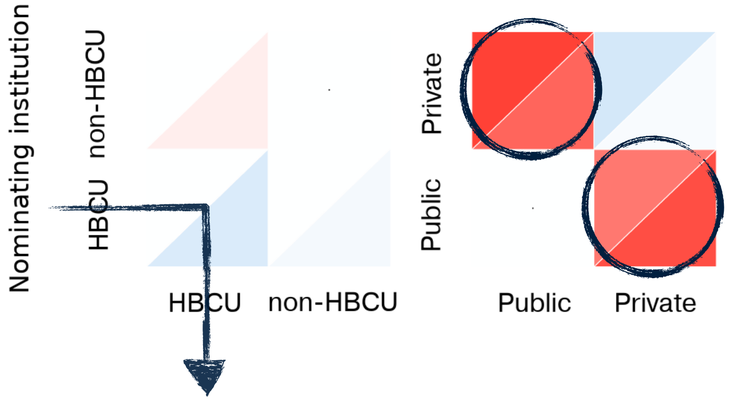
Private schools don't choose public schools (vv).

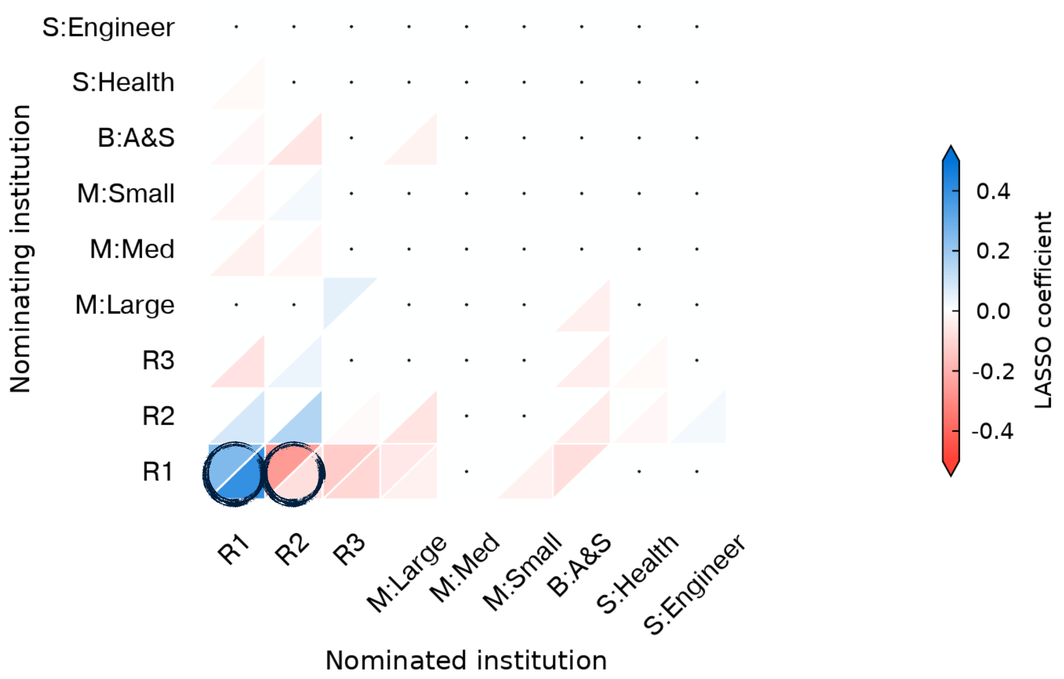
*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

Rich peer decision patterns (categorical features)



◸ : higher prestige
◿ : lower prestige





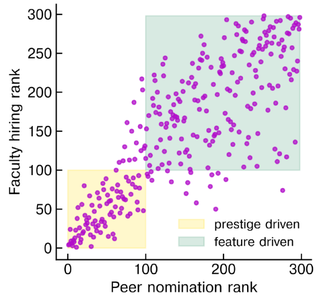
HBCU tends (slightly) to choose other HBCUs.

Private schools don't choose public schools (vv).

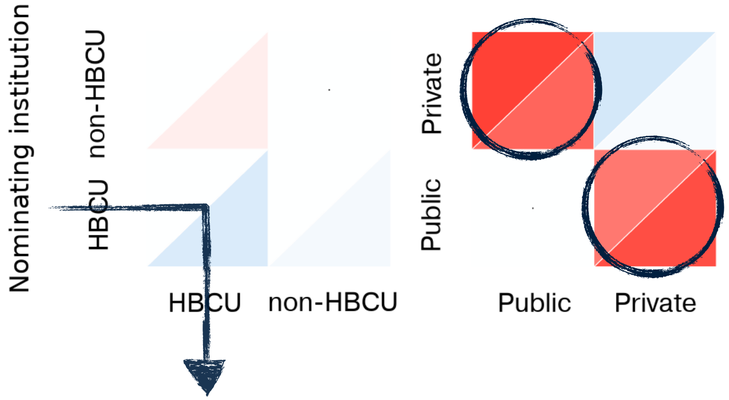
R1 chooses other R1, but **not** R2.

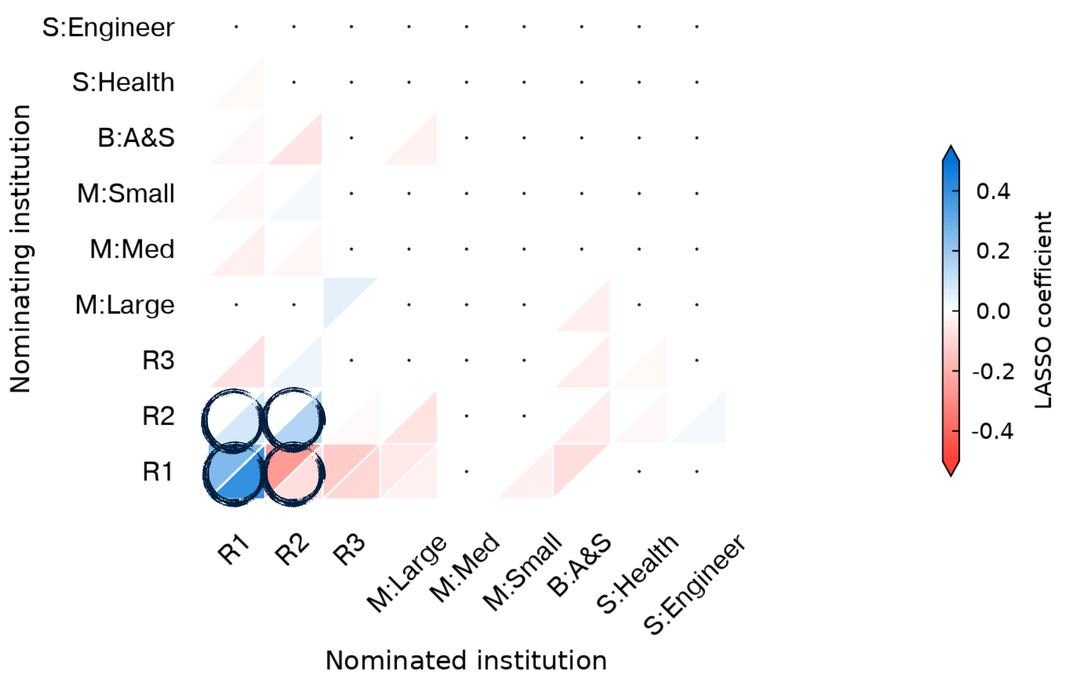
*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

Rich peer decision patterns (categorical features)



◸ : higher prestige
◿ : lower prestige





HBCU tends (slightly) to choose other HBCUs.

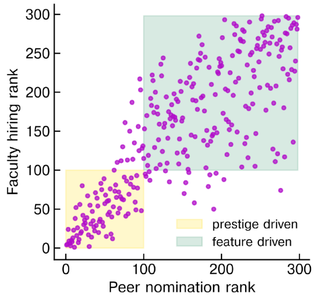
Private schools don't choose public schools (vv).

R1 chooses other R1, but **not** R2.

R2 chooses other R2, but also chooses R1.

*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

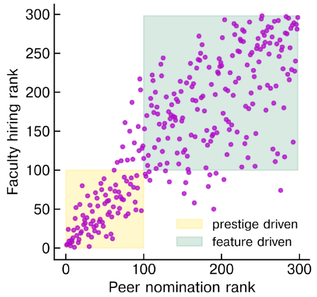
Prestige determines peer decision (numeric features)



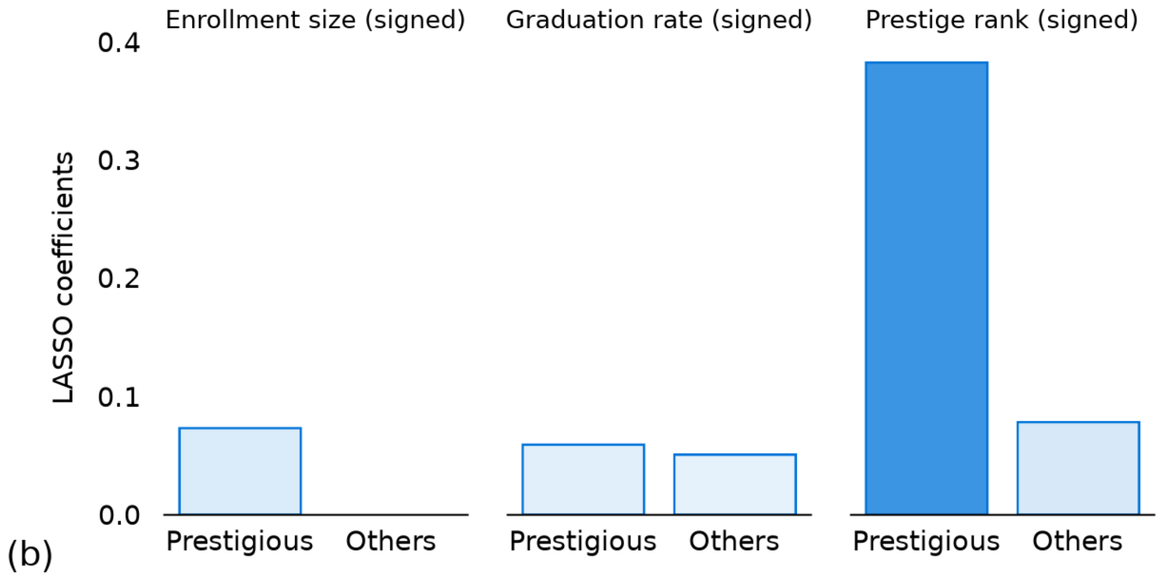
$i \to j$	Adm	Size	Grad	Prestige
Similarity (unsigned) $(x_j - x_i)^2$	∅	∅	∅	∅
Difference (signed) $x_j - x_i$	∅	✓	✓	✓

*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

Prestige determines peer decision (numeric features)



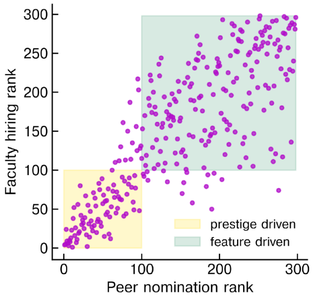
$i \to j$	Adm	Size	Grad	Prestige
Similarity (unsigned) $(x_j - x_i)^2$	∅	∅	∅	∅
Difference (signed) $x_j - x_i$	∅	✓	✓	✓



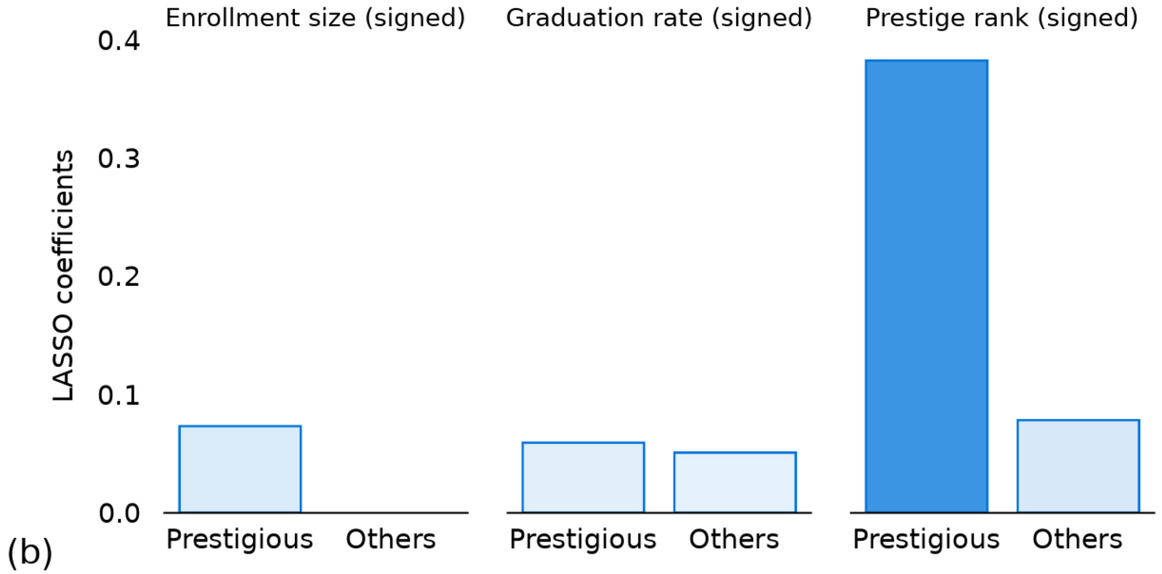
(b)

*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

Prestige determines peer decision (numeric features)



$i \to j$	Adm	Size	Grad	Prestige
Similarity (unsigned) $(x_j - x_i)^2$	∅	∅	∅	∅
Difference (signed) $x_j - x_i$	∅	✓	✓	✓

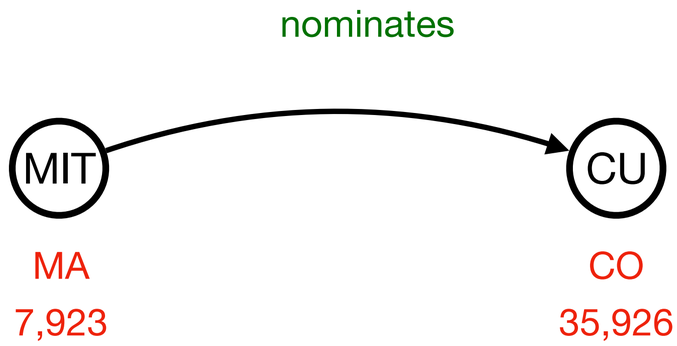


Outcome: Aspiration for a higher prestige rank is a significant predictive variable (for the elite institutions)

*Model validated via the average negative log likelihood (ANLL): stratified model (0.863); separate model (0.864); common model (0.912)

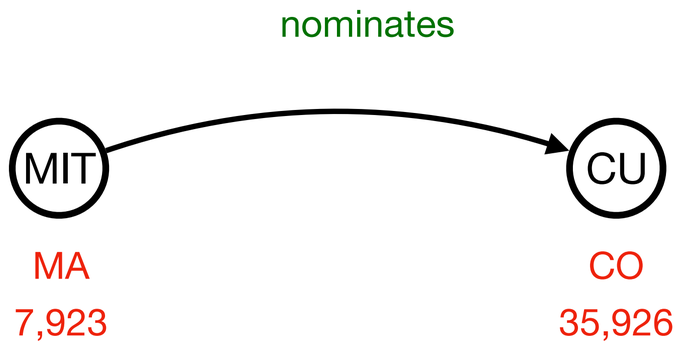
Wait… What about *other* schools?

Nomination network



Wait… What about *other* schools?

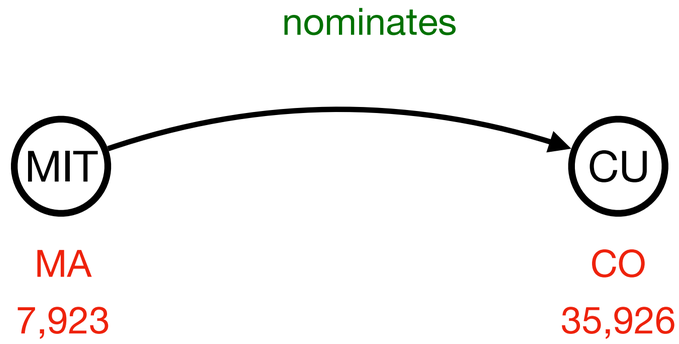
Nomination network



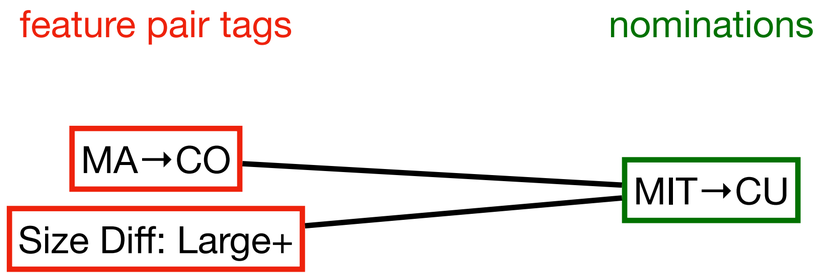


Wait… What about *other* schools?

Nomination network



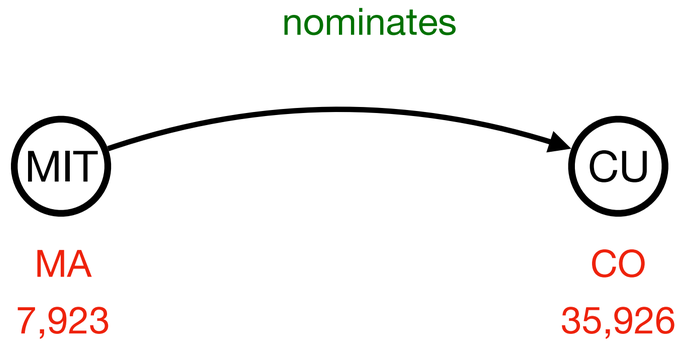
Bipartite expanded feature network



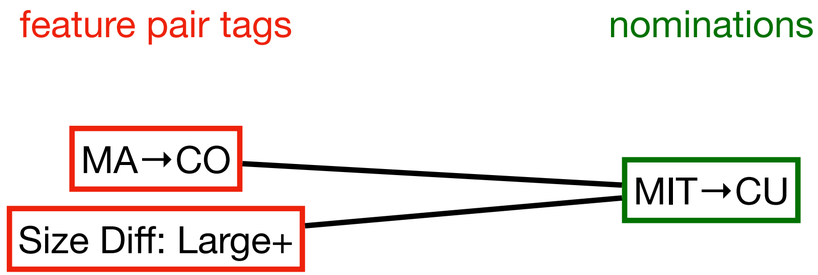


Wait… What about *other* schools?

Nomination network



Bipartite expanded feature network





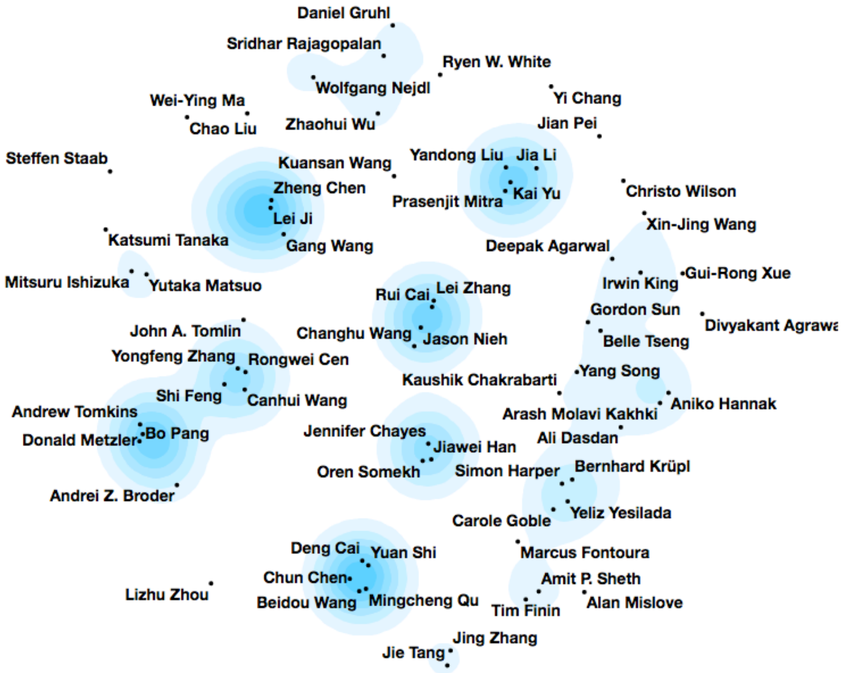
Method (clustering via the bipartite stochastic block model)

Conventional.

Bipartite network. of conferences and authors.

Nonnegative matrix factorization. Clustering who attend what conference.

Problems. *How many groups to choose? Sometimes just outputs 1 group (e.g., scarce data)* 😭



Lin *et al.*, SIAM Conference on Data Mining (2010)

Method (clustering via the bipartite stochastic block model)



Conventional.

Bipartite network. of conferences and authors.

Nonnegative matrix factorization. Clustering who attend what conference.

Problems. *How many groups to choose? Sometimes just outputs 1 group (e.g., scarce data)* 😭

Novel.

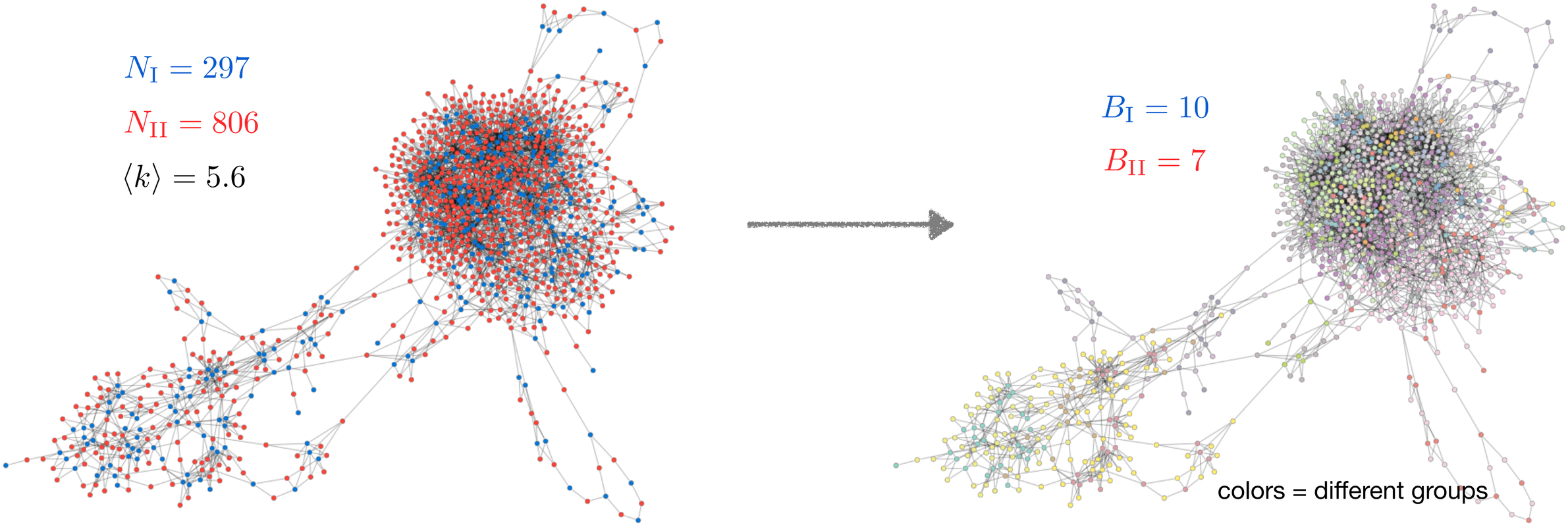
Nonparametric Bayesian modeling. Probabilistic generative model that detects communities. 😎



Communities with statistical validation (e.g., description length, posterior likelihood)

Known: The bipartite structure, i.e., which node is of which type. Edges are given (measurement is perfect).

Unknown: Of which group should a node be assigned to.



SBMs formalize the concept of “large-scale structure”

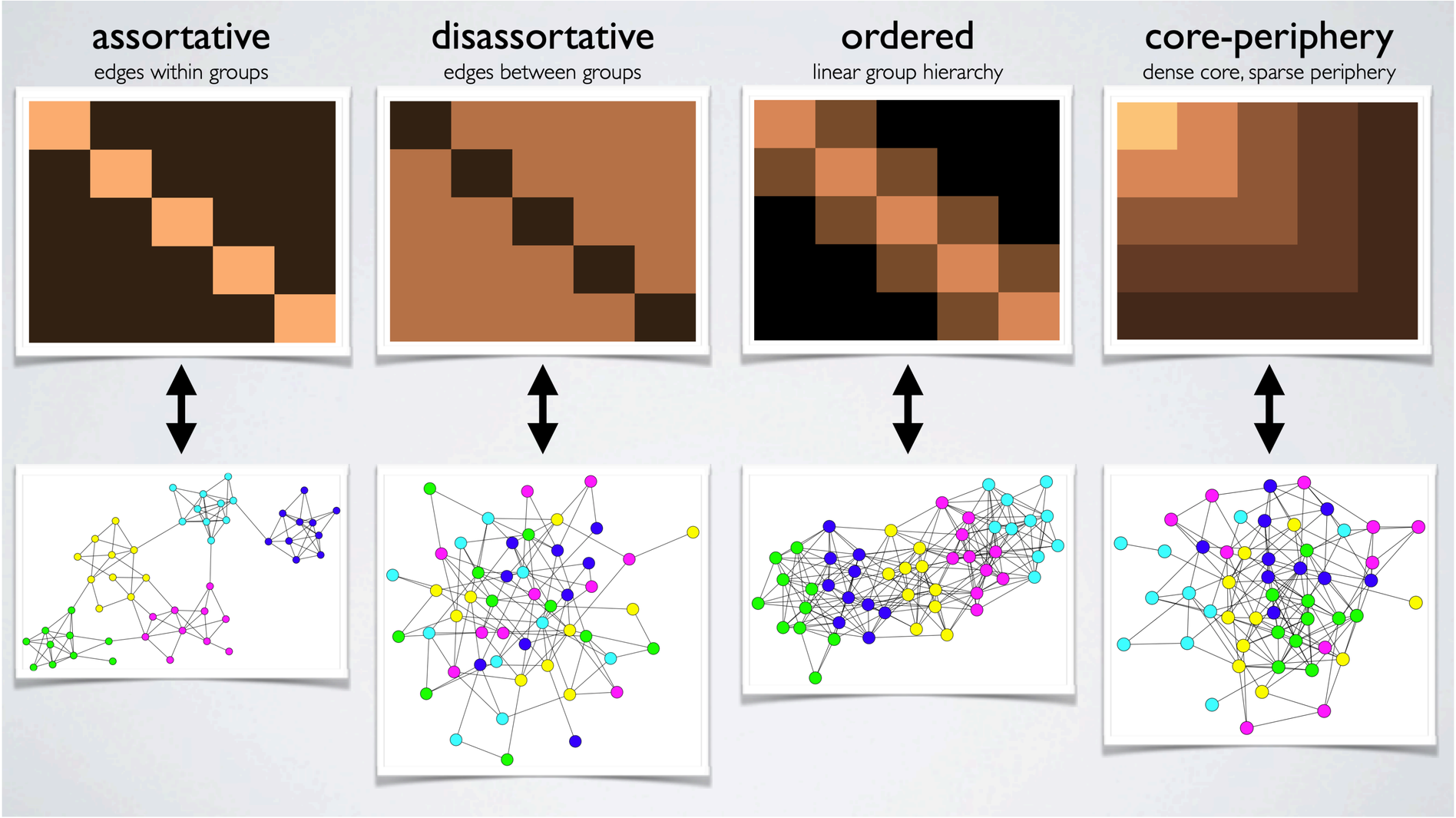


Image credit: Aaron Clauset

Bipartite stochastic block model

$$P(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = P(\boldsymbol{A} \mid \boldsymbol{k},\boldsymbol{e},\boldsymbol{b})P(\boldsymbol{k} \mid \boldsymbol{e},\boldsymbol{b})P(\boldsymbol{e} \mid \boldsymbol{b})P(\boldsymbol{b})$$

Likelihood

Prior

Bipartite stochastic block model

$$P_{\text{bi}}(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \frac{\prod_i k_i! \prod_{r<s} e_{rs}!}{\prod_r e_r! \prod_{i<j} A_{ij}!} \prod_r \frac{\prod_k \eta_k^r!}{n_r!} \frac{1}{q(e_r,n_r)} \left(\!\!\binom{B_{\text{I}}B_{\text{II}}}{E}\!\!\right)^{-1} \frac{\prod_r n_r!}{N_{\text{I}}!N_{\text{II}}!} \binom{N_{\text{I}}-1}{B_{\text{I}}-1}^{-1} \binom{N_{\text{II}}-1}{B_{\text{II}}-1}^{-1} \frac{1}{N_{\text{I}}N_{\text{II}}}.$$

$$P(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \underbrace{P(\boldsymbol{A} \mid \boldsymbol{k},\boldsymbol{e},\boldsymbol{b})}_{\text{Likelihood}} \underbrace{P(\boldsymbol{k} \mid \boldsymbol{e},\boldsymbol{b}) P(\boldsymbol{e} \mid \boldsymbol{b}) P(\boldsymbol{b})}_{\text{Prior}}$$

Bipartite stochastic block model

$$P_{\text{bi}}(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \frac{\prod_i k_i! \prod_{r<s} e_{rs}!}{\prod_r e_r! \prod_{i<j} A_{ij}!} \prod_r \frac{\prod_k \eta_k^r!}{n_r!} \frac{1}{q(e_r,n_r)} \left(\!\!\binom{B_{\text{I}}B_{\text{II}}}{E}\!\!\right)^{-1} \frac{\prod_r n_r!}{N_{\text{I}}!N_{\text{II}}!} \binom{N_{\text{I}}-1}{B_{\text{I}}-1}^{-1} \binom{N_{\text{II}}-1}{B_{\text{II}}-1}^{-1} \frac{1}{N_{\text{I}}N_{\text{II}}}.$$

$$P(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \underbrace{P(\boldsymbol{A} \mid \boldsymbol{k},\boldsymbol{e},\boldsymbol{b})}_{\text{Likelihood}} \underbrace{P(\boldsymbol{k} \mid \boldsymbol{e},\boldsymbol{b}) P(\boldsymbol{e} \mid \boldsymbol{b}) P(\boldsymbol{b})}_{\text{Prior}} = P(\mathbf{A}, \{b_i\})$$



Optimized with Markov chain Monte Carlo (Metropolis-Hastings)

Bipartite stochastic block model

$$P_{\text{bi}}(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \frac{\prod_i k_i! \prod_{r<s} e_{rs}!}{\prod_r e_r! \prod_{i<j} A_{ij}!} \prod_r \frac{\prod_k \eta_k^r!}{n_r!} \frac{1}{q(e_r,n_r)} \left(\!\!\binom{B_{\text{I}}B_{\text{II}}}{E}\!\!\right)^{-1} \frac{\prod_r n_r!}{N_{\text{I}}!N_{\text{II}}!} \binom{N_{\text{I}}-1}{B_{\text{I}}-1}^{-1} \binom{N_{\text{II}}-1}{B_{\text{II}}-1}^{-1} \frac{1}{N_{\text{I}}N_{\text{II}}}.$$

$$P(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \underbrace{P(\boldsymbol{A}\,|\,\boldsymbol{k},\boldsymbol{e},\boldsymbol{b})}_{\text{Likelihood}} \underbrace{P(\boldsymbol{k}\,|\,\boldsymbol{e},\boldsymbol{b})P(\boldsymbol{e}\,|\,\boldsymbol{b})P(\boldsymbol{b})}_{\text{Prior}} = P(\mathbf{A}, \{b_i\})$$



Optimized with Markov chain Monte Carlo (Metropolis-Hastings)

Enhanced model sensitivity: More detailed prior (e.g., we know *a priori* that the network is bipartite) gives more sensitive model to detect structure.

Bipartite stochastic block model

$$P_{\text{bi}}(\boldsymbol{A},\boldsymbol{k},\boldsymbol{e},\boldsymbol{b}) = \frac{\prod_i k_i! \prod_{r<s} e_{rs}!}{\prod_r e_r! \prod_{i<j} A_{ij}!} \prod_r \frac{\prod_k \eta_k^r!}{n_r!} \frac{1}{q(e_r,n_r)} \left(\!\!\binom{B_{\text{I}}B_{\text{II}}}{E}\!\!\right)^{-1} \frac{\prod_r n_r!}{N_{\text{I}}!N_{\text{II}}!} \binom{N_{\text{I}}-1}{B_{\text{I}}-1}^{-1} \binom{N_{\text{II}}-1}{B_{\text{II}}-1}^{-1} \frac{1}{N_{\text{I}}N_{\text{II}}}.$$

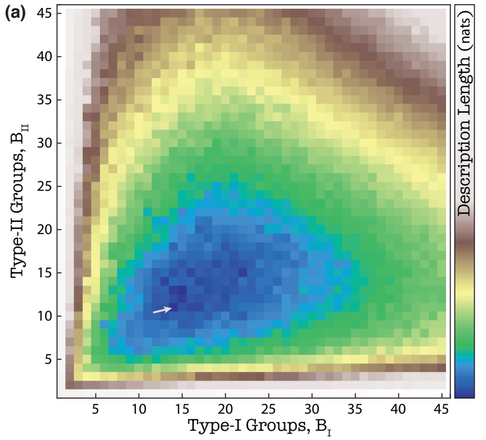
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Optimized with Markov chain Monte Carlo (Metropolis-Hastings)

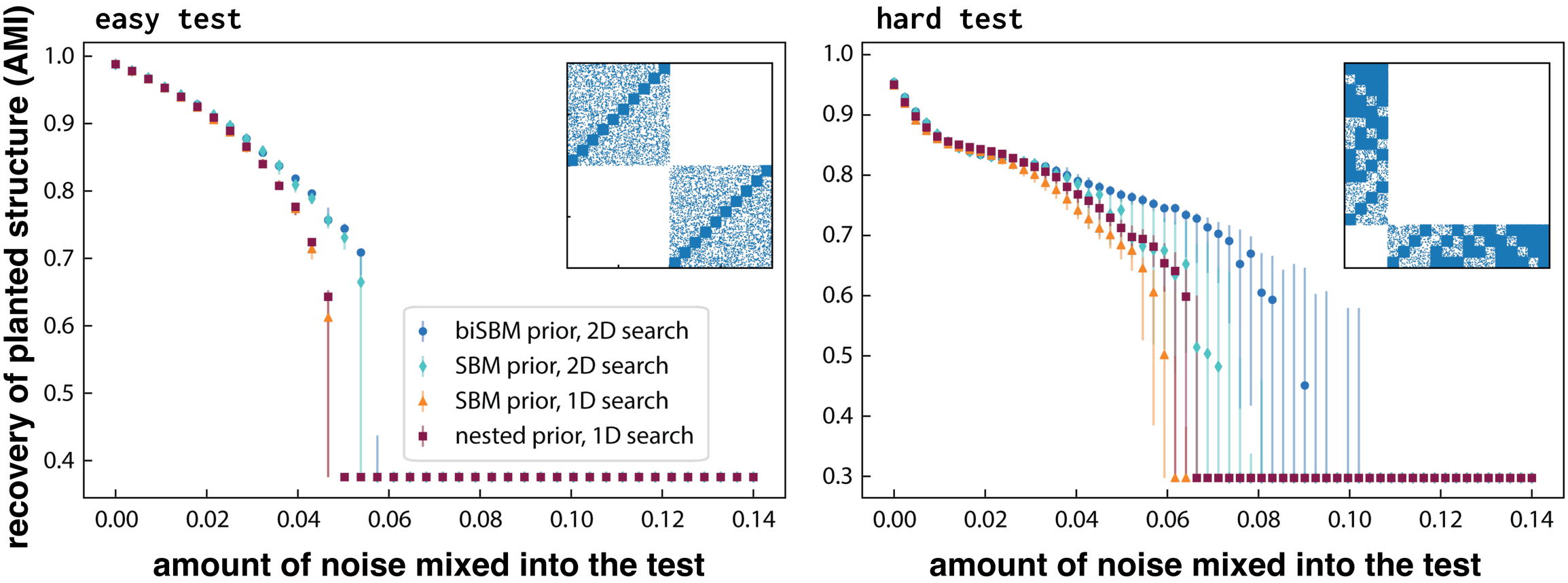
Enhanced model sensitivity: More detailed prior (e.g., we know *a priori* that the network is bipartite) gives more sensitive model to detect structure.

New algorithm comes with the new prior: Prior may introduce new variables, hence a new algorithm is needed.

Use dynamic programming to navigate the landscape



Testing performance: bipartite priors & search matter



vs effect of bipartite priors

vs effect of our search algorithm

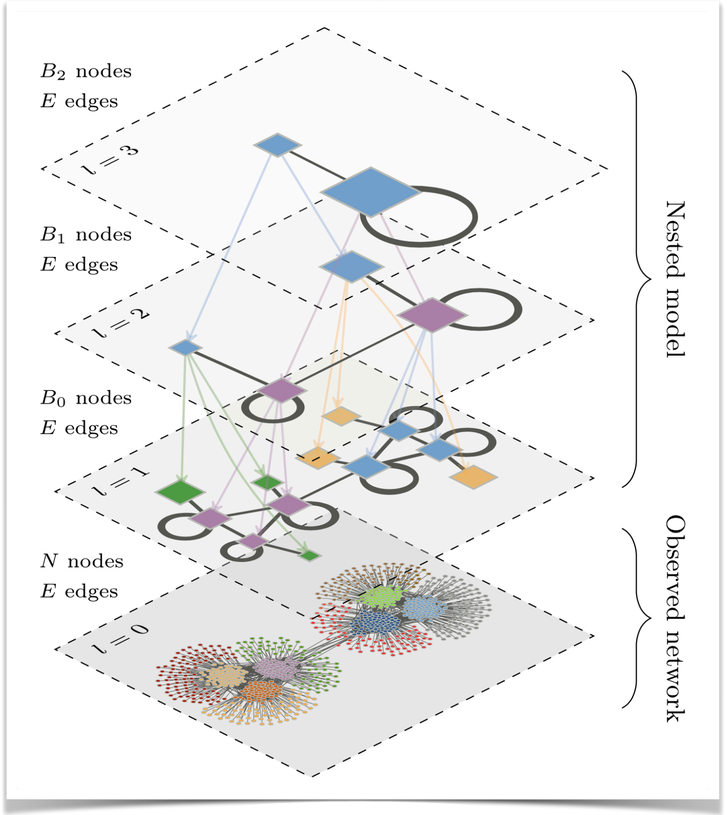
Yen & Larremore, Phys. Rev. E 102, 032309 (2020)

Comparison with hierarchical SBM

Table I. Results for 24 empirical networks. Number of nodes $n_{\rm I}$, $n_{\rm II}$, mean degree $\langle k\rangle$, number of type-I groups $B_{\rm I}$, and number of type-II groups $B_{\rm II}$, and description length per edge Σ/E. Superscripts: b-biSBM, g-SBM, h-hSBM. L indicates the number of levels found by the hSBM. Reported values indicate best of 100 independent runs. Unless otherwise noted, data are accessible from the Colorado Index of Complex Networks (ICON) [52]. The confidence level is marked with asterisks[a].

Dataset	$N_{\rm I}$	$N_{\rm II}$	$\langle k\rangle$	$(B_{\rm I}^{\rm b},B_{\rm II}^{\rm b})$	$(B_{\rm I}^{\rm g},B_{\rm II}^{\rm g})$	$(B_{\rm I}^{\rm h},B_{\rm II}^{\rm h})$	$\langle L+1\rangle$	$\Sigma^{\rm b}/E$	$\Sigma^{\rm h}/E$
Southern women interactions [53]	18	14	5.56	(1, 1)	(1, 1)	(1, 1)	2.0	**2.15***	2.26
Joern plant-herbivore web [54]	22	52	4.97	(2, 2)	(1, 1)	(1, 1)	2.0	**2.64***	2.74
Swingers and parties [55]	57	39	4.83	(1, 1)	(1, 1)	(1, 1)	2.0	**2.92***	2.97
McMullen pollination web [56]	54	105	2.57	(2, 2)	(2, 2)	(1, 1)	2.0	**2.87***	3.02
Ndrangheta criminals [57]	156	47	4.48	(3, 4)	(3, 3)	(3, 4)	2.87	**3.44***	3.49
Abu Sayyaf kidnappings[b] [58]	246	105	2.28	(2, 2)	(1, 1)	(1, 1)	2.0	**4.50***	4.54
Virus-host interactome [59]	53	307	2.52	(2, 2)	(1, 1)	(1, 1)	2.0	**3.78***	3.81
Clements-Long plant-pollinator [60]	275	96	4.98	(1, 1)	(1, 1)	(1, 1)	2.0	**3.45***	3.47
Human musculoskeletal system [61]	173	270	4.30	(7, 8)	(5, 5)	(8, 8)	4.01	**3.94**	3.94
Mexican drug trafficking[b] [62]	765	10	16.1	(12, 8)	(8, 7)	(10, 6)	3.11	**1.26***	1.29
Country-language network [63]	254	614	2.89	(4, 5)	(2, 2)	(4, 3)	2.11	**4.53***	4.56
Malaria gene similarity [44]	297	806	5.38	(15, 16)	(6, 6)	(25, 20)	4.95	4.73	**4.67***
Protein complex-drug [64]	739	680	5.20	(20, 22)	(14, 14)	(35, 39)	5.06	3.65	**3.50****
Robertson plant-pollinator [65]	456	1428	16.2	(20, 18)	(11, 11)	(20, 19)	4.0	**3.10***	3.10
Human gene-disease network [66]	1419	516	4.06	(13, 14)	(9, 9)	(35, 36)	5.04	5.02	**4.80****
Food ingredients-flavors web [67]	1525	1107	27.9	(27, 69)	(20, 29)	(42, 130)	4.91	2.55	**2.51****
Wikipedia doc-word network [68]	63	3140	24.8	(22, 206)	(18, 23)	(29, 71)	4.17	1.58	**1.51****
Foursquare check-ins [69]	2060	2876	11.0	(65, 66)	(40, 40)	(244, 248)	5.2	5.92	**5.09****
Ancient metabolic network [70]	5651	5252	4.22	(18, 22)	(5, 5)	(17, 21)	4.26	**5.68****	5.82
Marvel Universe characters [71]	6486	12942	9.95	(68, 72)	(67, 62)	(365, 314)	6.24	4.70	**4.42*****
Reuters news stories [72]	19757	38677	33.5	(396, 440)	(87, 108)	(294, 463)	6.25	4.22	**4.16*****
IMDb movie-actor dataset[c]	53158	39768	6.49	(91, 92)	(69, 68)	(264, 265)	6.22	7.40	**7.30*****
YouTube group memberships [73]	94238	30087	4.72	(62, 66)	(37, 38)	(221, 238)	5.9	**7.07****	7.13
DBpedia writer network [74]	89355	46213	2.13	(22, 26)	(2, 3)	(2, 3)	2.16	**10.32****	10.41

[a] Via the posterior odds ratio: * : $\Lambda < 10^{-2}$; ** : $\Lambda < 10^{-100}$; *** : $\Lambda < 10^{-10000}$.
[b] Temporal data with timestamps are aggregated, making a multigraph.
[c] Data available at http://www.imdb.com/interfaces. IMDb copyright permits redistribution of data only in unaltered form.



See Peixoto, Phys. Rev. X, 4, 011047 (2014) for the hierarchical SBM.

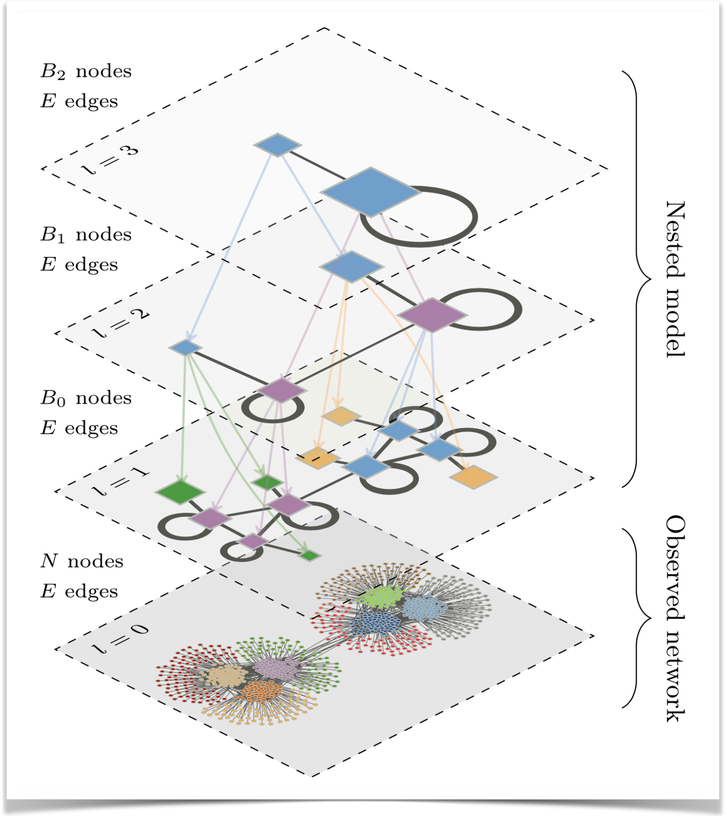
Comparison with hierarchical SBM

Avg. description length, the lower the better

Table I. Results for 24 empirical networks. Number of nodes $n_{\rm I}$, $n_{\rm II}$, mean degree $\langle k\rangle$, number of types $B_{\rm I}$, $B_{\rm II}$, and description length per edge Σ/E. Superscripts: b-biSBM, g-SBM, h-hSBM. L indicates the number of levels found by the hSBM. Reported values indicate best of 100 independent runs. Unless otherwise noted, data are accessible [...] Networks (ICON) [52]. The confidence level is marked with asterisks[a].

Dataset	$N_{\rm I}$	$N_{\rm II}$	$\langle k\rangle$	$(B^{\rm b}_{\rm I}, B^{\rm b}_{\rm II})$	$(B^{\rm g}_{\rm I}, B^{\rm g}_{\rm II})$	$(B^{\rm h}_{\rm I}, B^{\rm h}_{\rm II})$	$\langle L+1\rangle$	$\Sigma^{\rm b}/E$	$\Sigma^{\rm h}/E$
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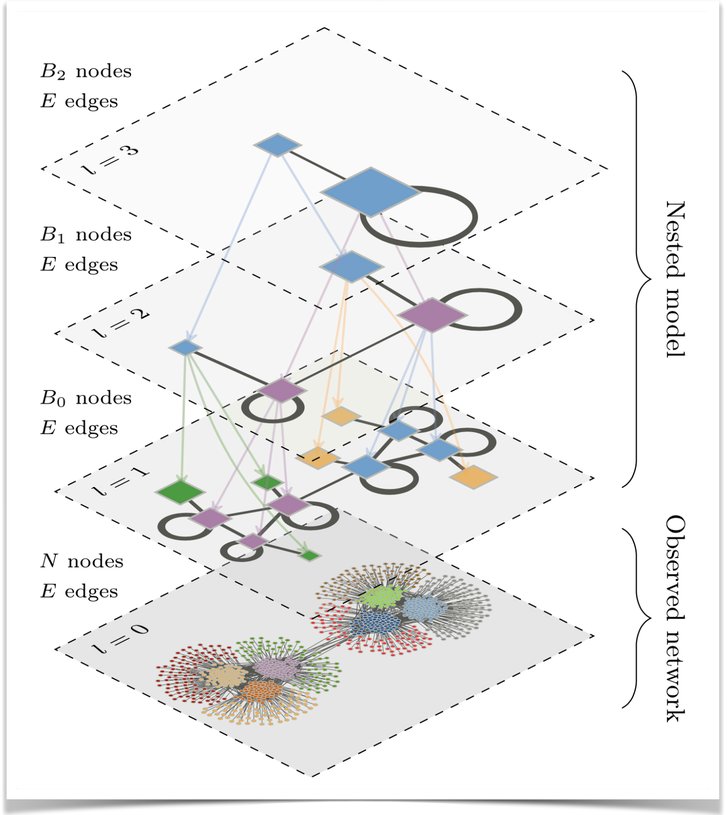
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For smaller networks, bipartite SBM is better.

See Peixoto, Phys. Rev. X, 4, 011047 (2014) for the hierarchical SBM.

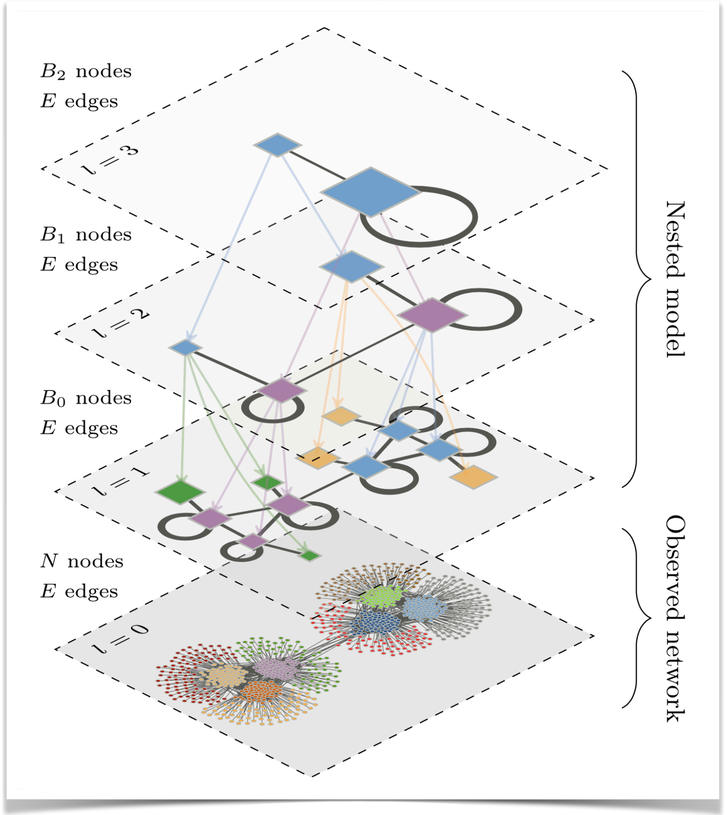
Comparison with hierarchical SBM

Table I. Results for 24 empirical networks. Number of nodes $n_{\rm I}$, $n_{\rm II}$, mean degree $\langle k\rangle$, number of types in each partition for the best fit of the bipartite SBM, $B_{\rm I}$, $B_{\rm II}$, and description length per edge Σ/E. Superscripts: b-biSBM, g-SBM, h-hSBM. L indicates the number of levels found by the hSBM. Reported values indicate best of 100 independent runs. Unless otherwise noted, data are accessible at the Index of Complex Networks (ICON) [52]. The confidence level is marked with asterisks[a].

Avg. description length, the lower the better

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McMullen pollination web [56]	54	105	2.57	(2, 2)	(2, 2)	(1, 1)	2.0	**2.87***	3.02
Ndrangheta criminals [57]	156	47	4.48	(3, 4)	(3, 3)	(3, 4)	2.87	**3.44***	3.49
Abu Sayyaf kidnappings[b] [58]	246	105	2.28	(2, 2)	(1, 1)	(1, 1)	2.0	**4.50***	4.54
Virus-host interactome [59]	53	307	2.52	(2, 2)	(1, 1)	(1, 1)	2.0	**3.78***	3.81
Clements-Long plant-pollinator [60]	275	96	4.98	(1, 1)	(1, 1)	(1, 1)	2.0	**3.45***	3.47
Human musculoskeletal system [61]	173	270	4.30	(7, 8)	(5, 5)	(8, 8)	4.01	**3.94**	3.94
Mexican drug trafficking[b] [62]	765	10	16.1	(12, 8)	(8, 7)	(10, 6)	3.11	**1.26***	1.29
Country-language network [63]	254	614	2.89	(4, 5)	(2, 2)	(4, 3)	2.11	**4.53***	4.56
Malaria gene similarity [44]	297	806	5.38	(15, 16)	(6, 6)	(25, 20)	4.95	4.73	**4.67***
Protein complex-drug [64]	739	680	5.20	(20, 22)	(14, 14)	(35, 39)	5.06	3.65	**3.50****
Robertson plant-pollinator [65]	456	1428	16.2	(20, 18)	(11, 11)	(20, 19)	4.0	**3.10***	3.10
Human gene-disease network [66]	1419	516	4.06	(13, 14)	(9, 9)	(35, 36)	5.04	5.02	**4.80****
Food ingredients-flavors web [67]	1525	1107	27.9	(27, 69)	(20, 29)	(42, 130)	4.91	2.55	**2.51****
Wikipedia doc-word network [68]	63	3140	24.8	(22, 206)	(18, 23)	(29, 71)	4.17	1.58	**1.51****
Foursquare check-ins [69]	2060	2876	11.0	(65, 66)	(40, 40)	(244, 248)	5.2	5.92	**5.09****
Ancient metabolic network [70]	5651	5252	4.22	(18, 22)	(5, 5)	(17, 21)	4.26	**5.68****	5.82
Marvel Universe characters [71]	6486	12942	9.95	(68, 72)	(67, 62)	(365, 314)	6.24	4.70	**4.42*****
Reuters news stories [72]	19757	38677	33.5	(396, 440)	(87, 108)	(294, 463)	6.25	4.22	**4.16*****
IMDb movie-actor dataset[c]	53158	39768	6.49	(91, 92)	(69, 68)	(264, 265)	6.22	7.40	**7.30*****
YouTube group memberships [73]	94238	30087	4.72	(62, 66)	(37, 38)	(221, 238)	5.9	**7.07****	7.13
DBpedia writer network [74]	89355	46213	2.13	(22, 26)	(2, 3)	(2, 3)	2.16	**10.32****	10.41

[a] Via the posterior odds ratio: $^{*}:\Lambda<10^{-2}$; $^{**}:\Lambda<10^{-100}$; $^{***}:\Lambda<10^{-10000}$.
[b] Temporal data with timestamps are aggregated, making a multigraph.
[c] Data available at http://www.imdb.com/interfaces. IMDb copyright permits redistribution of data only in unaltered form.



For smaller networks, bipartite SBM is better.

For larger+sparser networks, bipartite SBM is better.

See Peixoto, Phys. Rev. X, 4, 011047 (2014) for the hierarchical SBM.

Implications

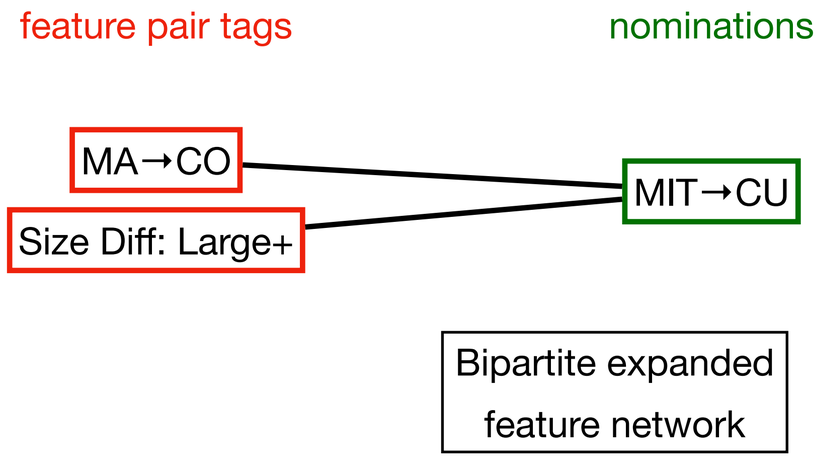
Bayesian framework. data becomes a part of the model, algorithm becomes data-dependent, i.e., some data may be harder to fit (opportunities for improvement).

Always choose a simpler model. If not possible to attain (e.g., no good definition of "simple-ness"), choose a more flexible one.

A handful of groups explain most nomination behaviors

Type-I nodes: feature pair tags, to cluster as B_I groups

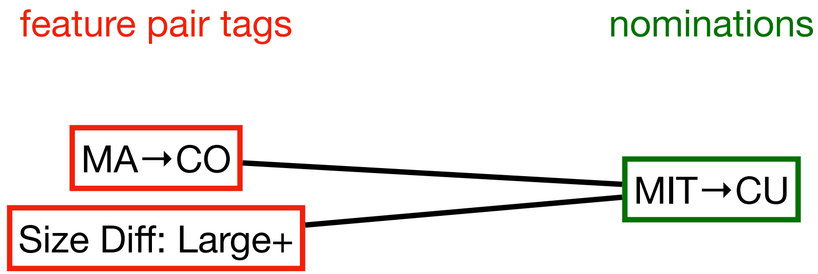
Type-II nodes: nominations, to cluster as B_{II} groups



A handful of groups explain most nomination behaviors

Type-I nodes: feature pair tags, to cluster as B_I groups

Type-II nodes: nominations, to cluster as B_{II} groups

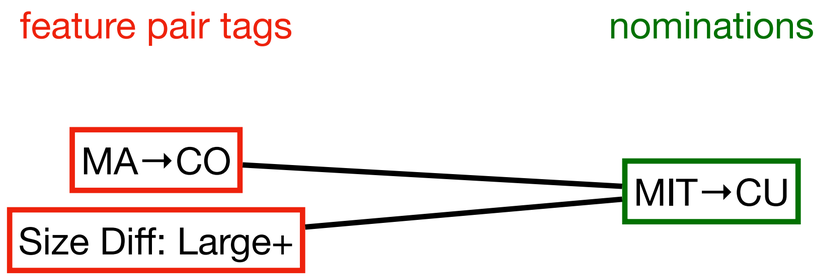


Code	Type of Institutions	N	N_{I}	N_{II}	E	B_{I}	B_{II}	Σ/E
15	Doctoral Universities: Highest Research Activity	117	946	1956	13692	5	2	2.45
16	Doctoral Universities: Higher Research Activity	112	833	1757	12299	8	2	2.67
17	Doctoral Universities: Moderate Research Activity	102	596	1815	12705	11	3	2.68
18	Master's Colleges & Universities: Larger Programs	251	958	4118	28825	16	3	2.73
19	Master's Colleges & Universities: Medium Programs	129	656	2082	14574	14	3	2.71
20	Master's Colleges & Universities: Small Programs	78	502	1169	8183	6	2	2.70
21	Baccalaureate Colleges: Arts & Sciences Focus	176	778	3105	21735	4	2	2.48
22	Baccalaureate Colleges: Diverse Fields	144	698	2129	14903	12	3	2.69
23	Baccalaureate/Associate's Colleges: Mixed Baccalaureate/Associate's	126	32	232	1624	4	2	2.45
24	Special Focus Four-Year: Faith-Related Institutions	1	9	2	14	1	1	1.31
26	Special Focus Four-Year: Other Health Professions Schools	5	53	42	293	1	1	2.55
27	Special Focus Four-Year: Engineering Schools	3	45	24	168	1	1	2.53
28	Special Focus Four-Year: Other Technology-Related Schools	3	53	38	266	1	1	2.37
29	Special Focus Four-Year: Business & Management Schools	6	47	122	854	1	1	2.27
30	Special Focus Four-Year: Arts, Music & Design Schools	18	138	196	1372	1	1	2.41
32	Special Focus Four-Year: Other Special Focus Institutions	2	38	30	209	1	1	2.34
		total = 1179						

A handful of groups explain most nomination behaviors

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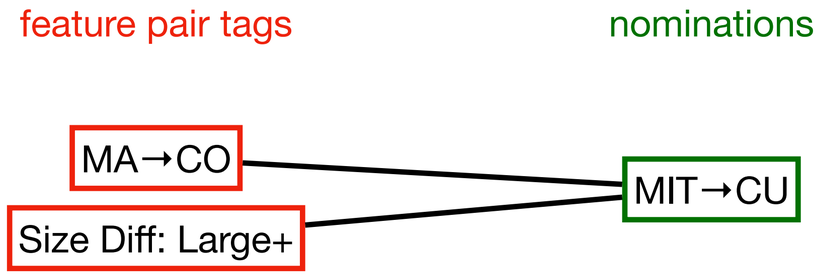


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A handful of groups explain most nomination behaviors (cont.)

Type	Top feature pairs	Group 1	Group 2
R1	non-HBCU to non-HBCU, to higher admission rate, to other R1	10.4%	36.8%
	78.9% intrastate, 93.5% interstate, non-HBCU to HBCU, to similar enrollment size, to R2 or to M:Large	2.5%	22.1%
	Public to Public/Private, to lower grad rate	0%	13.2%
	5.3% intrastate, to higher grad rate, to similar admission rate	3.9%	6.1%
	15.8% intrastate, 6.5% interstate, Private to Public/Private	4.9%	0.1%
R2	non-HBCU to non-HBCU, to higher admission rate, to R1, to M:Large	28.4%	12.7%
	to lower enrollment size, to higher graduation rate, to similar admission rate, to other R2	19.7%	4.7%
	69.6% intrastate, 90.7% interstate, HBCU to HBCU/non-HBCU, non-HBCU to HBCU, to M:Small, to Bacc. Colleges (diverse fields), Private to Public/Private for-profit	11.5%	1.3%
	Public to Public	9.6%	0%
	to higher admission rate, to R3	1.9%	2.1%
	Private to Private	0%	3.7%
	17.4% intrastate, 4% interstate, to M:Med, S:Engineer, Public to Private	0.6%	1.8%
	13% intrastate, 5.3% interstate, to B:A&S, to Special Focus Four-Year (Arts/Music/Design)	0%	1.9%

*See dissertation for clustering of other Carnegie classifications

A handful of groups explain most nomination behaviors (cont.)

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Niche effect. R1 wants to increase grad rate than other intrastate R1s; R2 aspires the same, but be fitter (lower enrollment size).

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Implications

Implications

All institutions. Name higher prestige institutions as their peers.

Implications

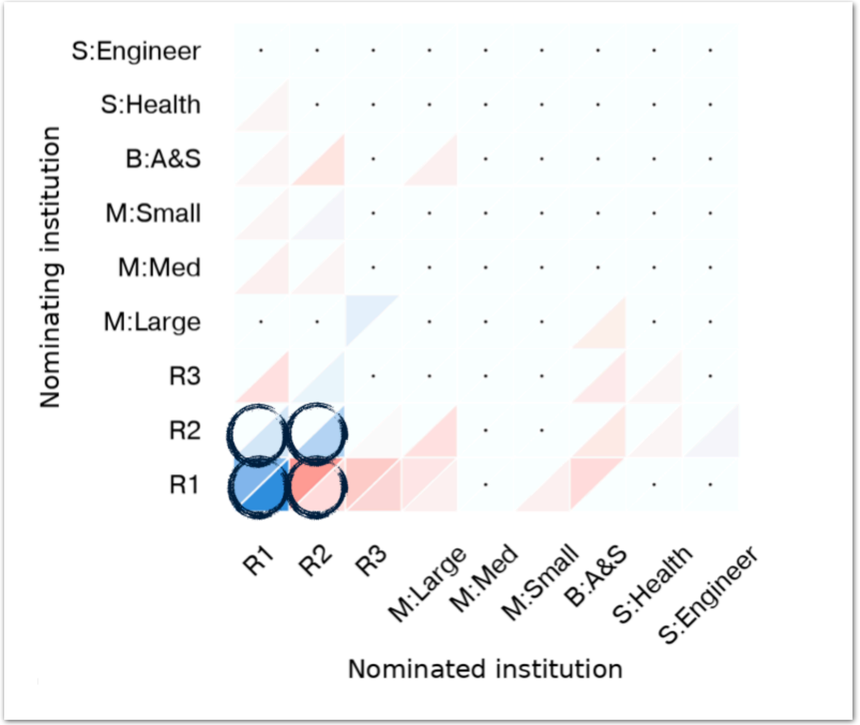
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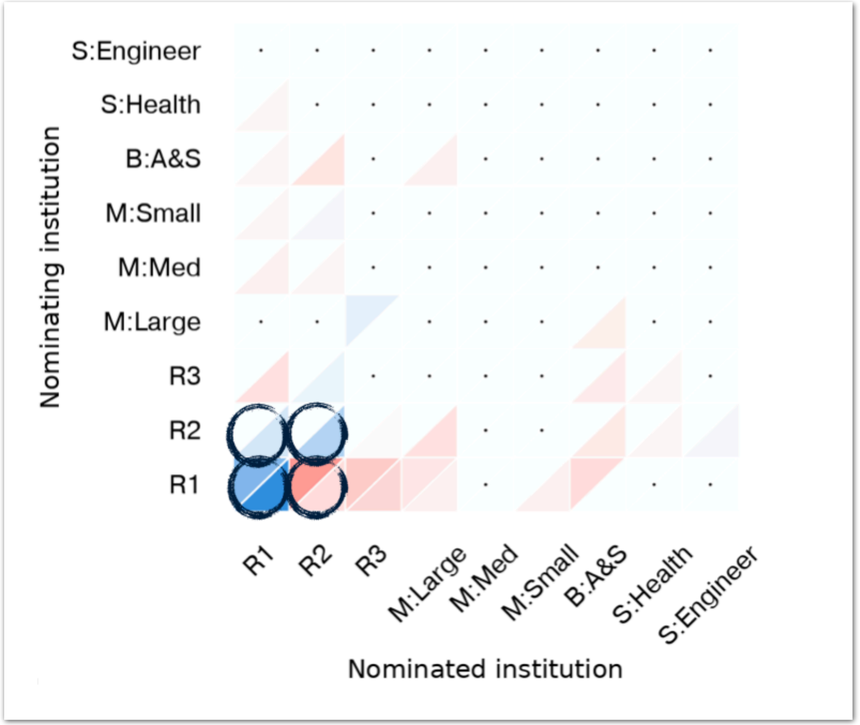


Implications

All institutions. Name higher prestige institutions as their peers.

Elite institutions. Particularly aspire prestige.

Others. Explainable by a handful of feature groups.



Outline

1. Context & motivation (chapter 1)
2. Aspiration of prestige in institutional peer selection (chapter 5)
3. Community detection in bipartite networks (chapter 2)
4. Regularized methods for efficient ranking (chapter 3)
5. A detour in higher-order structures (chapter 4)
6. Conclusions & future research (chapter 6)



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M. E. J. Newman & Aaron Clauset

Nature Communications **7**, Article number: 11863 (2016)

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Darko Hric, Tiago P. Peixoto, and Santo Fortunato
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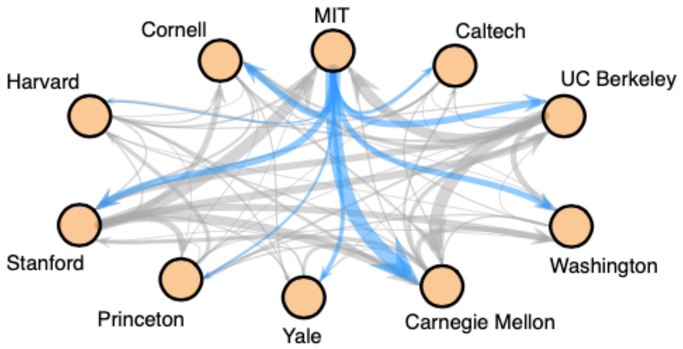
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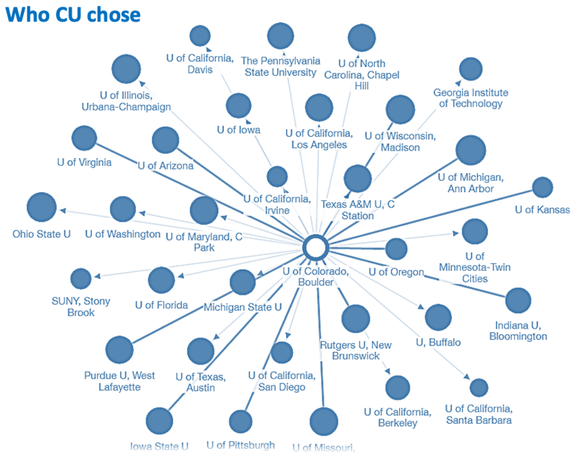
SpringRank

Each directed edge $u \to v$ implies PhD from u becomes faculty at v



Computer science faculty hiring network; http://tuvalu.santafe.edu/~aaronc/facultyhiring/. See also: *Sci. Adv.* 1(1), e1400005, 2015.

Each directed edge $u \to v$ implies institution u selects institution v



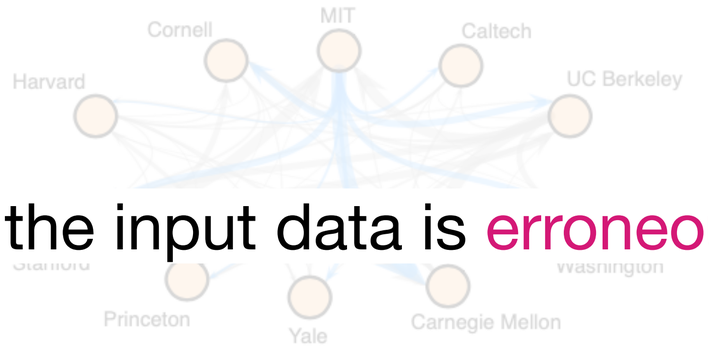
SpringRank: Let $\mathbf{A} = \{A_{ij}\}$ be the adjacency matrix of a directed multigraph.

The SpringRank Model finds the ranking $\mathbf{s}^*$ of the nodes by solving:

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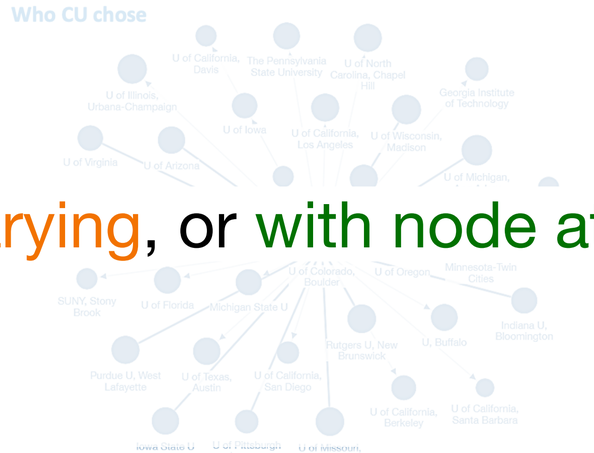
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When the input data is erroneous, time-varying, or with node attributes

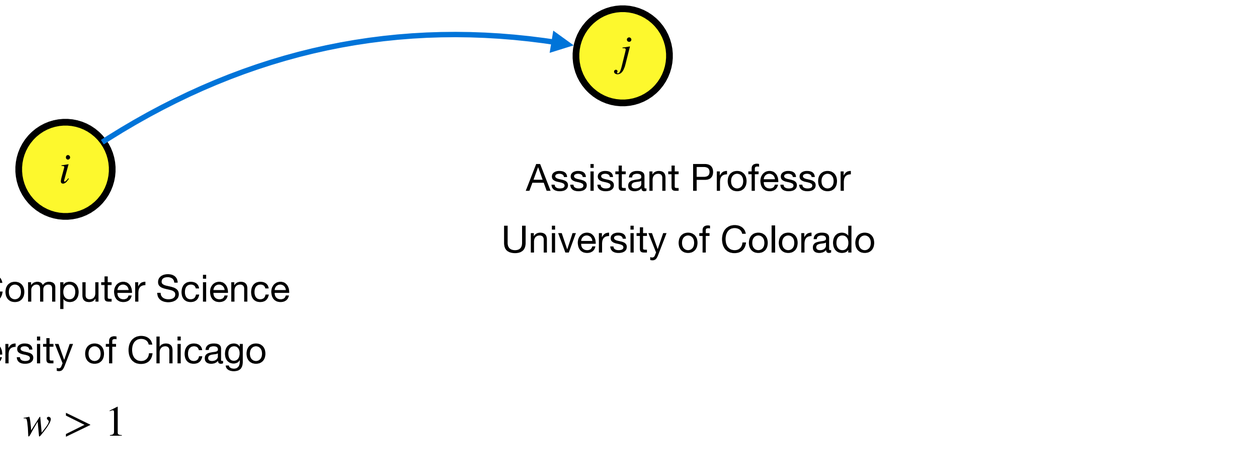
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Math PhD Exchange Dataset: Proxy for university i hiring a graduate from university j at a time near t. We view this as an endorsement by j that graduates of t are of high quality.

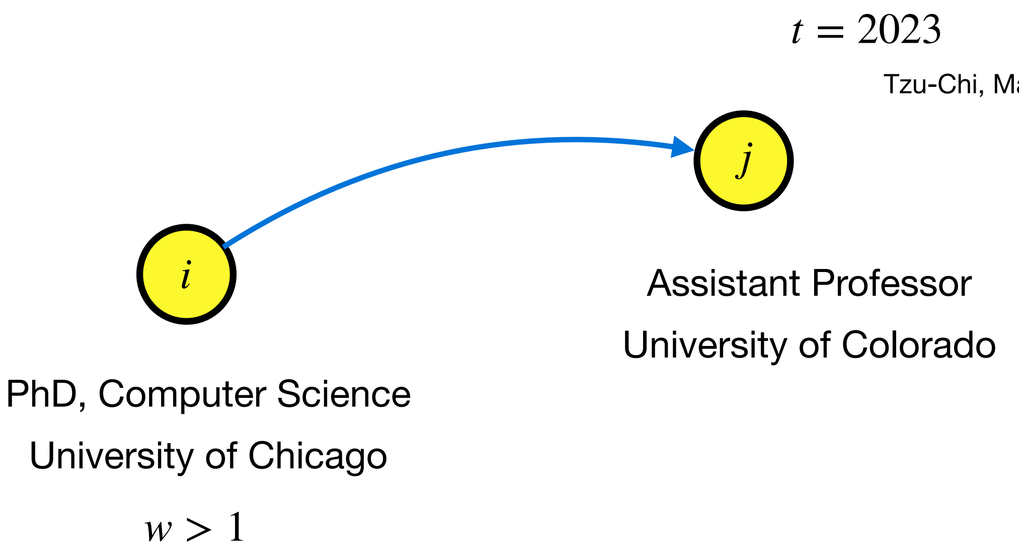


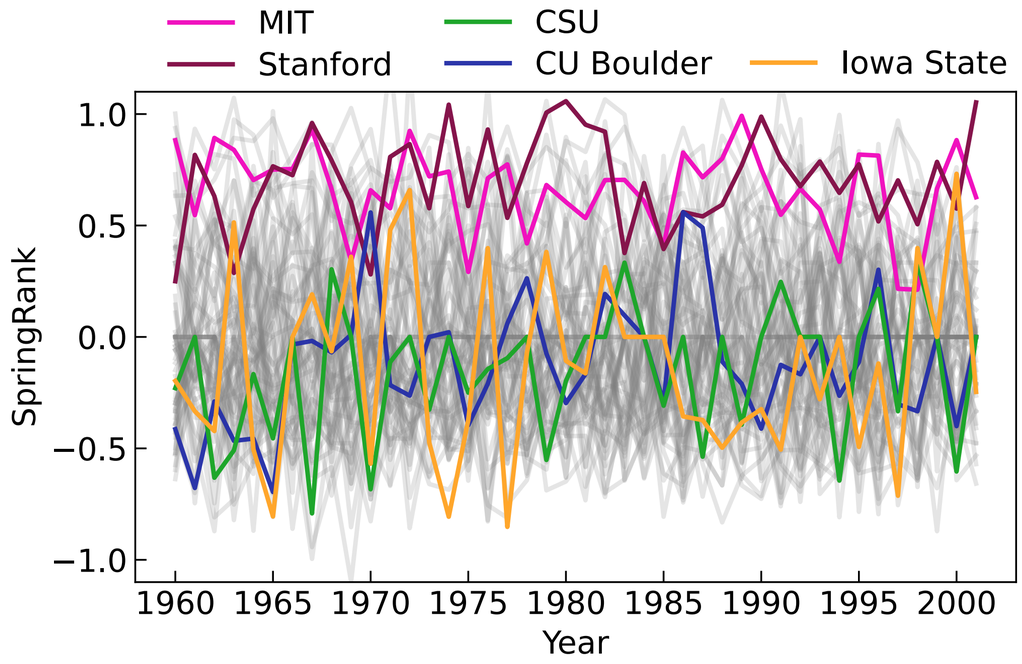


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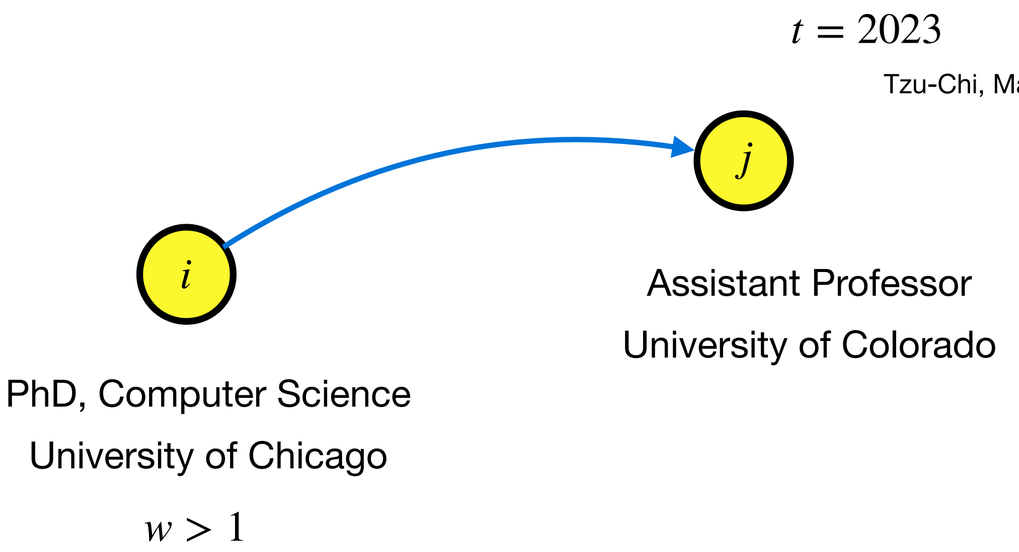




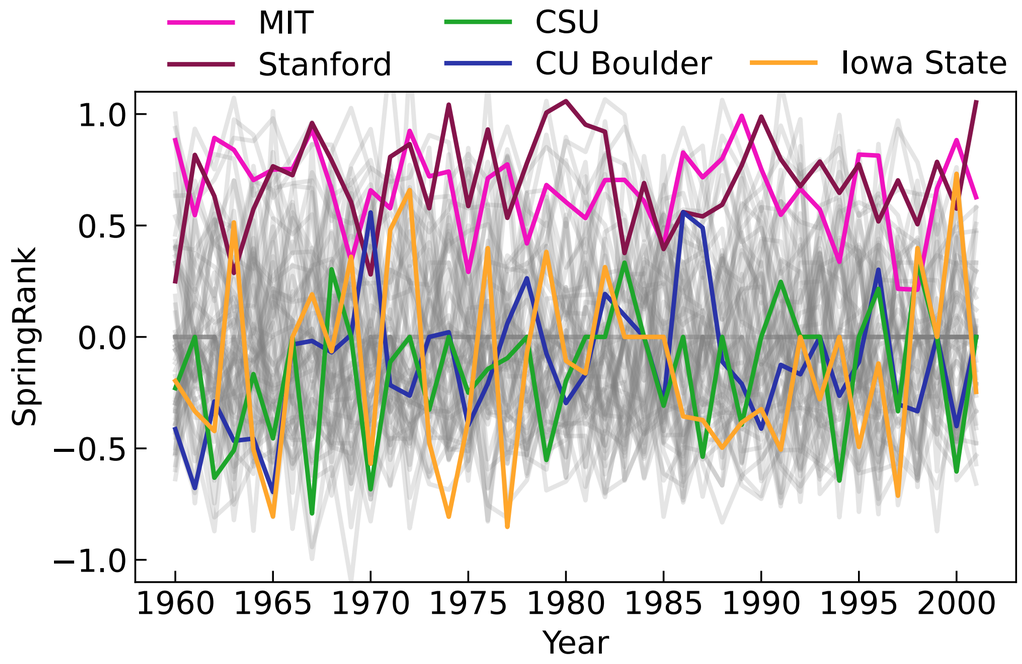
Motivation

Math PhD Exchange Dataset: Proxy for university i hiring a graduate from university j at a time near t. We view this as an endorsement by j that graduates of t are of high quality.





Problem: Fluctuating rankings!



Idea: Optimization with Sparsity-Inducing Penalties

Sparsity through the $\ell 1$ norm: a number of coefficients of $\mathbf{w}^*$, depending on the strength of the regularization, will be exactly equal to zero.

For details, see Bach *et al.*, “Optimization with Sparsity-Inducing Penalties ” (2011).

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Sparsity through the ℓ1/ℓq norm (group norm): sometimes coefficients of $\mathbf{w}^*$ are naturally partitioned in subsets, or groups, of variables. Through regularization, some groups of coefficients will be exactly equal to zero.

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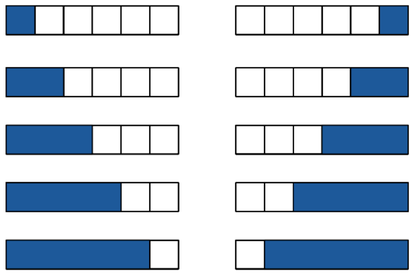
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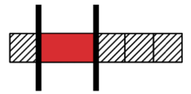
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Sparsity through overlapping groups: groups can even overlap, resulting in more exotic structures to be selected.

example group setup



example coefficients selected



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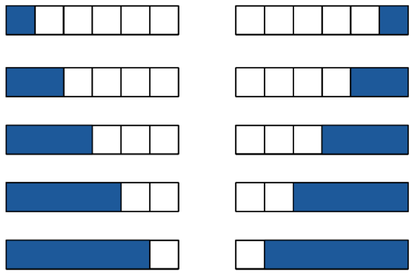
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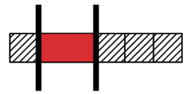
Examples. Regression, graphical modeling, de-noising, dictionary learning, etc.

(common theme: convex optimization!)

example group setup



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Specific regularizations (1/3)

Regularize time dependency: apply $\ell 1$ or $\ell 2$ norm to the rank gradient in adjacent time window

$$\Omega_1(\boldsymbol{s}) \coloneqq \sum_t \|\boldsymbol{s}_t - \boldsymbol{s}_{t-1}\|_1$$

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$\ell 2$ encourages $\boldsymbol{s}_t \approx \boldsymbol{s}_{t-1}$

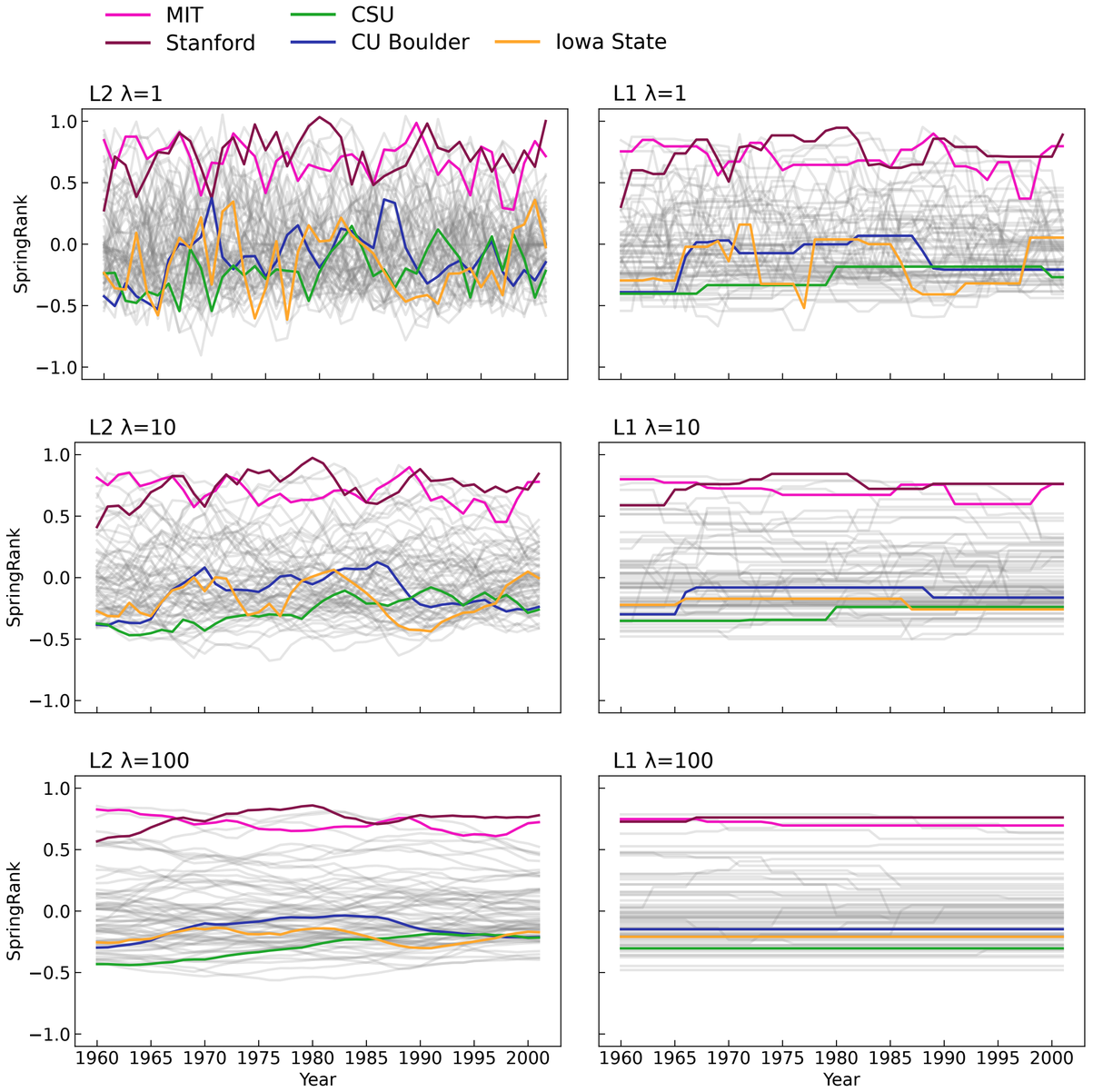
$\ell 1$ encourages $\boldsymbol{s}_t = \boldsymbol{s}_{t-1}$ (sparsity in ranking difference)

Result (1/3): Ranking over time

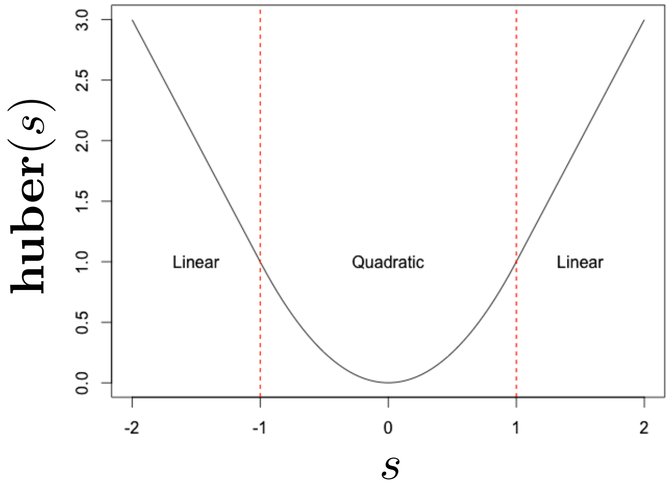
$$\underset{s}{\text{minimize}}\, \mathcal{L}(s) + \alpha\|s\|_2^2 + \lambda\Omega(Ls)$$

Benefits. Reduce the S/N-ratio to reveal the trends (through $\ell 2$), and possibly also reveal "specific events" (through $\ell 1$).

For smaller schools (lacking data), we can assign non-zero ranks.



Specific regularizations (2/3)



Robust to outliers: substitute the quadratic loss with the Huber loss

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Result (2/3): Robust ranking

$$\underset{s}{\text{minimize}}\, \mathcal{L}(\boldsymbol{s}) + \alpha \|\boldsymbol{s}\|_2^2 + \lambda \Omega(L\boldsymbol{s})$$

Error bar averages over 100 random nodes.

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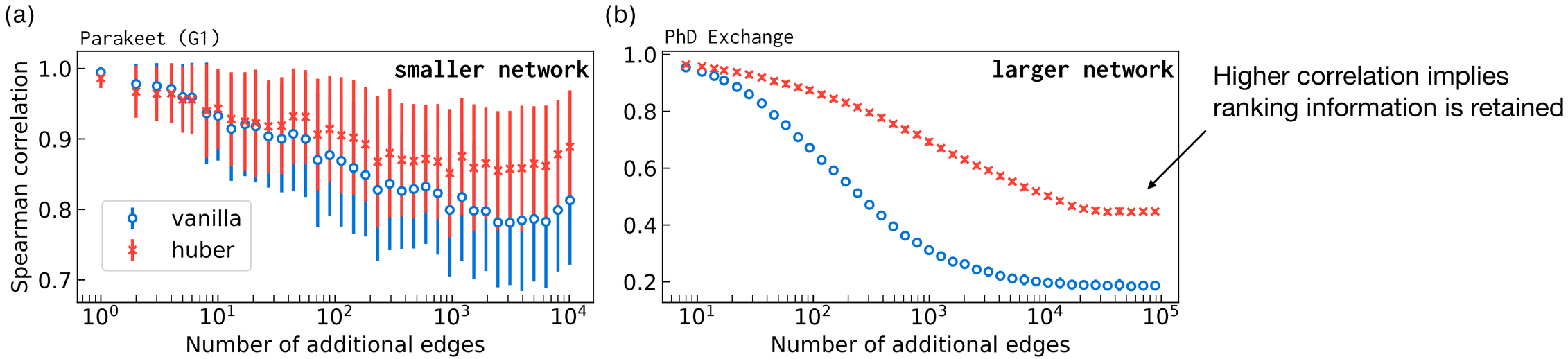
“Single-point mutation” style noise: A random node receives edges $|E|$ pointed from other nodes.

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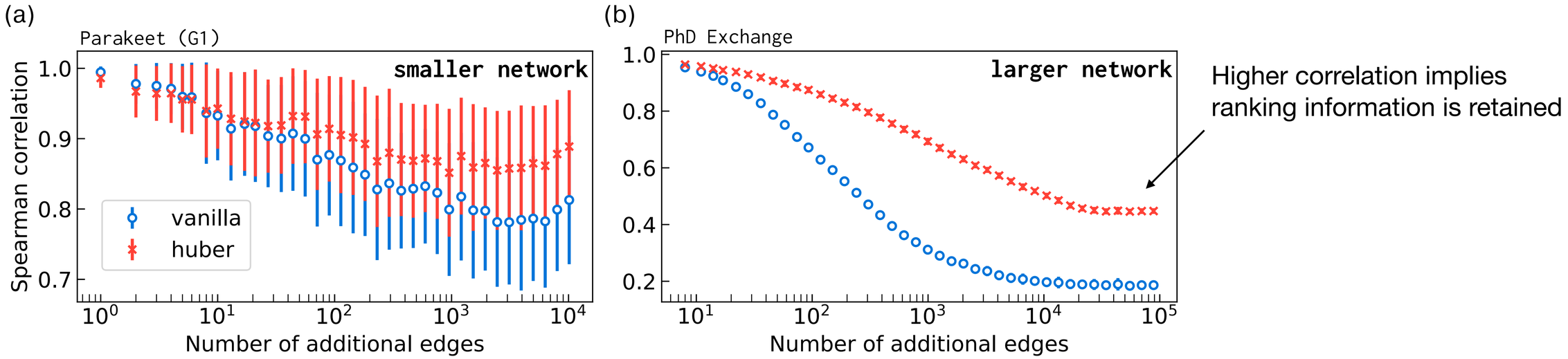
Higher correlation implies ranking information is retained

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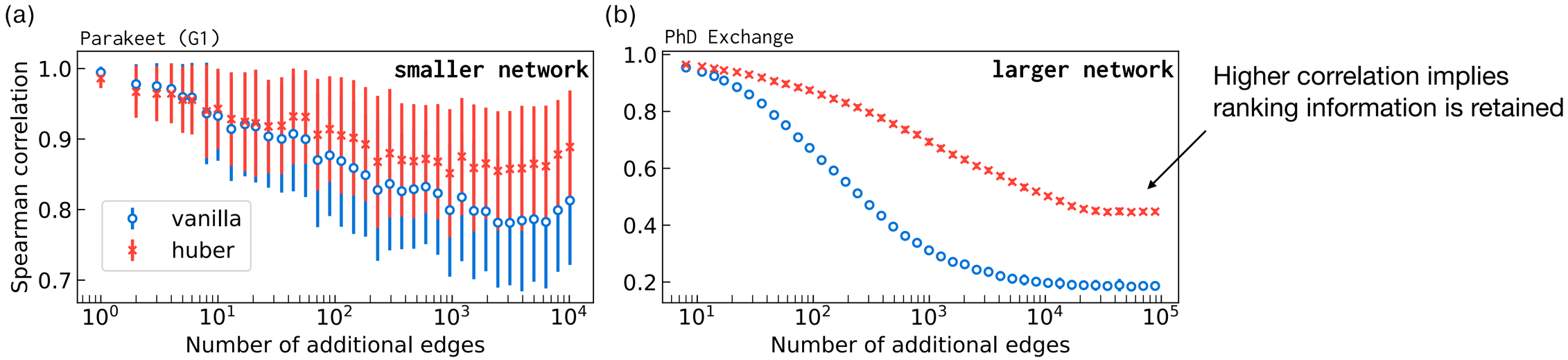
Other forms of noise: Randomly added/removed edges

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Benefits: Huber loss is less sensitive to outliers in the data.

Error bar averages over 100 random nodes.

Solution method

$$\underset{\boldsymbol{s}\in\mathbb{R}^N}{\text{minimize}}\ \underbrace{\frac{1}{2}\sum_{ij} A_{ij}(s_i - s_j - 1)^2}_{\mathcal{L}_{\text{quad}}} + \alpha \sum_{i=1}^{N} s_i^2$$

Generic form: two regularization functions, one makes the objective strongly convex (easier to solve), the other encourages certain structure.

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* The original SpringRank paper uses this!

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First-order methods. we may turn to generalizations of gradient decent

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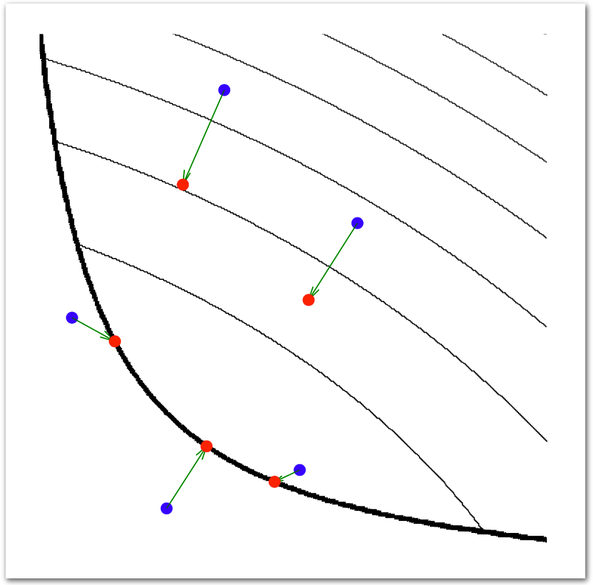
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Composite model: requires that f has a nice gradient and g has a easy-to-compute proximal operator

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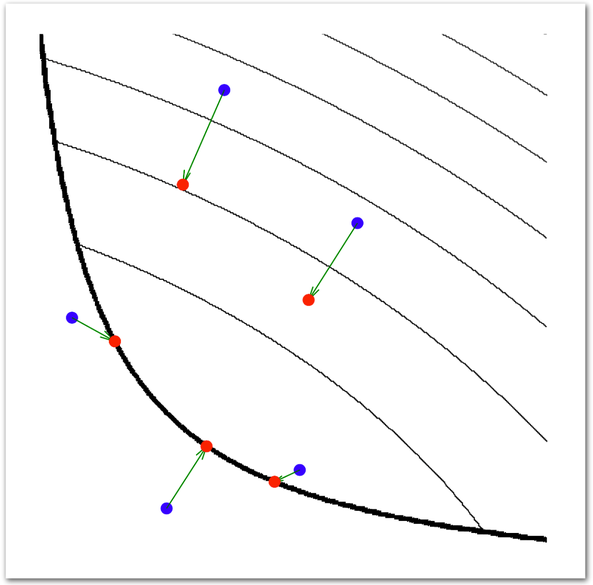
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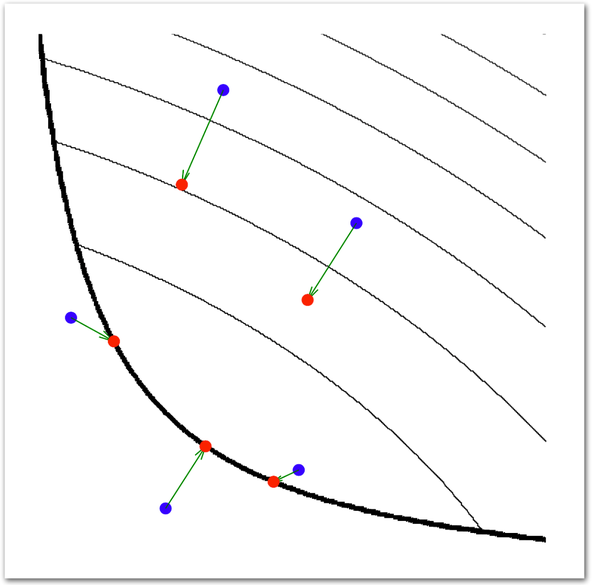
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Dual problem: easier to solve, as the linear operator L goes to the part that relies on the gradient.

(Primal) $\underset{\boldsymbol{s}\in\mathbb{R}^N}{\text{minimize}}\, f(\boldsymbol{s}) + g(L\boldsymbol{s})$

(Dual) $\underset{\boldsymbol{v}\in\mathcal{K}}{\text{minimize}}\, f^*(-L^*\boldsymbol{v}) + g^*(\boldsymbol{v})$

$$f^*(s) = \max_x \langle s, x\rangle - f(x)$$

The Proximal Gradient Method

Initialization: pick $\mathbf{x}^0 \in \text{int}(\text{dom}(f))$.
General step: for any $k = 0, 1, 2, \ldots$ execute the following steps:

(a) pick $L_k > 0$;

(b) set $\mathbf{x}^{k+1} = \text{prox}_{\frac{1}{L_k}g}\left(\mathbf{x}^k - \frac{1}{L_k}\nabla f(\mathbf{x}^k)\right)$.

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Specific regularizations

Robust to outliers: substitute the quadratic loss with the Huber loss

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Same node category, same mean ranking: encourage “no bias across categories” unless necessary

$$\Omega_{\text{group}}(\boldsymbol{s}) \coloneqq \sum_{z(i)\neq z(j)} w_{ij} |\langle s_i \rangle - \langle s_j \rangle|$$

Result (3/3): Ranking to learn group-dependent phenomena

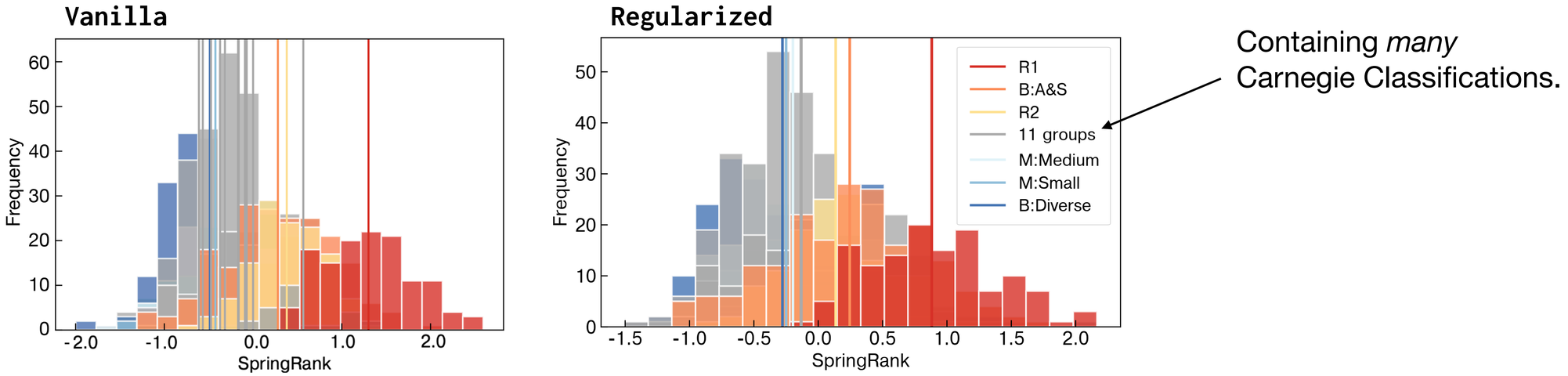
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We used α=0.01, λ=0 or λ=10 (regularized).

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Peer institution network (large)



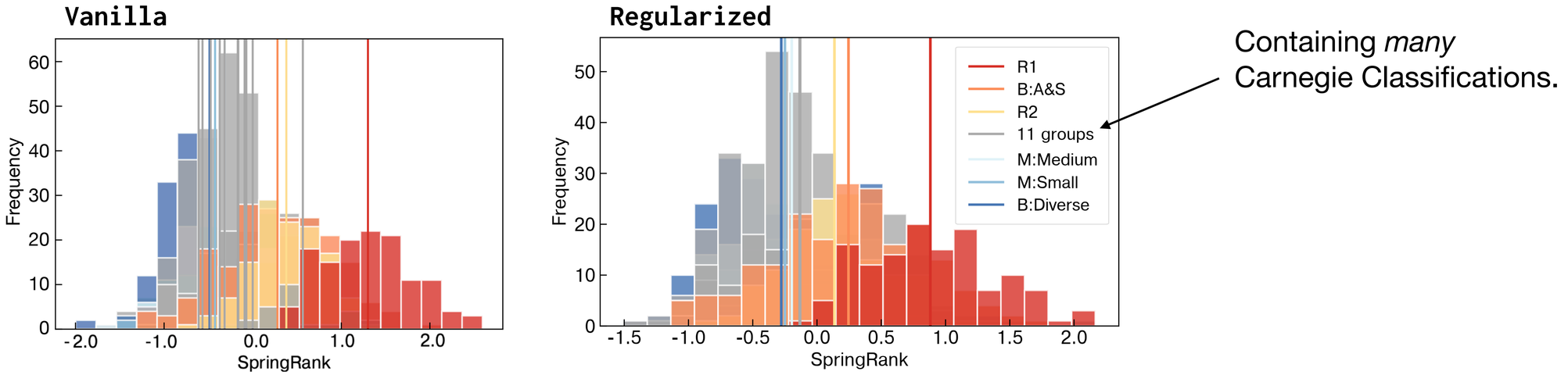
Benefits: By encouraging nodes of different groups to have the same, mean ranking, we *select* the groups that are special, or biased.

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Caveats: *Is this a better model?* Not always. We use a cross-validated model to predict out-of-sample edge directions (worse) and compare their likelihoods (better) with the vanilla SpringRank. But "better" is subjective. We expect the model to outperform for smaller categories though.

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Mix-and-match losses with regularizations allow new modeling capabilities.



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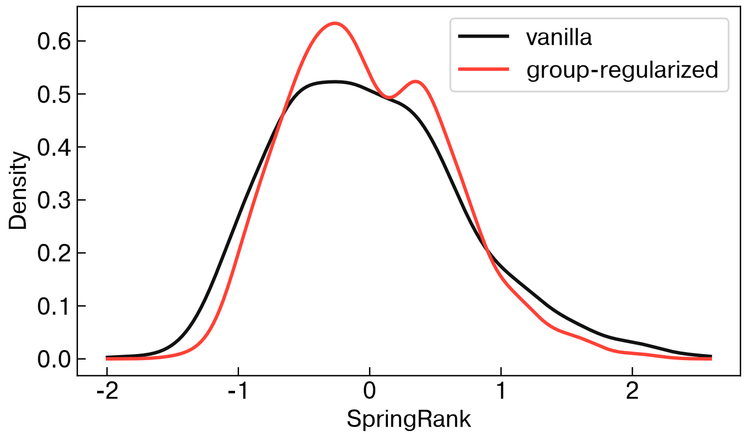
SpringRank can now select group-dependent (multi-modal) ranking distributions. Other fancier choice models do the same (e.g., contextual repeated selection model), but not conventional ones (e.g., Bradley-Terry-Luce model & vanilla SpringRank).

$$\mathbf{huber}(s) = \begin{cases} (1/2)s^2 & |s| \le 1 \\ |s| - (1/2) & |s| > 1 \end{cases}.$$

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$$\Omega_2(\boldsymbol{s}) \coloneqq \sum_t \|\boldsymbol{s}_t - \boldsymbol{s}_{t-1}\|_2^2$$

$$\Omega_{\text{group}}(\boldsymbol{s}) \coloneqq \sum_{z(i)\neq z(j)} w_{ij} |(\langle s_i \rangle - \langle s_j \rangle)|$$



Implications

$$\underset{\boldsymbol{s}\in\mathbb{R}^N}{\text{minimize}} \underbrace{\frac{1}{2}\sum_{ij} A_{ij}(s_i - s_j - 1)^2}_{\mathcal{L}_{\text{quad}}} + \alpha \sum_{i=1}^{N} s_i^2$$

Mix-and-match losses with regularizations allow new modeling capabilities.

SpringRank can now select group-dependent (multi-modal) ranking distributions. Other fancier choice models do the same (e.g., contextual repeated selection model), but not conventional ones (e.g., Bradley-Terry-Luce model & vanilla SpringRank).

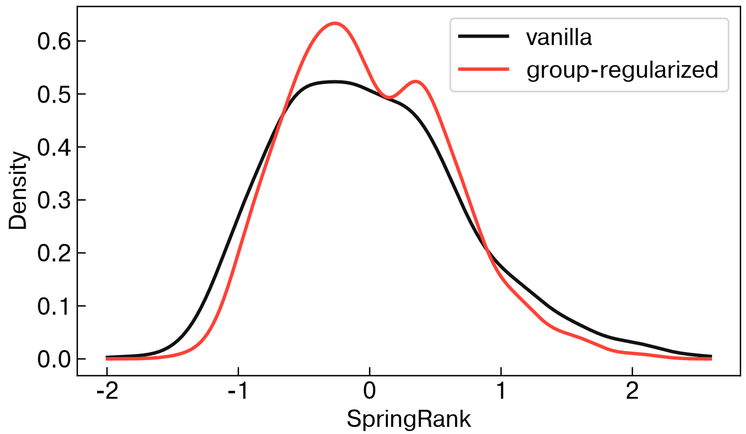
Limitations. No natural way to apply to numeric groups (think: how does admission rate relate to the hierarchy?); Cross-validating >2 hyperparameters is slow.

$$\mathbf{huber}(s) = \begin{cases} (1/2)s^2 & |s| \le 1 \\ |s| - (1/2) & |s| > 1 \end{cases}.$$

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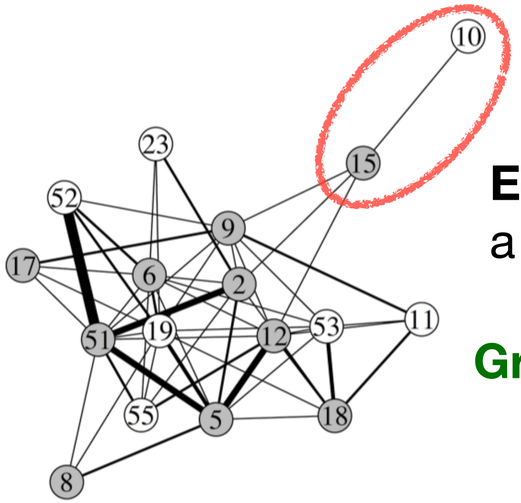
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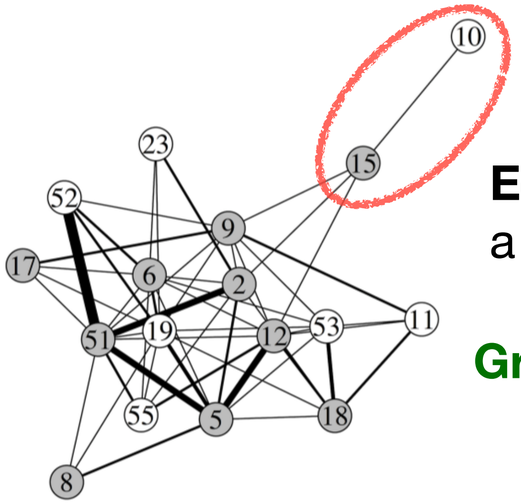
Outline

1. Context & motivation (chapter 1)
2. Aspiration of prestige in institutional peer selection (chapter 5)
3. Community detection in bipartite networks (chapter 2)
4. Regularized methods for efficient ranking (chapter 3)
5.  A detour in higher-order structures (chapter 4)
6. Conclusions & future research (chapter 6)



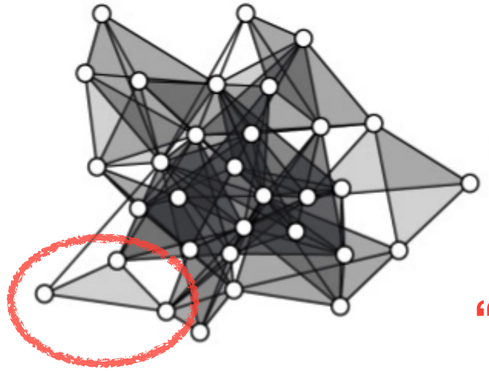
Edges. These 2 authors have written a paper together.

Graph



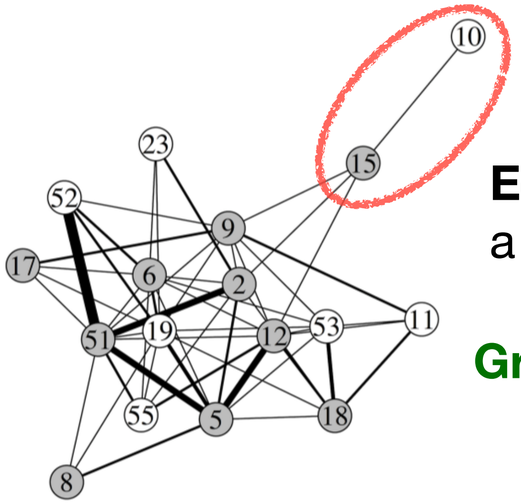
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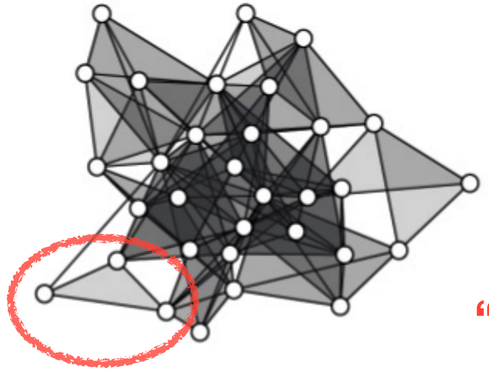
“Higher-order” graph

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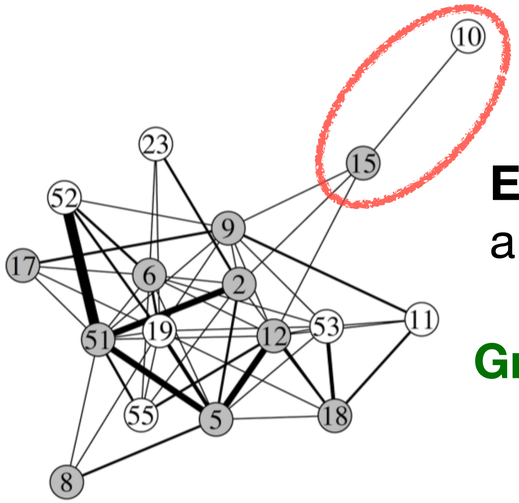
Letter

Construction of simplicial complexes with prescribed degree-size sequences

Tzu-Chi Yen*

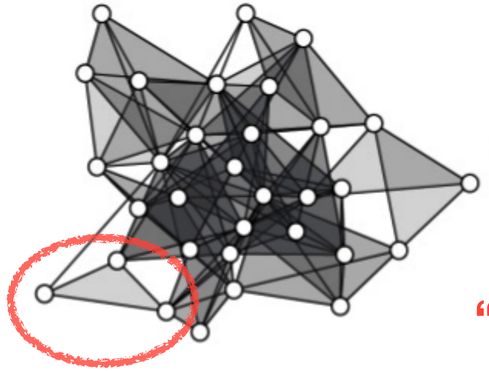
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(Received 31 May 2021; accepted 30 September 2021; published 28 October 2021)



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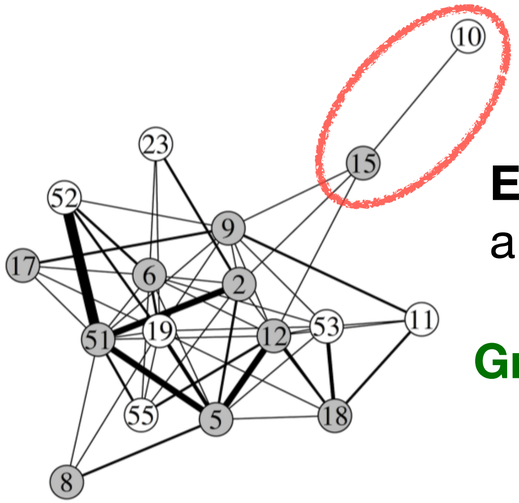
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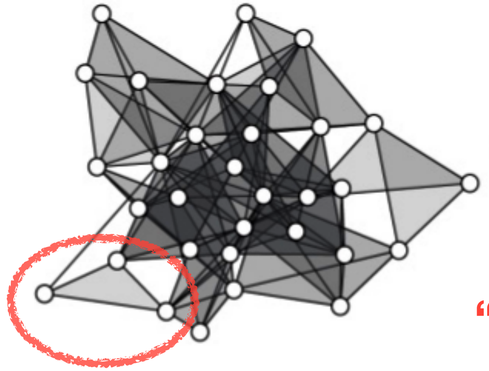
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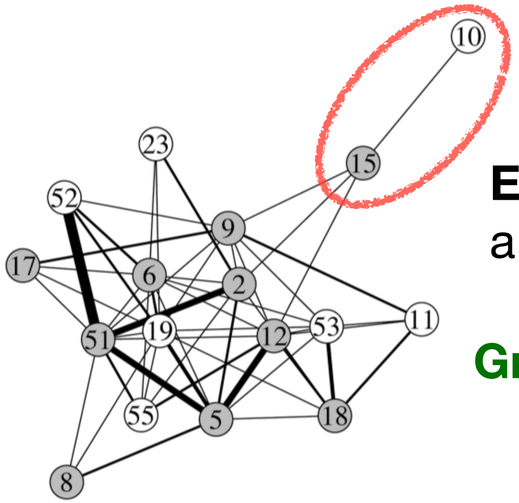
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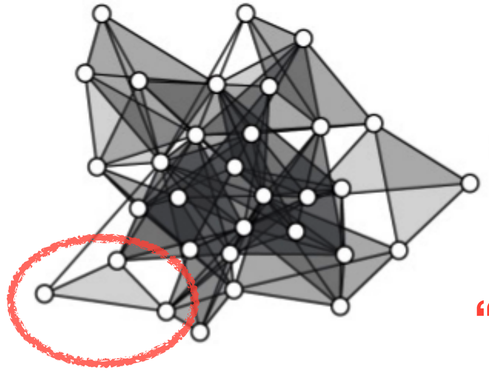
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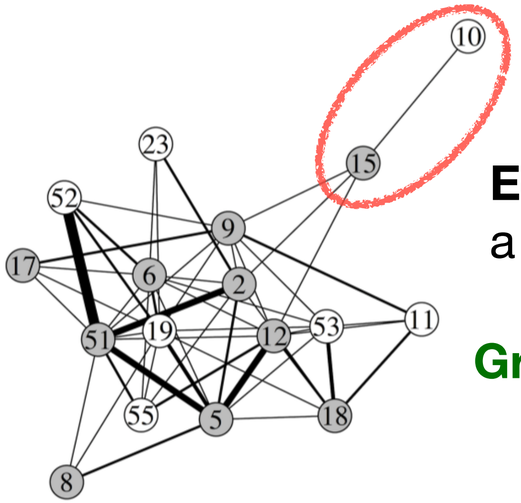
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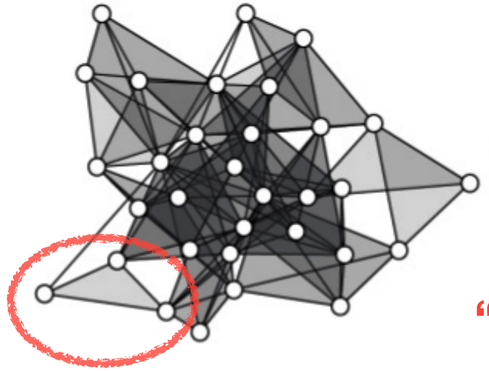
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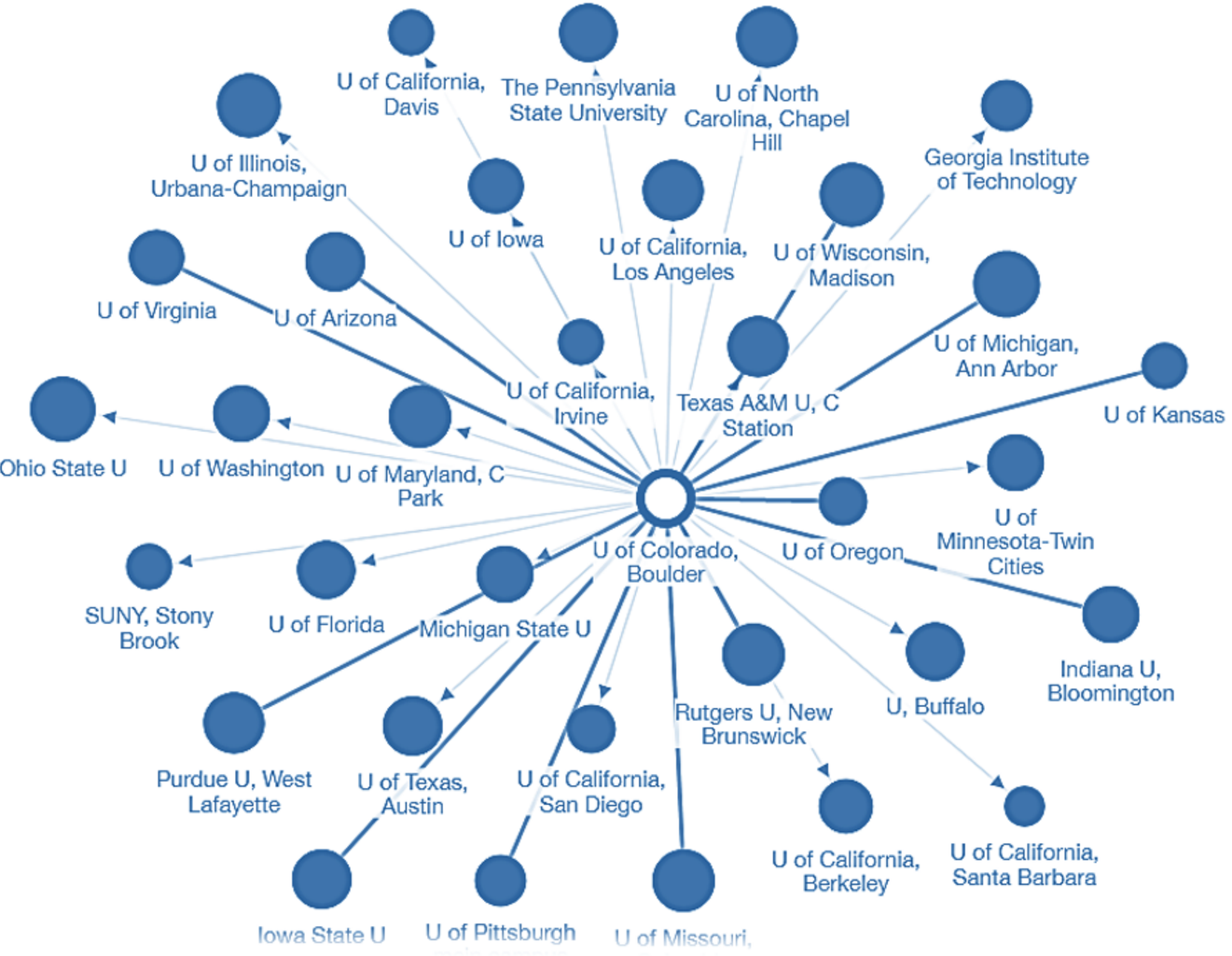
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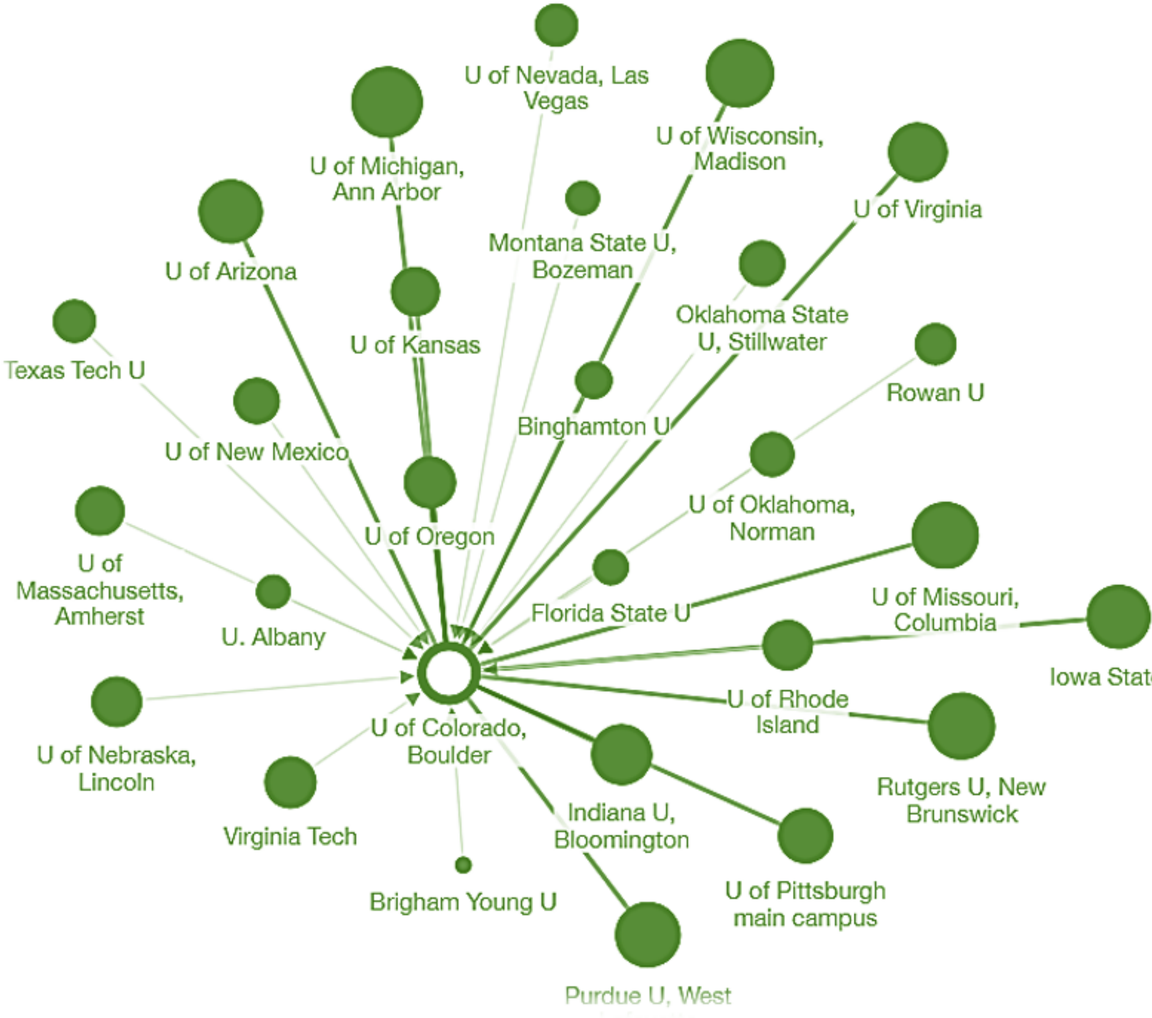
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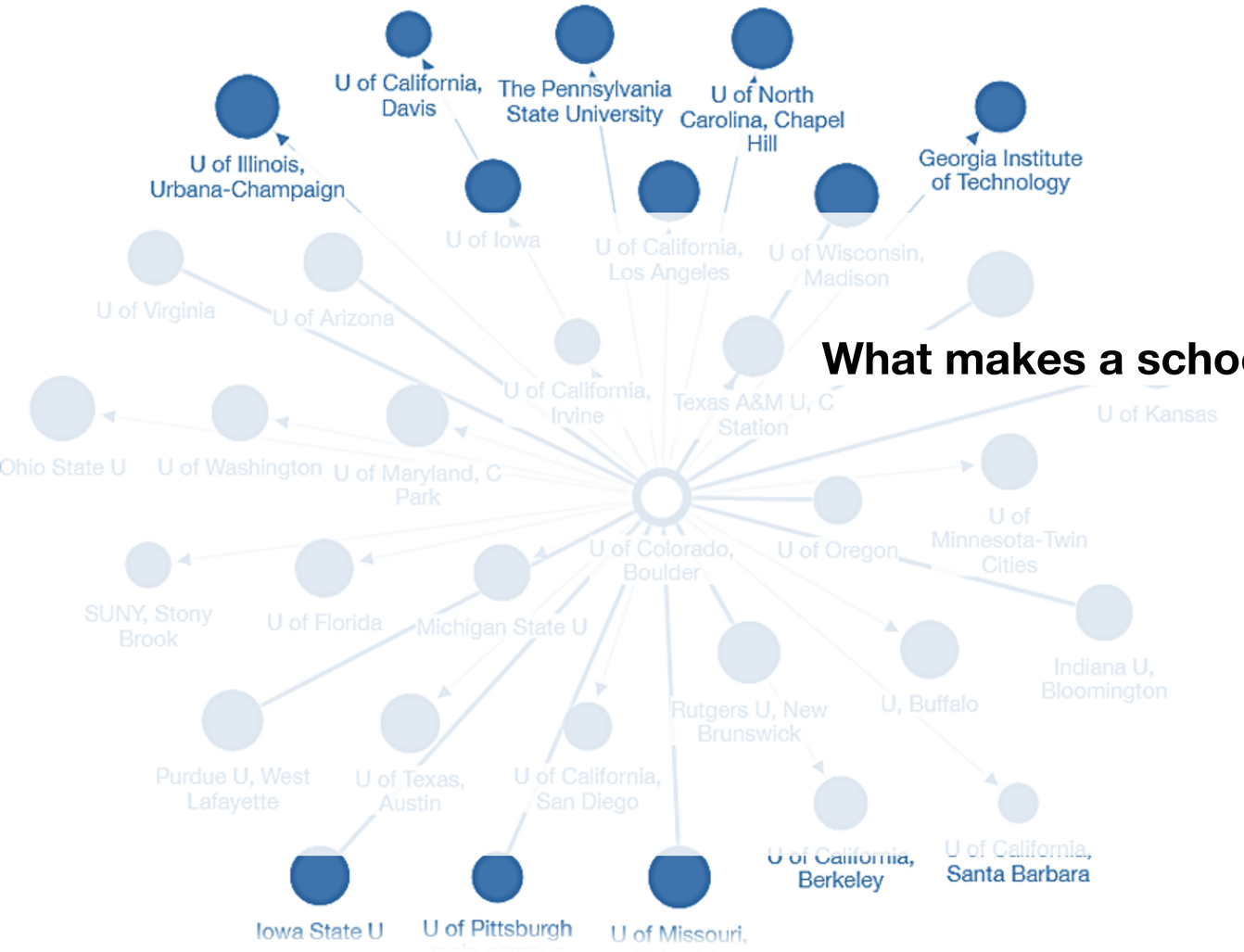
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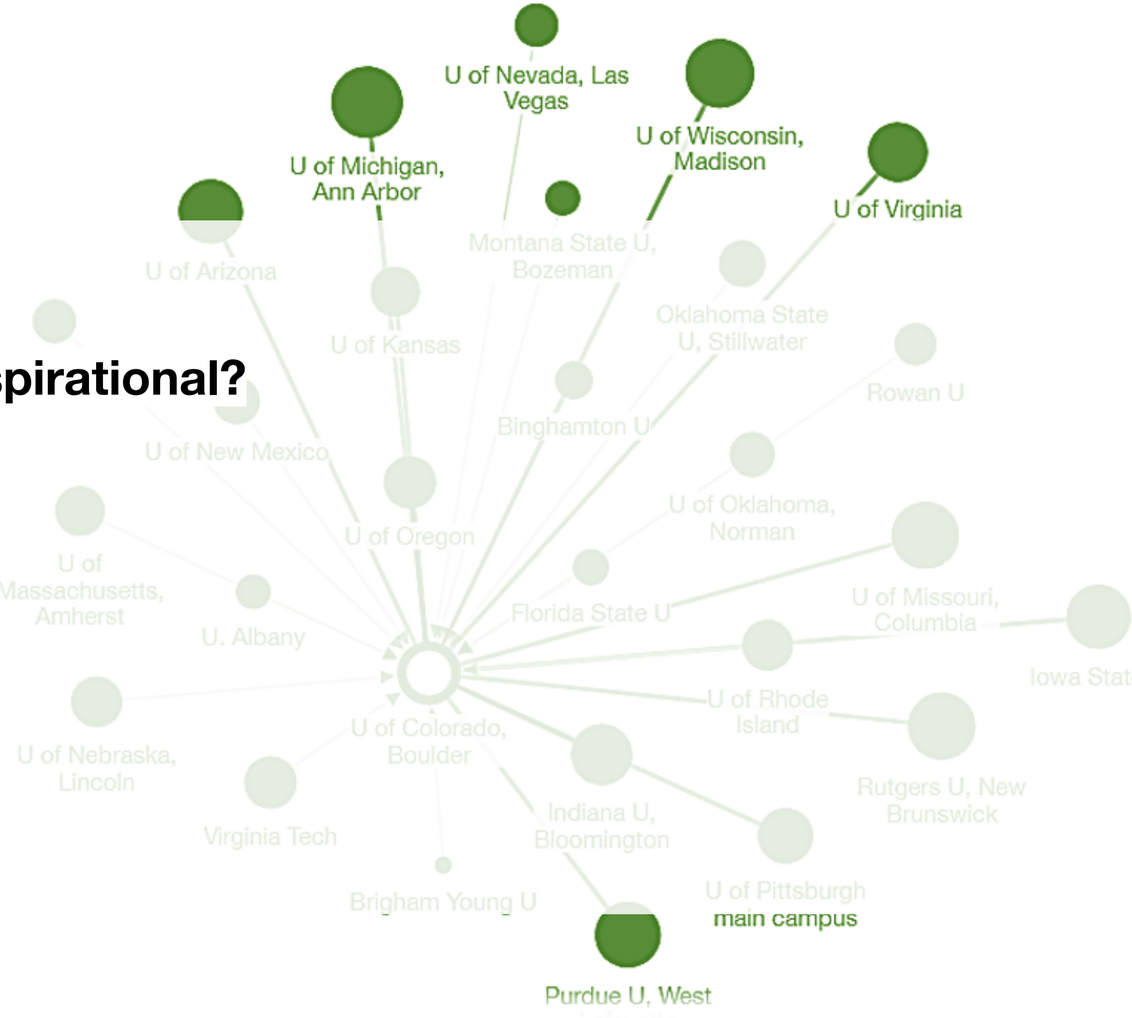


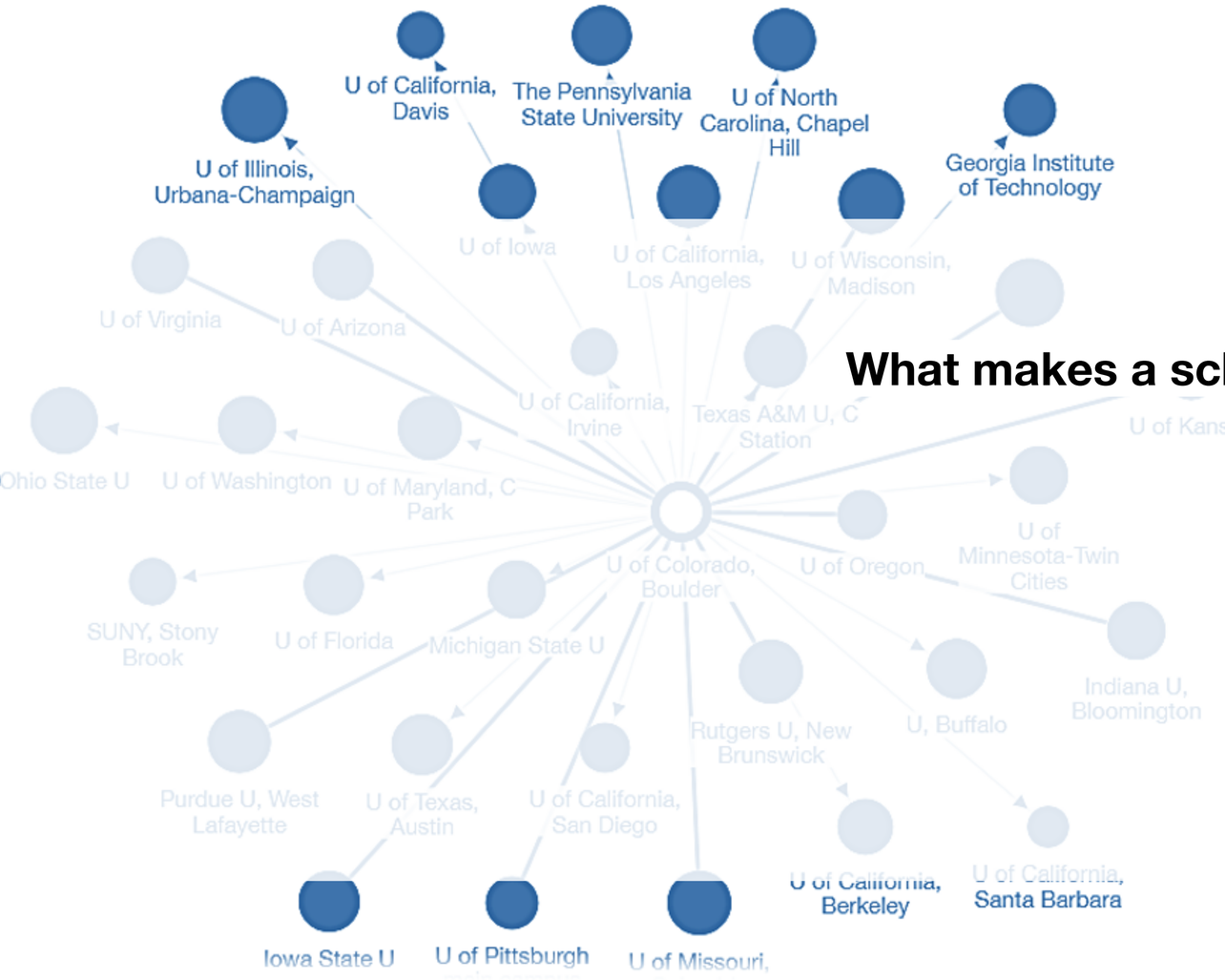

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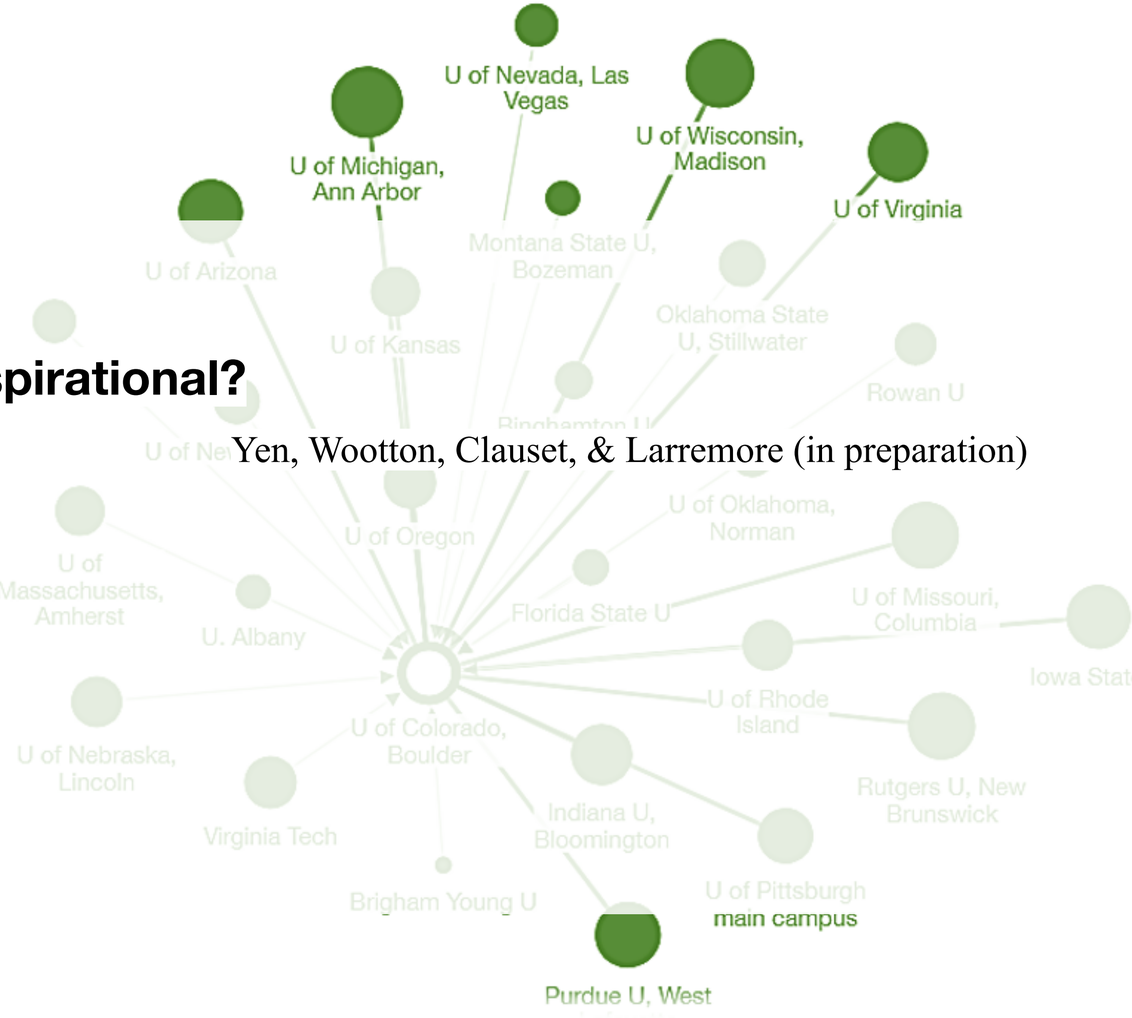
What makes a school aspirational?

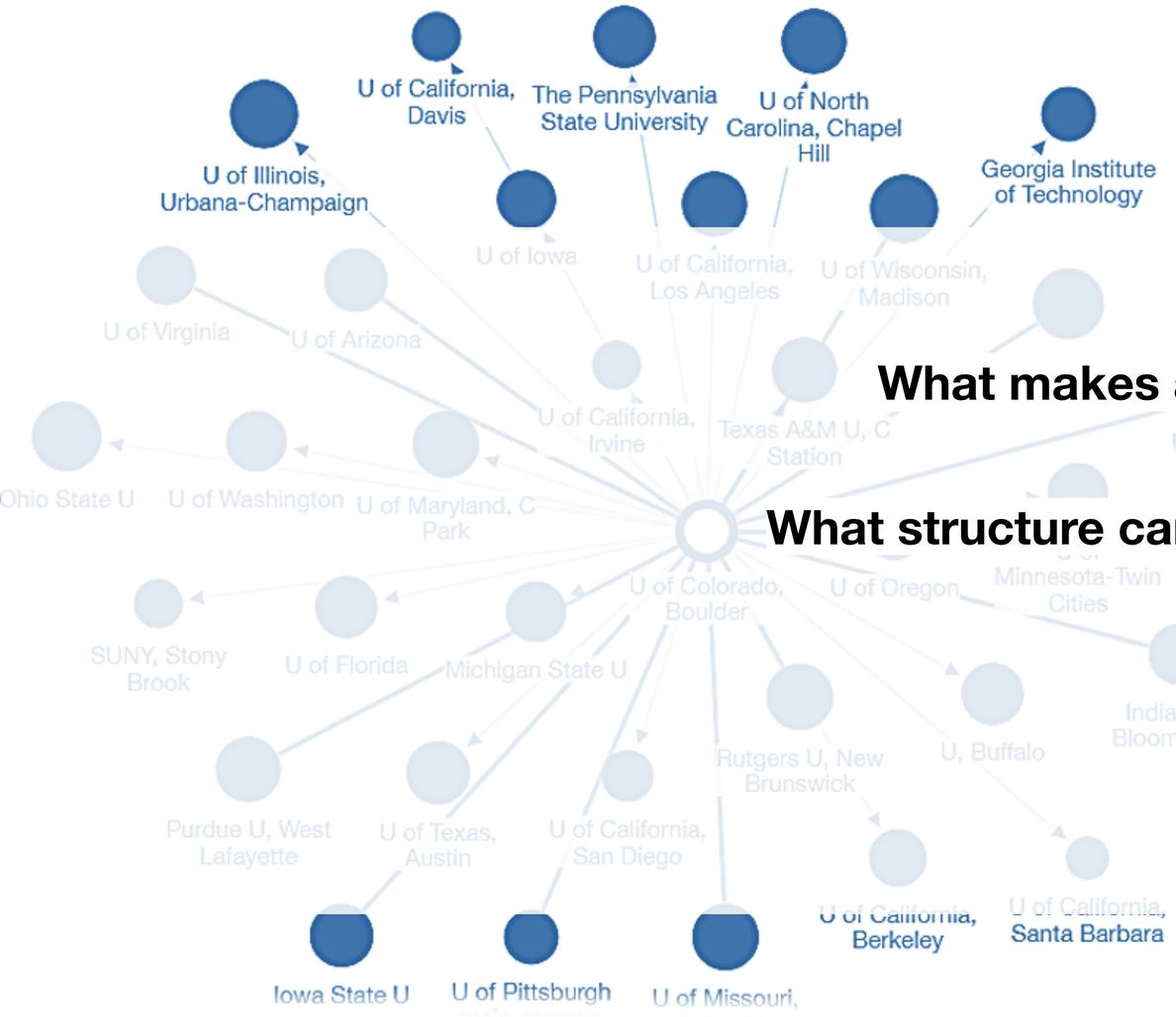


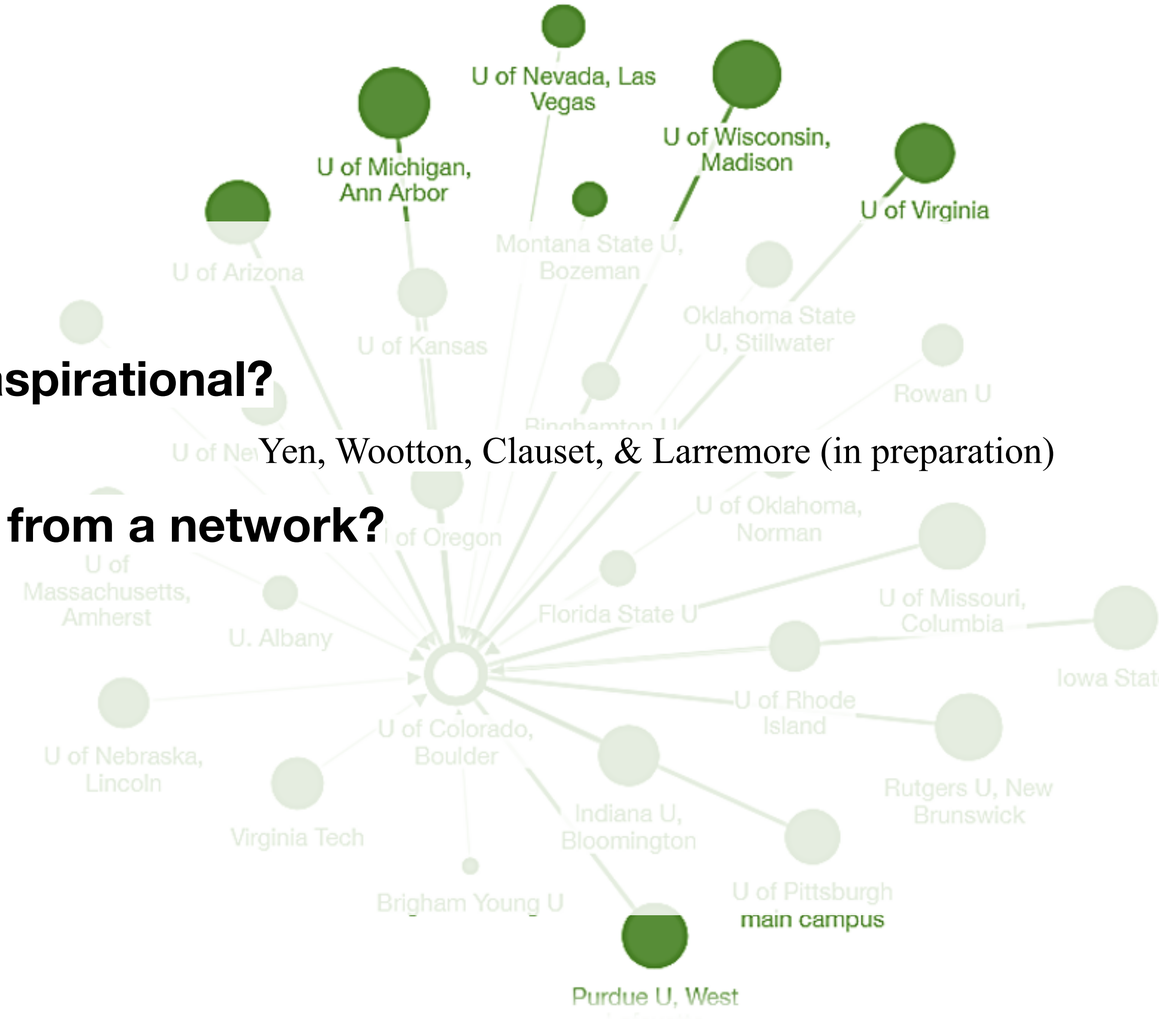


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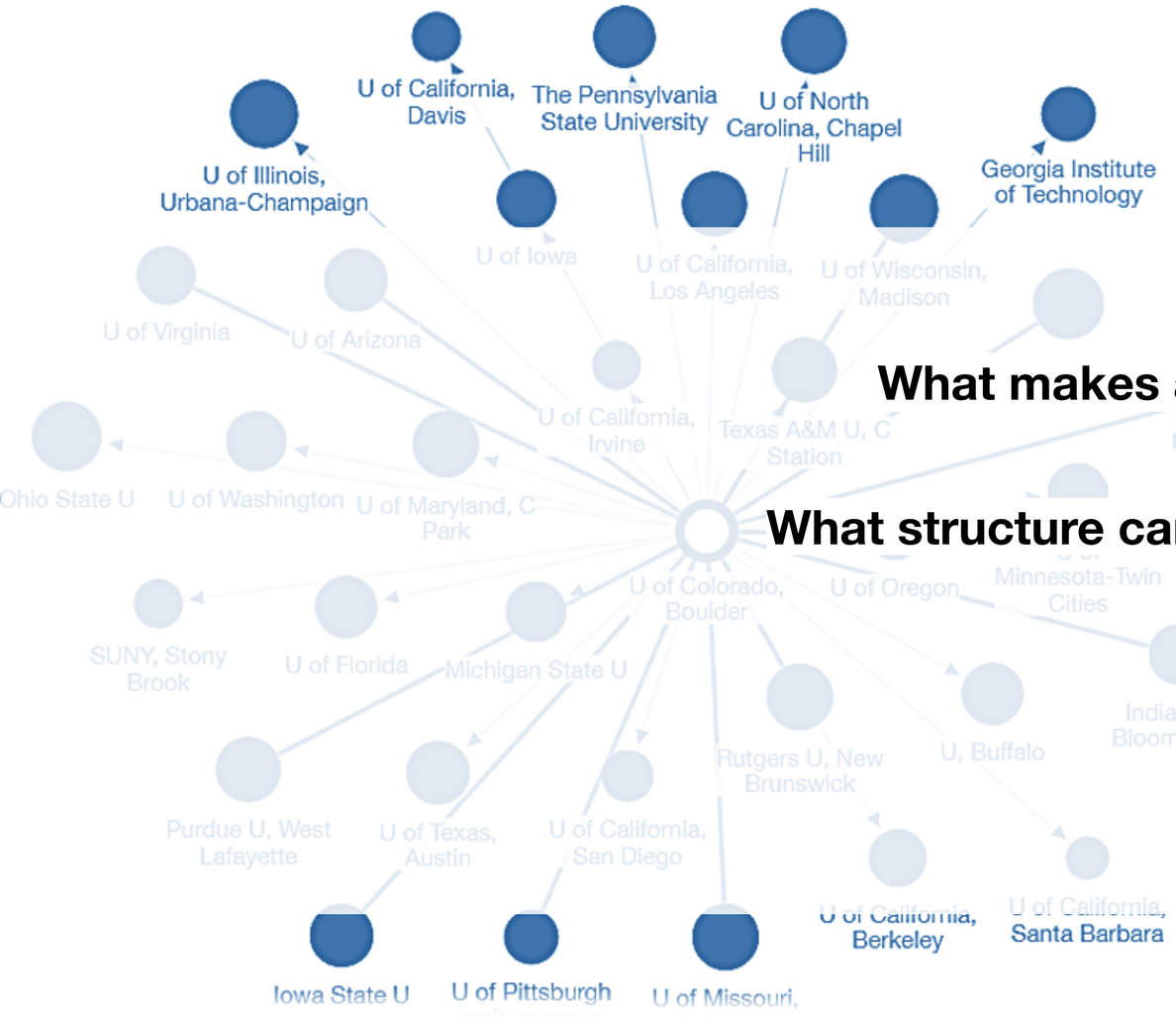


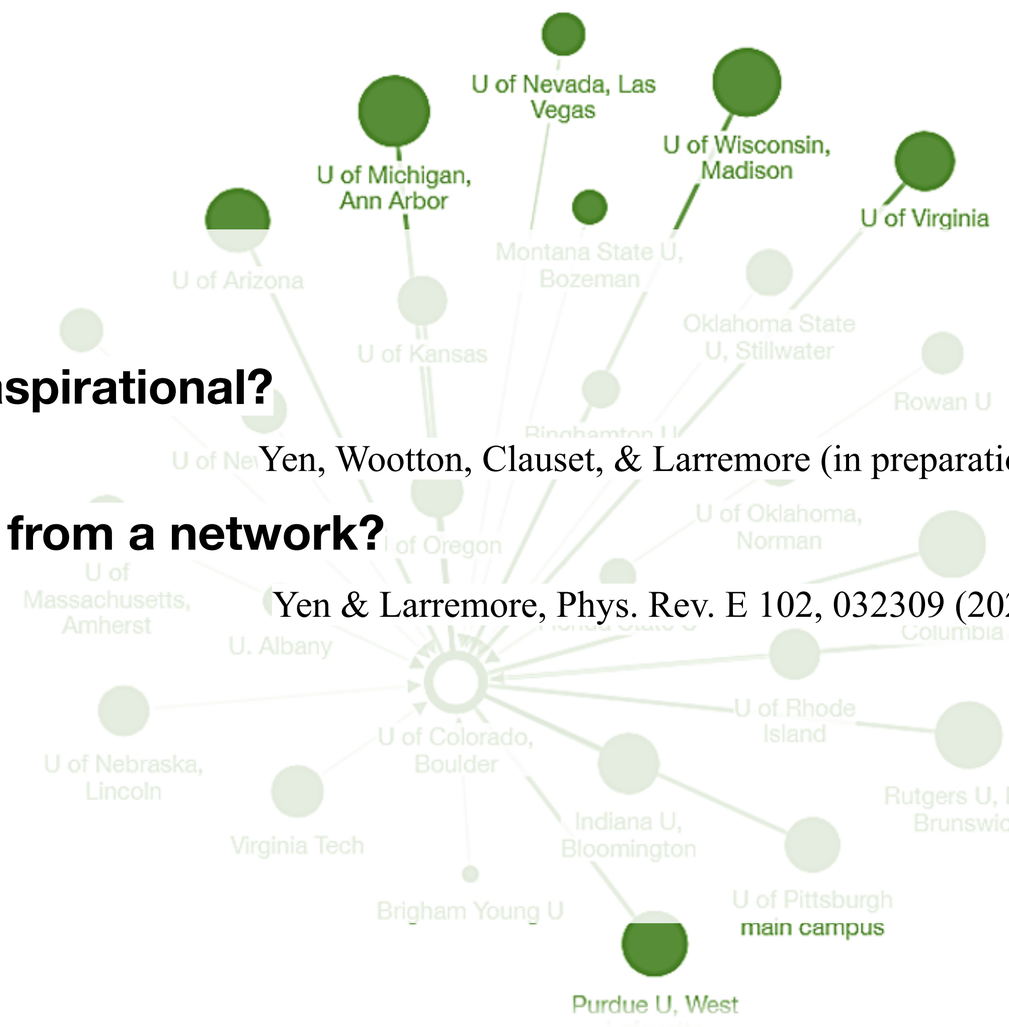


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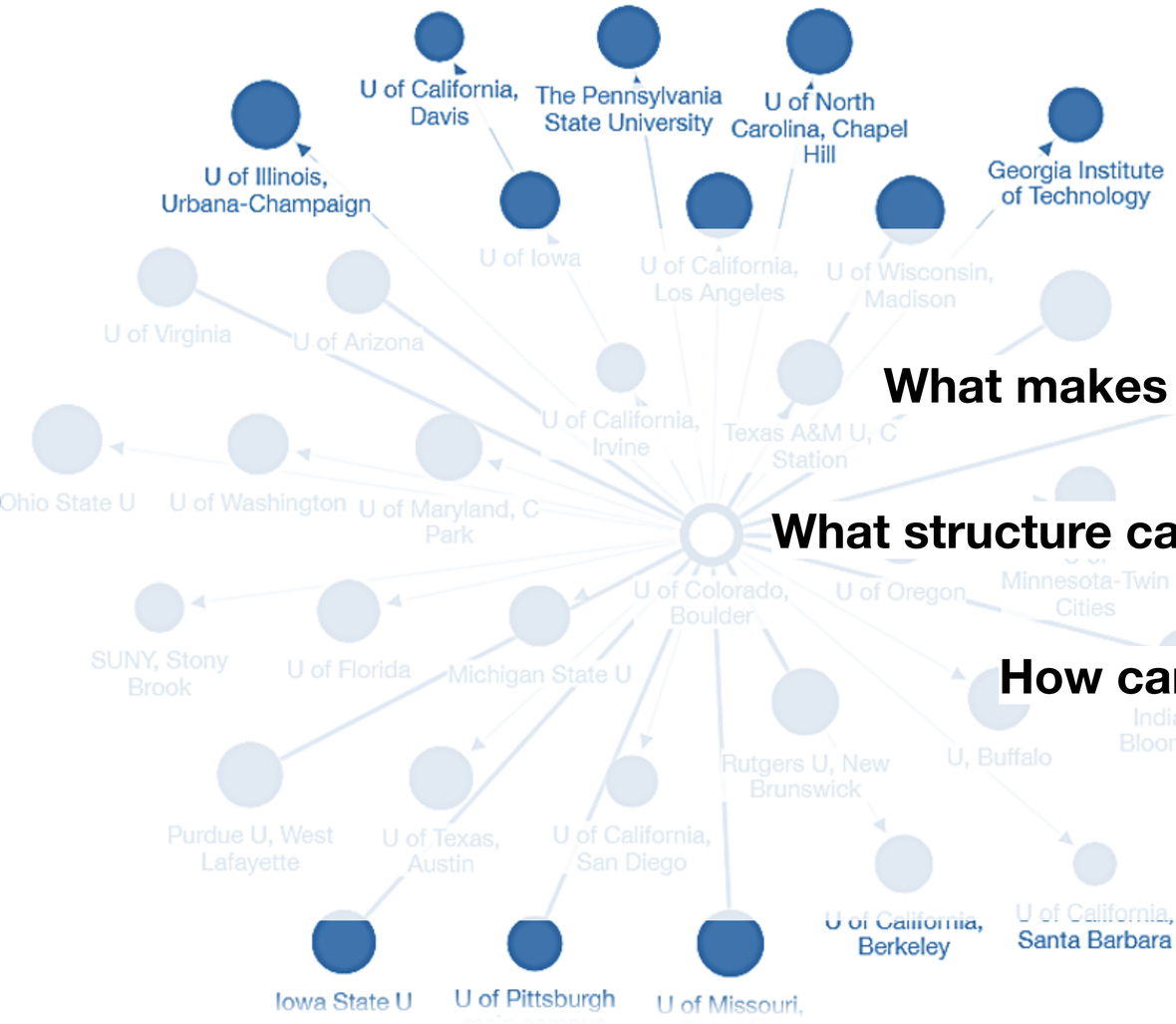


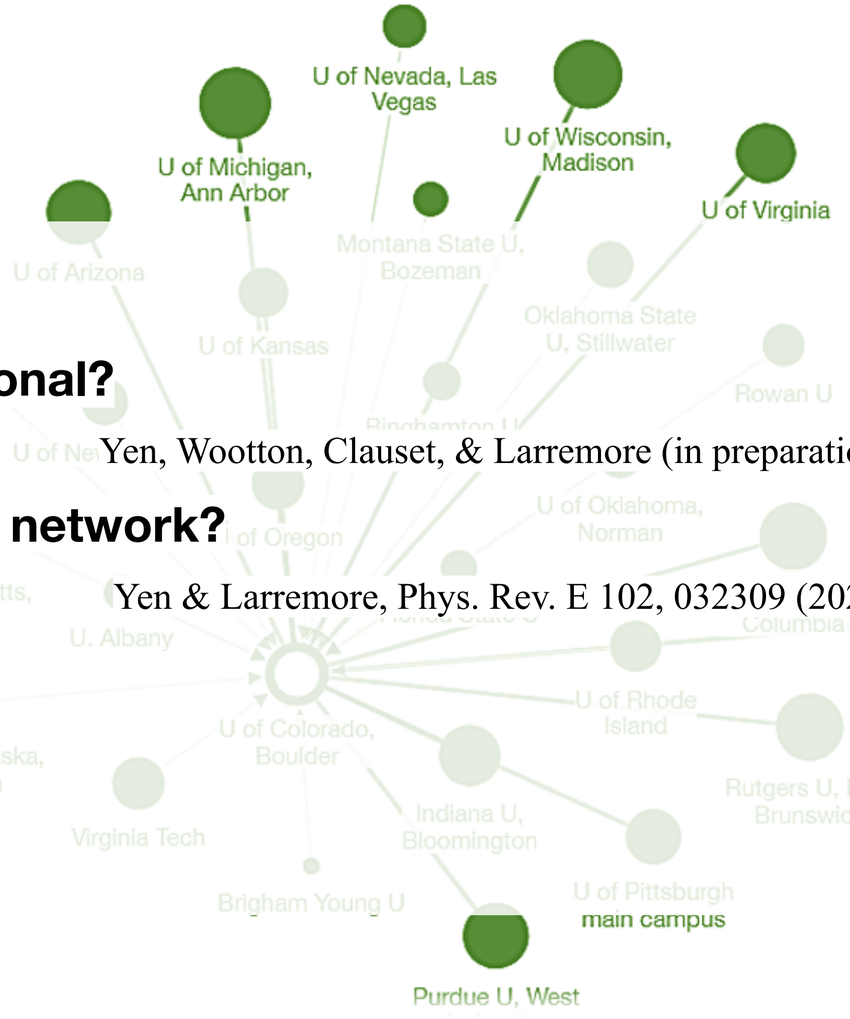
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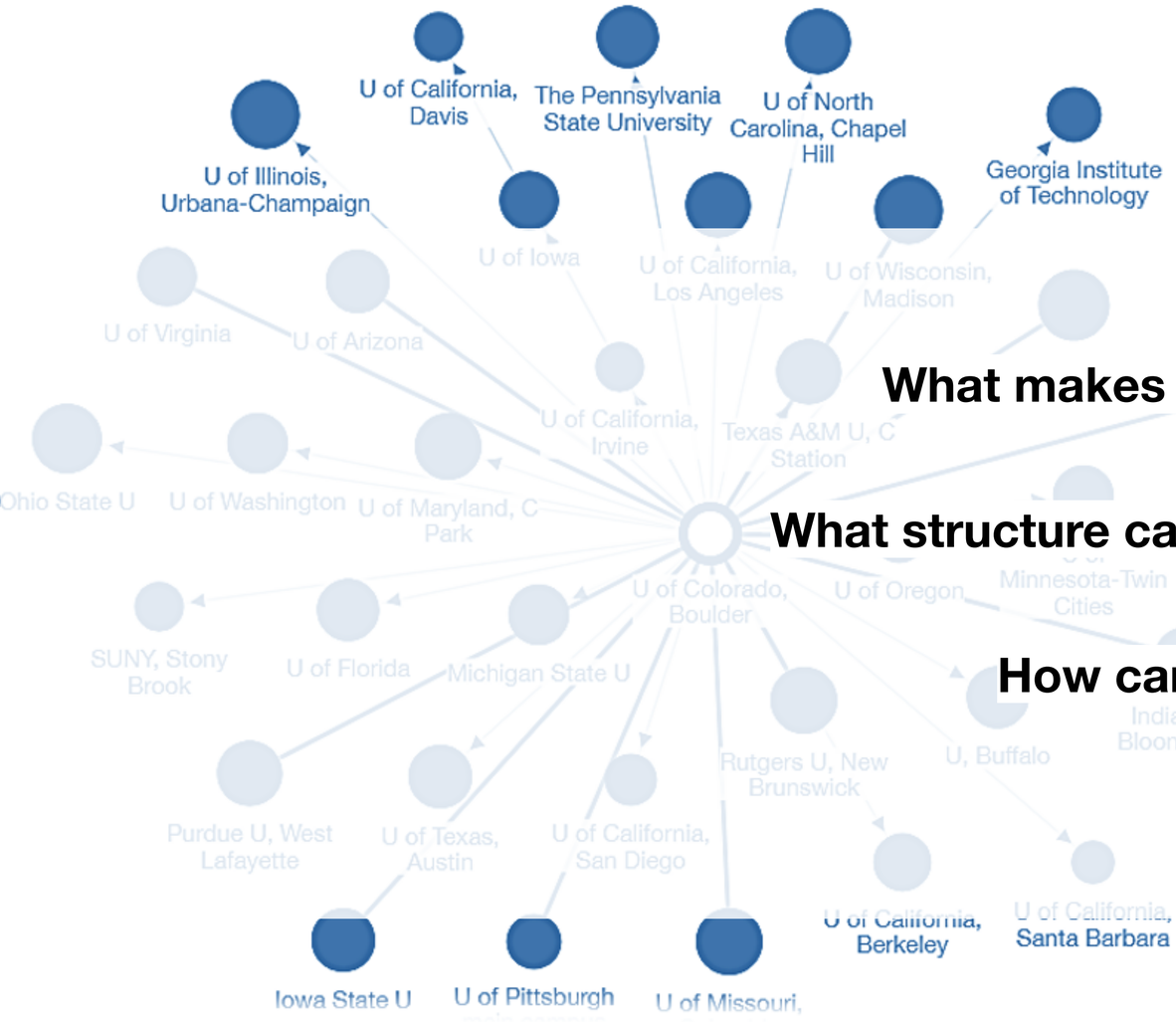
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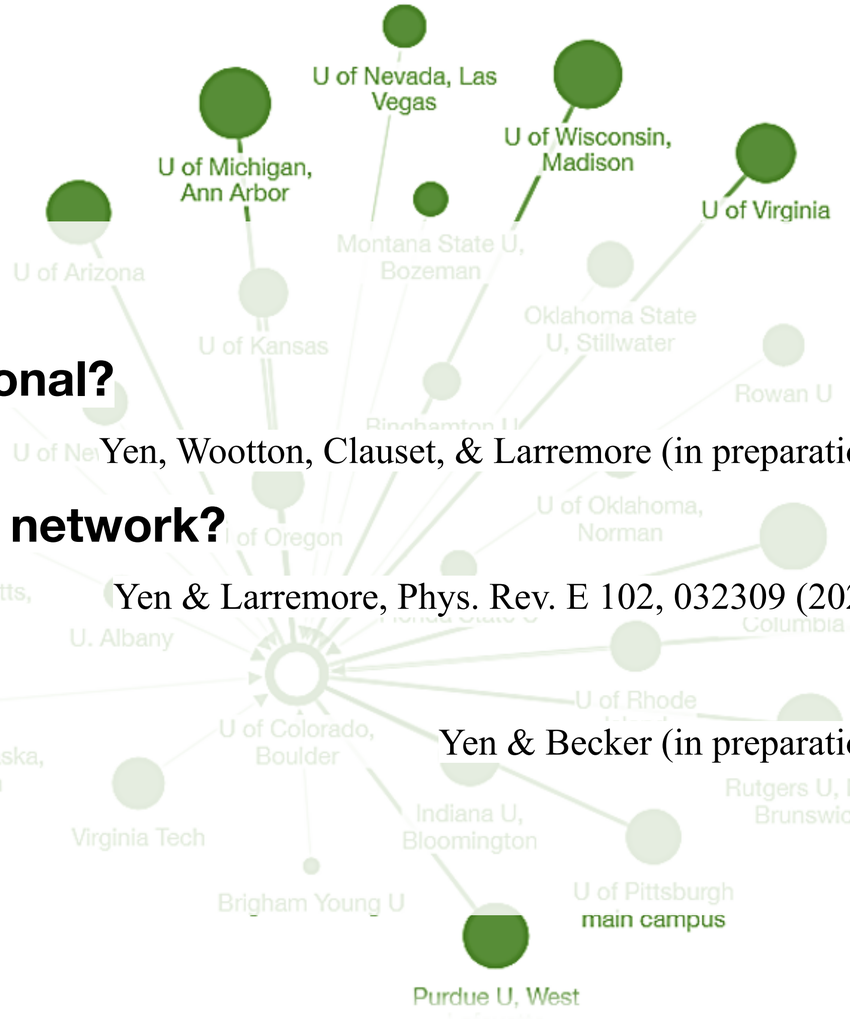
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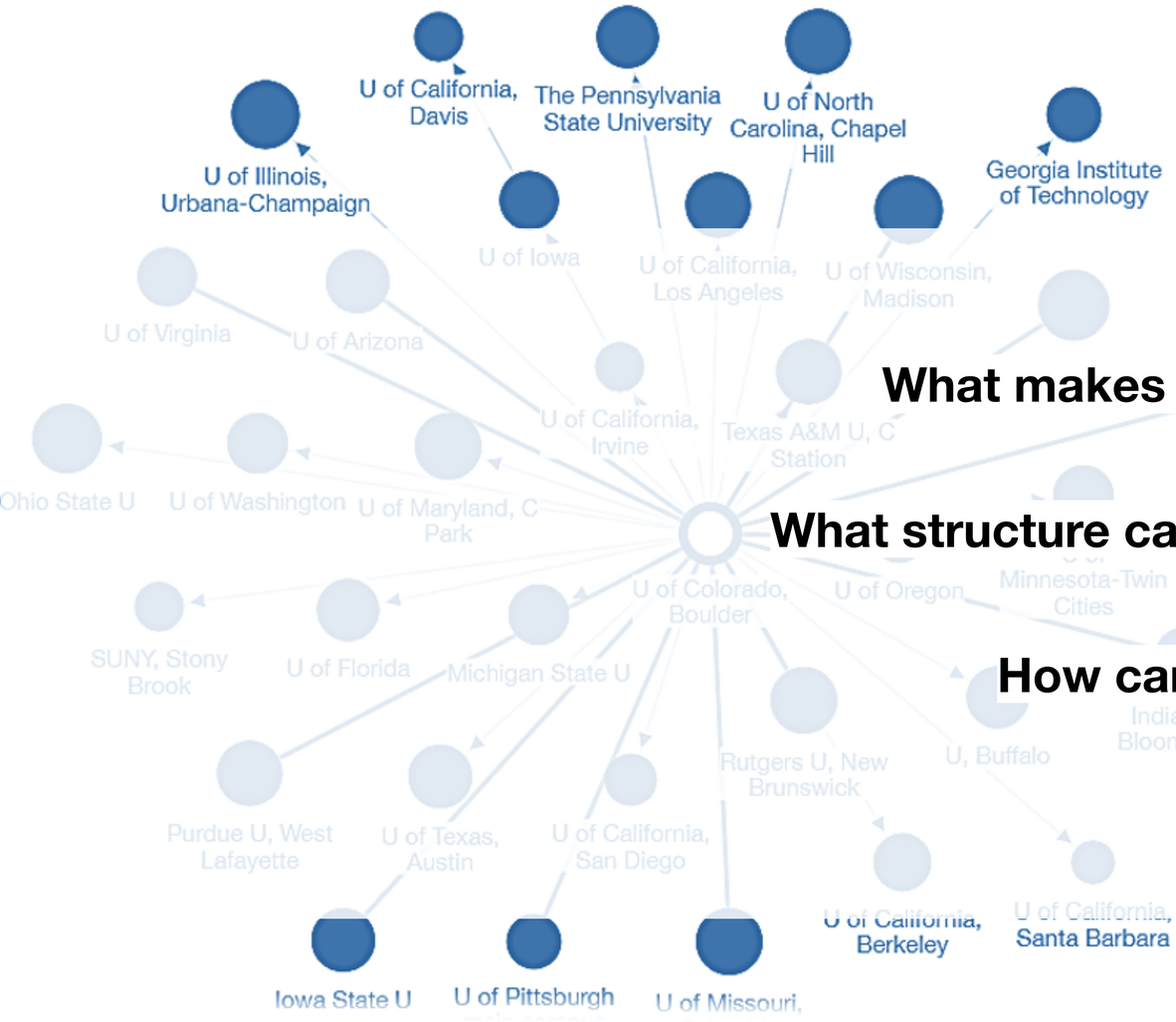
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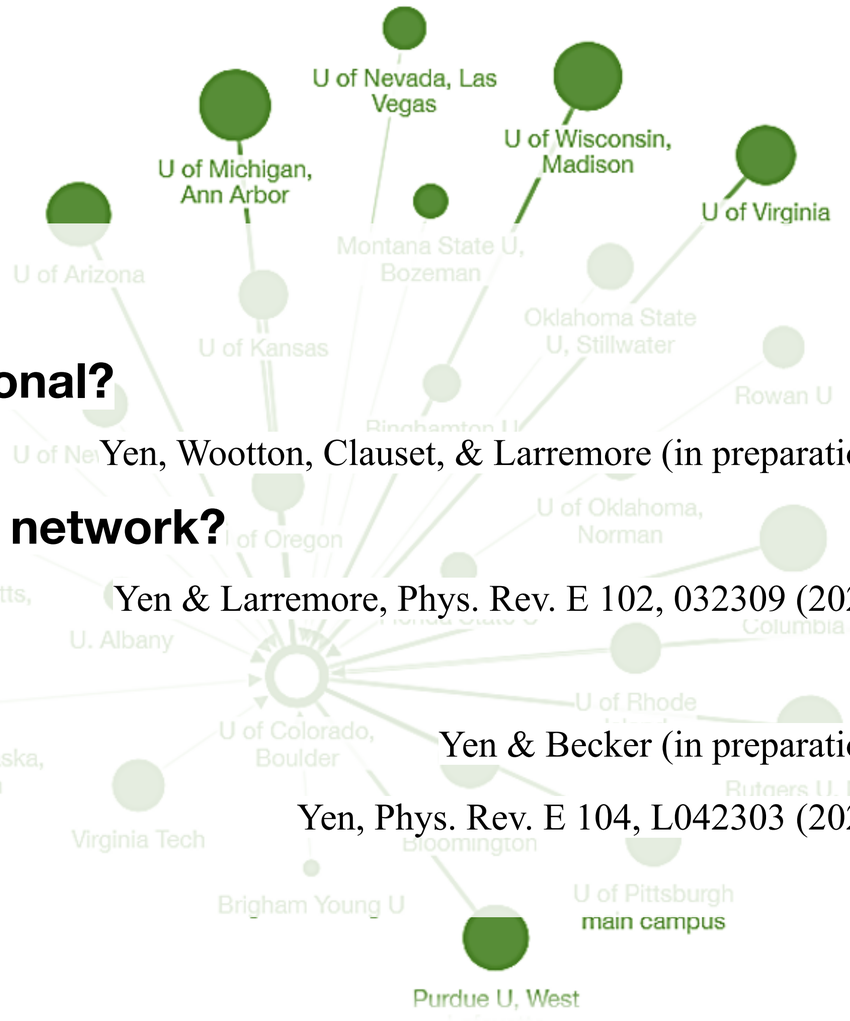
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Future research

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Mix-and-match. Network science + □□□□□□.

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Structure is mundane, psychology is alive.

- Directed edge. Action verbs.
- Metadata. Show intent.

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Reproducible results. Statistically grounded methodologies.

Statistical inference links data and theory in network science

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Exploiting sparsity. Combinatorial problems often admits a natural (convex) relaxation.

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A unified perspective on convex structured sparsity:
Hierarchical, symmetric, submodular norms and beyond

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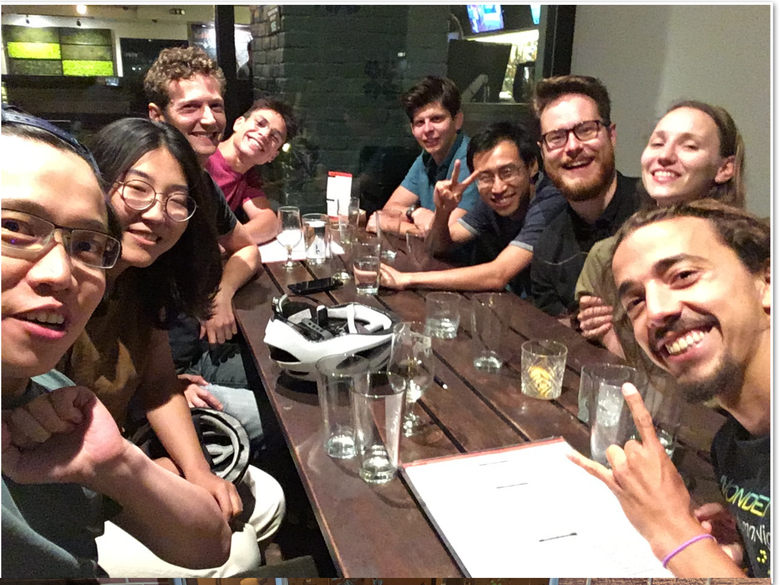
December 8, 2016







Thanks!





Jose Cuervo
BEST MARGARITAS
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