Nearly-optimal prediction of missing links in networks

joint work with Amir Ghasemian (Yale), Homa Hosseinmardi (Penn),
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what is link prediction? ⚠️

most real-world networks are *incomplete*

▶ social networks	all are sampled some edges hidden intentionally some simply unobserved/able
▶ biological networks	observed by expensive experiments edges must often be inferred
▶ communication networks	different types of interactions missing all off-platform interactions

what is link prediction?

most real-world networks are *incomplete*

link prediction helps fill in the missing connections

- useful for comparing models
  which model is better at out-of-sample predictions?
- useful for marshaling resources
  which connections should we sample next?
- useful for predicting the future (dynamic networks)
  which connections will form next?

predicting missing links

- the general setting :
  - a *latent* network $G = (V, E)$, and
  - an *observed* network $G' = (V, E')$ where $E' \subset E$
  - given G' :
    - learn how observed links E' correlate with $X = E - E'$
    - within $\underbrace{(V \times V) - E'}_{\text{haystack : } O(n^2)}$, predict $\underbrace{X}_{\text{all needles : } O(n)}$

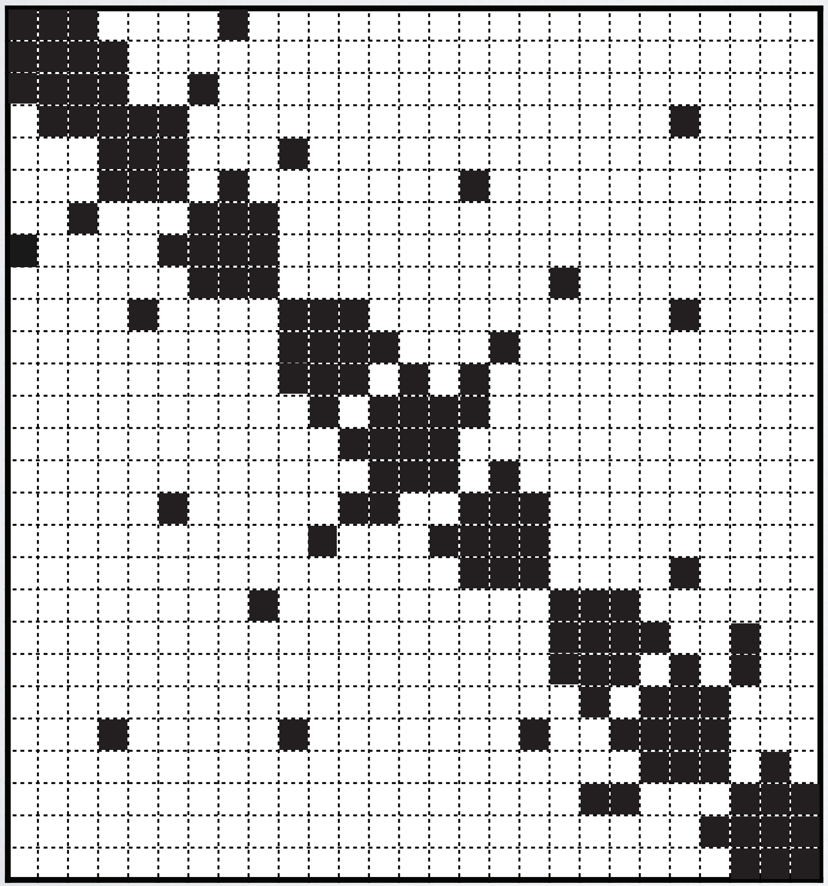
baseline accuracy : $O(1/n)$

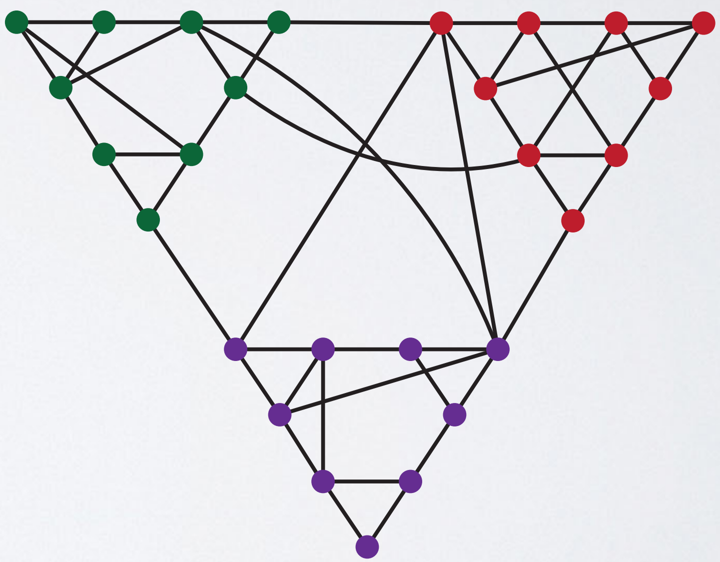
* we assume all nodes are known, and just edges are missing. predicting missing nodes is a harder problem because nodes are correlated bundles of edges
* baseline: assume the network is sparse, with mean degree $\langle k \rangle = O(1)$ and guessing uniformly at random

predicting missing links

for example:

latent $\quad G = (V, E)$

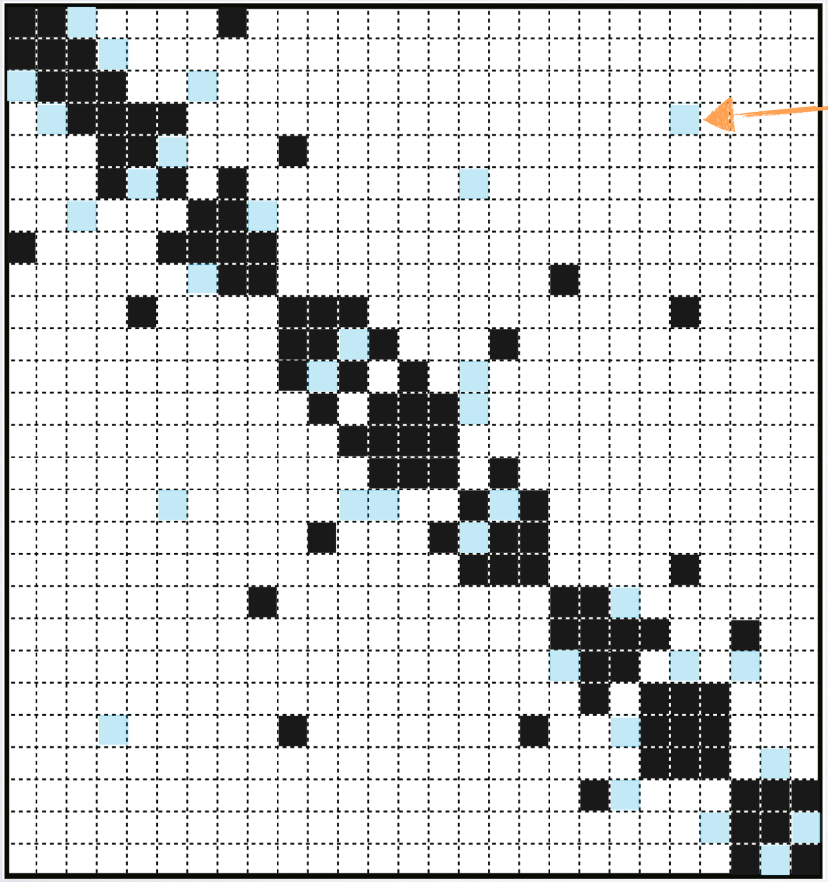




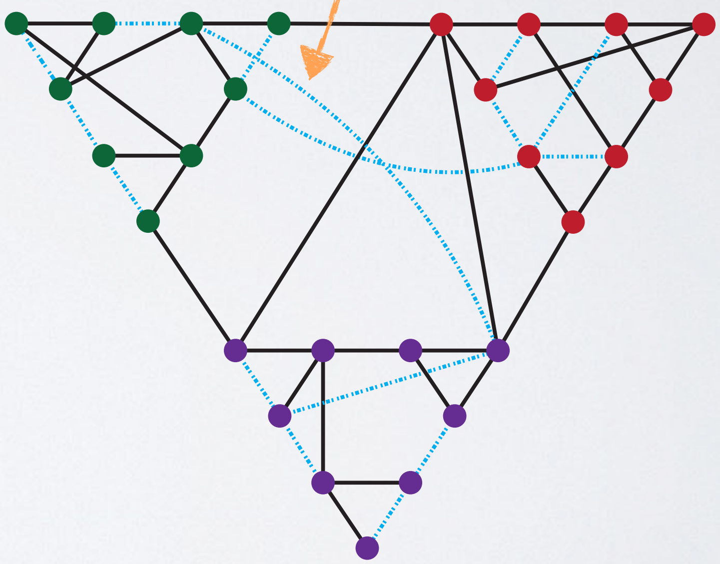
predicting missing links

for example:

observed $G' = (V, E')$



missing links $X = E - E'$



predicting missing links

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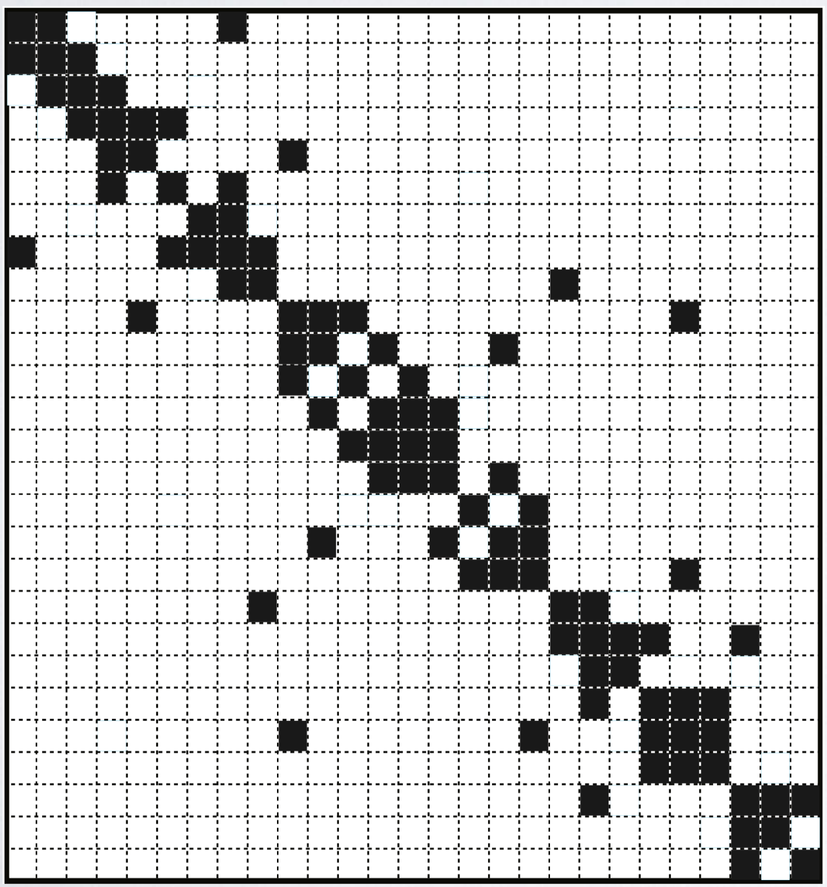


prediction task:

for every in G'

guess or

non-edge

missing link $\in X$

predicting missing links

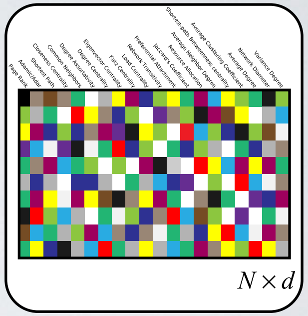
- by other names :
  - recommendation algorithms [bipartite networks]
  - matrix completion
- all good approaches, slightly different problem formulations

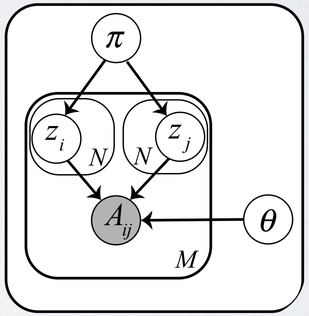
in networks, we can only learn from the observed connections

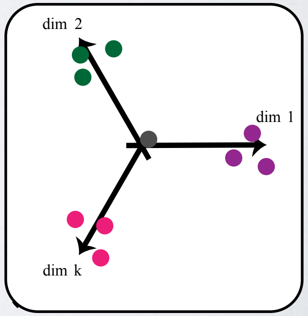
* recommendation algorithms and matrix completion have literatures far too large to summarize here
* no metadata (node attributes) allowed for learning here

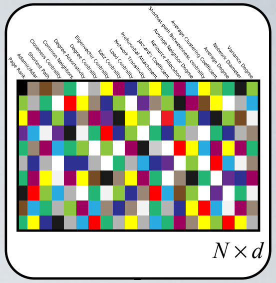
predicting missing links

- in practice : huge number of link prediction methods
  - **topological features**
    degree, common neighbors, Jaccard, short paths, etc.
  - **model-based methods**
    probabilistic models, stochastic block models, modularity, Infomap, etc.
  - **embedding methods**
    spectral embedding, latent spaces, neural embeddings, node2vec, etc.
  - **and more**









predicting missing links

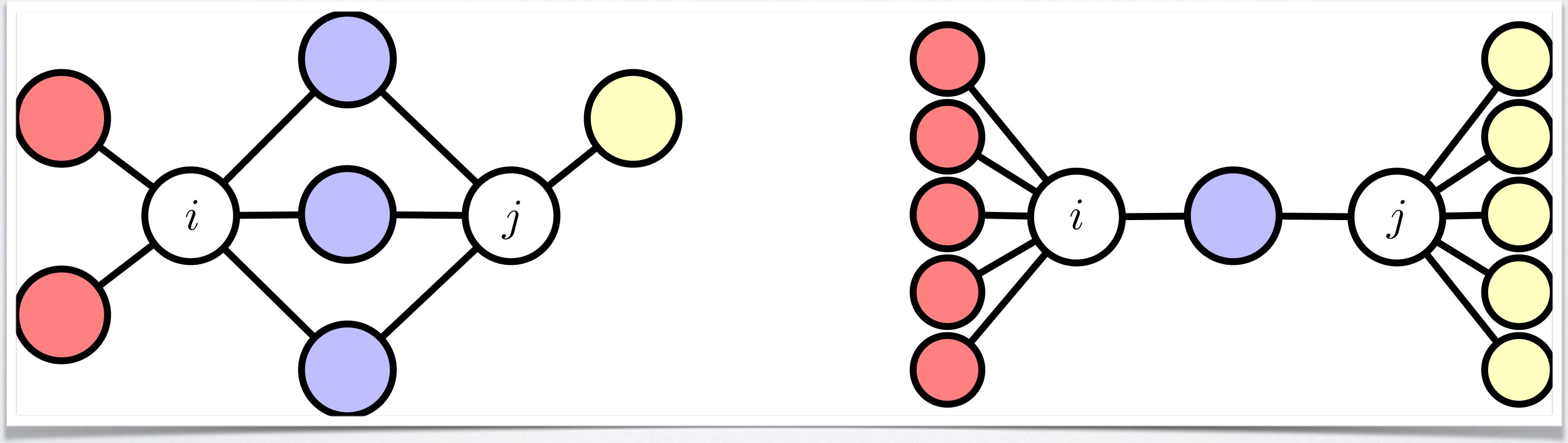
- examples of "topological" score functions:

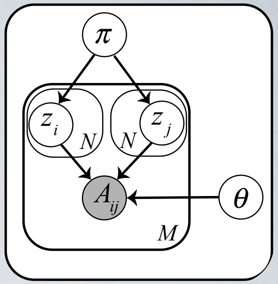
$$\text{Jaccard}(i,j) = \frac{|\nu(i) \cap \nu(j)|}{|\nu(i) \cup \nu(j)|}$$

$\nu(i)$: set of neighbors of i

$$\text{Degree-product}(i,j) = k_i \times k_j$$

k_i : num. of neighbors of i



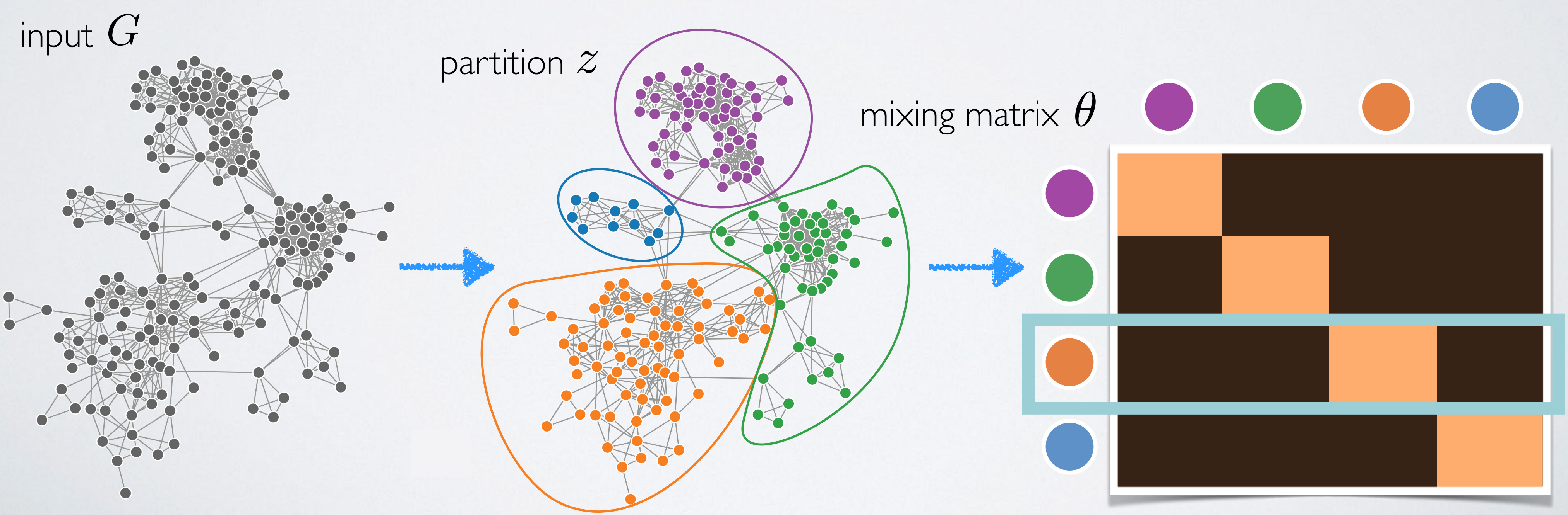


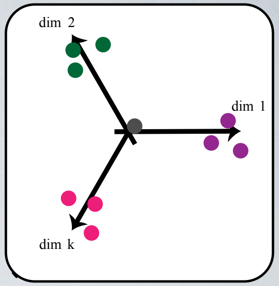
predicting missing links

- example of "mode-based" score functions:

stochastic block model: probabilistic generative network model

$\mathrm{SBM}(i,j) = \Pr(A_{ij} = 1 \mid z, \theta)$ [score is probability under learned model]



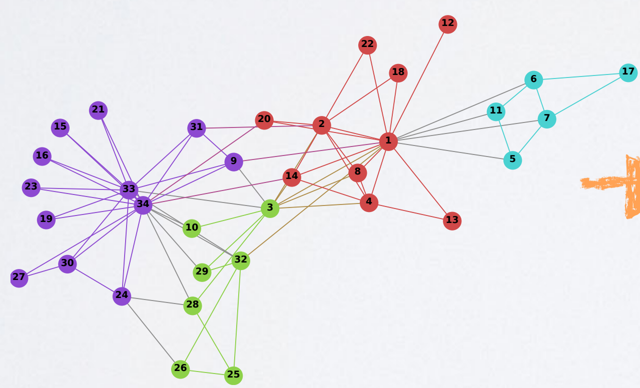


predicting missing links

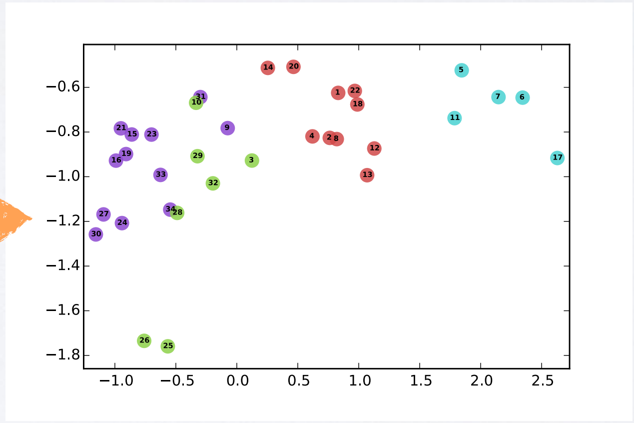
- example of "embedding-based" score functions:

  learn a latent space embedding of nodes ϕ

  $\mathrm{DeepWalk}(i,j) = d(i,j\,|\,\phi)^{-1}$ [score is *closeness* in learned embedding]



input graph G



learned embedding ϕ

* Perozzi et al., "DeepWalk: Online Learning of Social Representations." *KDD* 2014

predicting missing links

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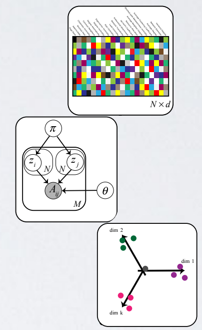
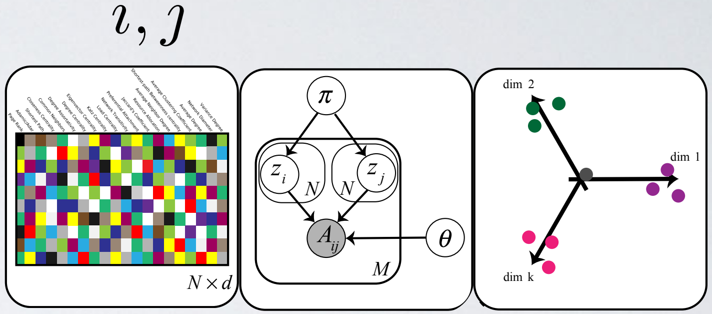
  - **topological features**
  - **model-based methods**
  - **embedding methods**



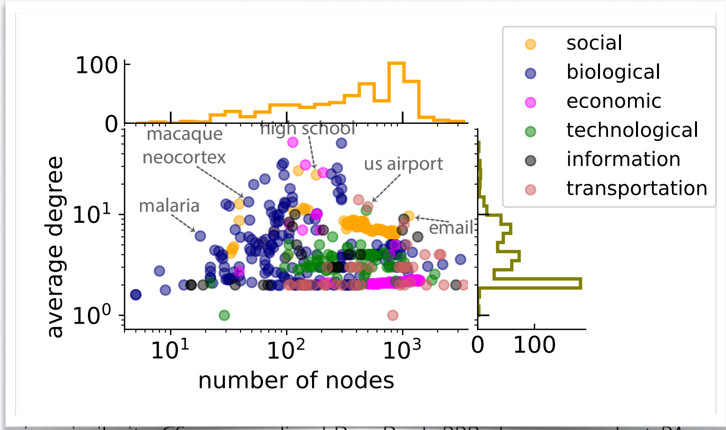
- ***all*** *published link prediction methods work well*
- are they all learning the same thing?
- is there one method that is *best overall*?
- or, does predictability vary *across* network types & settings?
- just how predictable *are* missing edges?

all the data, all the methods

- *methods* : 203 features of a candidate pair
  - 42 topological features
  - 11 probabilistic network models
  - 150 features from graph embeddings



- *data* : 550 structurally diverse networks
  - from icon.colorado.edu
  - social, biological, economic, technological, information, & transportation



* **topological features**: node count *N*, edge count *OE*, degree distribution variance *VD*, common neighbors *CN*, shortest path *SP*, cosine similarity *CS*, personalized PageRank *PPR*, degree product *PA*, Jaccard coefficient *JC*, Adamic-Adar index *AA*, resource allocation index *RA*, dot product of low-rank approx *dLRA*, mean neighbor degree *AND*, betweenness centrality *SPBC*, closeness centrality *CC*, PageRank *PR*, and load centrality *LC*.
* **probabilistic models**: modularity *Q*, multi-resolution modularity *Q-MR*, msg. passing modularity *Q-MP*, Bayesian Newman-Reinert *B-NR (SBM)*, Bayesian Newman Reinert *B-NR (DC-SBM)*, Bayesian Hayashi-Konishi-Kawamoto *B-HKK (SBM)*, corrected int. class. likelihood *cICL-HKK (SBM)*, *Infomap*, min. descr. length *MDL (SBM)*, and min. descr. length *MDL (DC-SBM)*, *S-NB*
* **embedding features**: {hadamard product, dot product, L2 distance} × 128-dimension DeepWalk and 16-dim variational graph auto-encoder
* **network corpus**: we omit 24 of original 572 networks because they are too small to support cross-validation

a diversity of errors

in practice, not one of 203 predictors best on all 550 networks

- *No Free Lunch* theorem[*] — no method *can* be best on all inputs
- different methods capture different aspects of structure
- performance varies by domain (soc, bio, etc.)

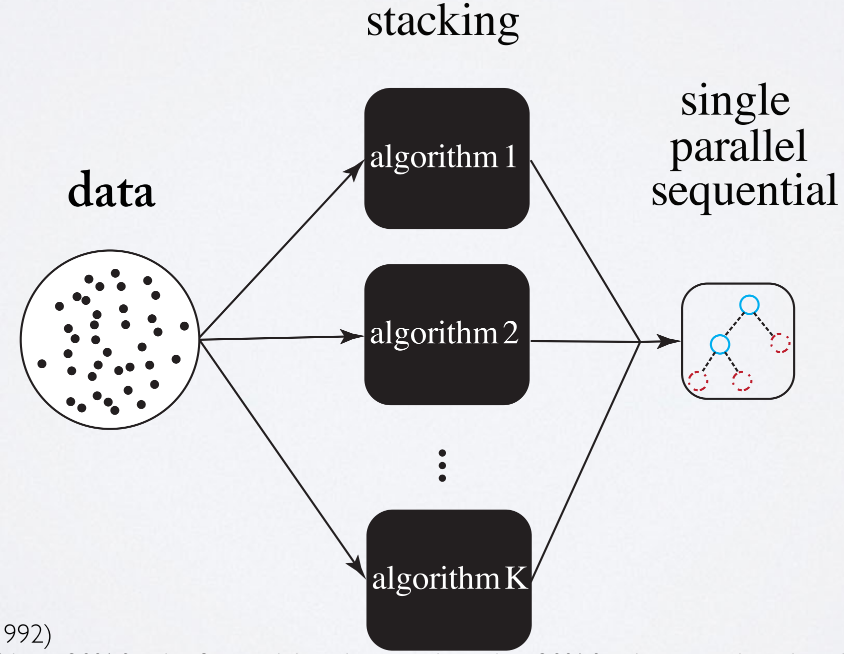
- methods make a *diversity of errors*
- let's *exploit* this diversity via *meta-learning* to *combine* methods to make *strictly better* predictions than any individual method

* Wolpert and Macready, "No Free Lunch Theorems for Optimization." *IEEE Transactions on Evolutionary Computation* **1** (1997)
* Peel et al. "The ground truth about metadata and community detection in networks." *Science Advances* **3** (2017)

learning to combine methods

learning to combine methods

- here, via stacked generalization [a la Netflix Prize]
  - *learn* which algorithm to apply to a given test case x_{ij}, based on its attributes $f(x_{ij})$
  - *leverages* the independence of the errors each method makes, to be better than any component method



* stacked generalization a la Wolpert, *Neural Networks* **5** (1992)
* this supervised technique has two training phases; we hold out 20% for the first, training phase, and another 20% for the second, testing phase

learning to combine methods

- here, via stacked generalization [a la Netflix Prize]
  - *claim: this method produces nearly-optimal link predictions*
  - testing this claim:
    - synthetic data with known structure (*a la* DC-SBM)
    - real-world data from large, diverse corpus (*a la* ICON)
    - accuracy saturation as more features are included?
    - do individual features satisfy AdaBoost theorem?

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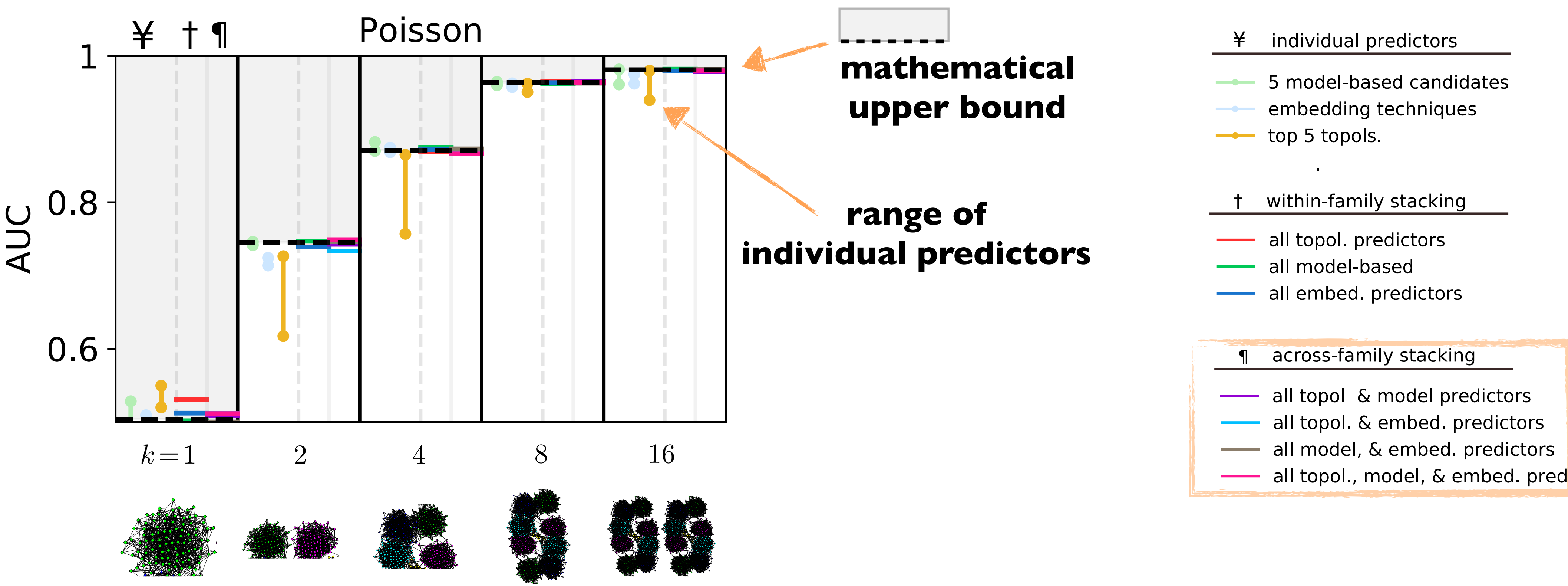
on synthetic data

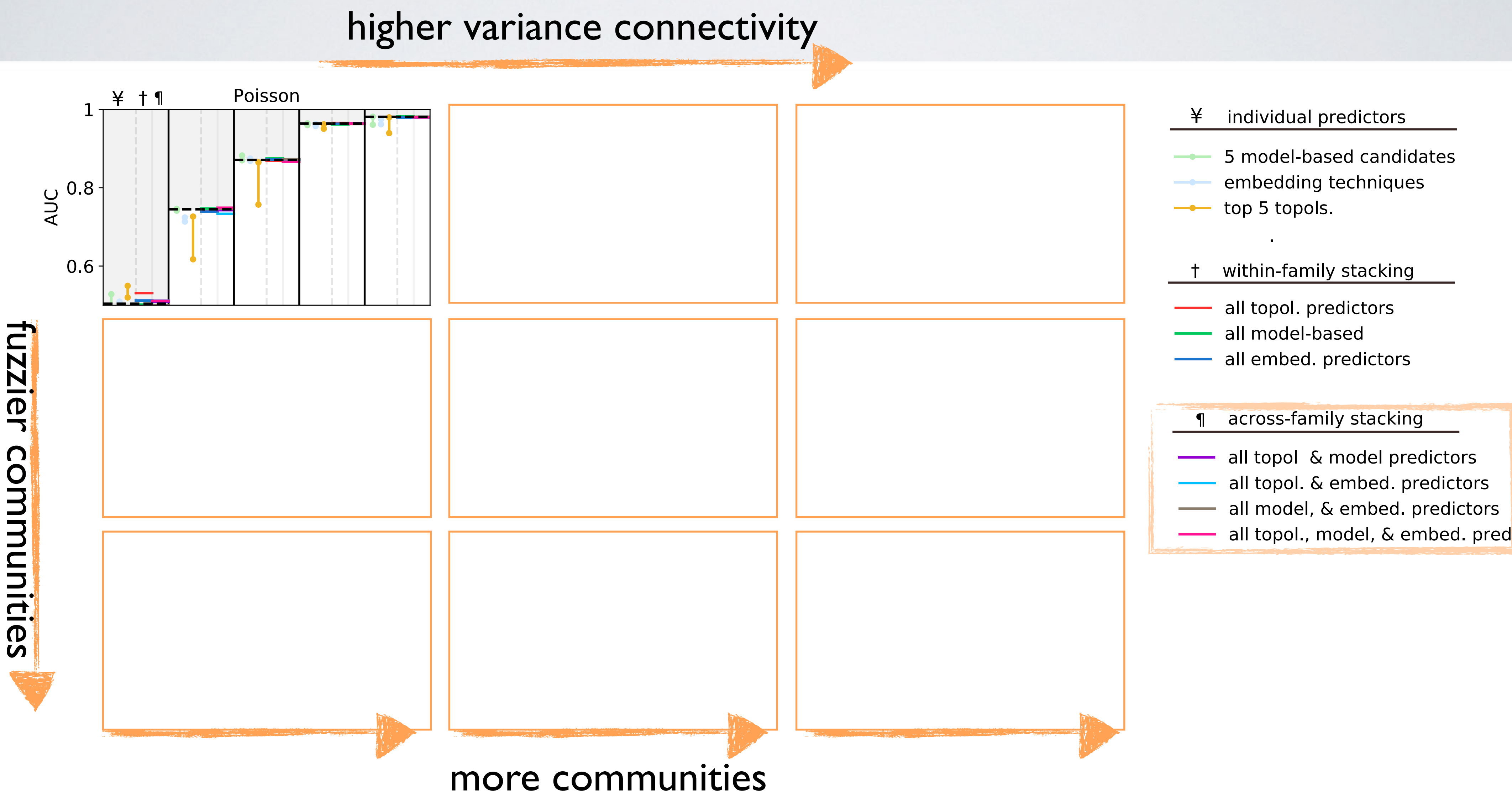
- warm-up (1 dimension) : low-variance in connectivity, sharp communities, and vary number of communities
- score by AUC on 20% holdout & compare w/ *mathematical upper bound*



degree-corrected SBM

on synthetic data

- vary by 3 dimensions : variance in connectivity, fuzziness of structure, and number of communities
- score by AUC on 20% holdout & compare w/ *mathematical upper bound*



on synthetic data

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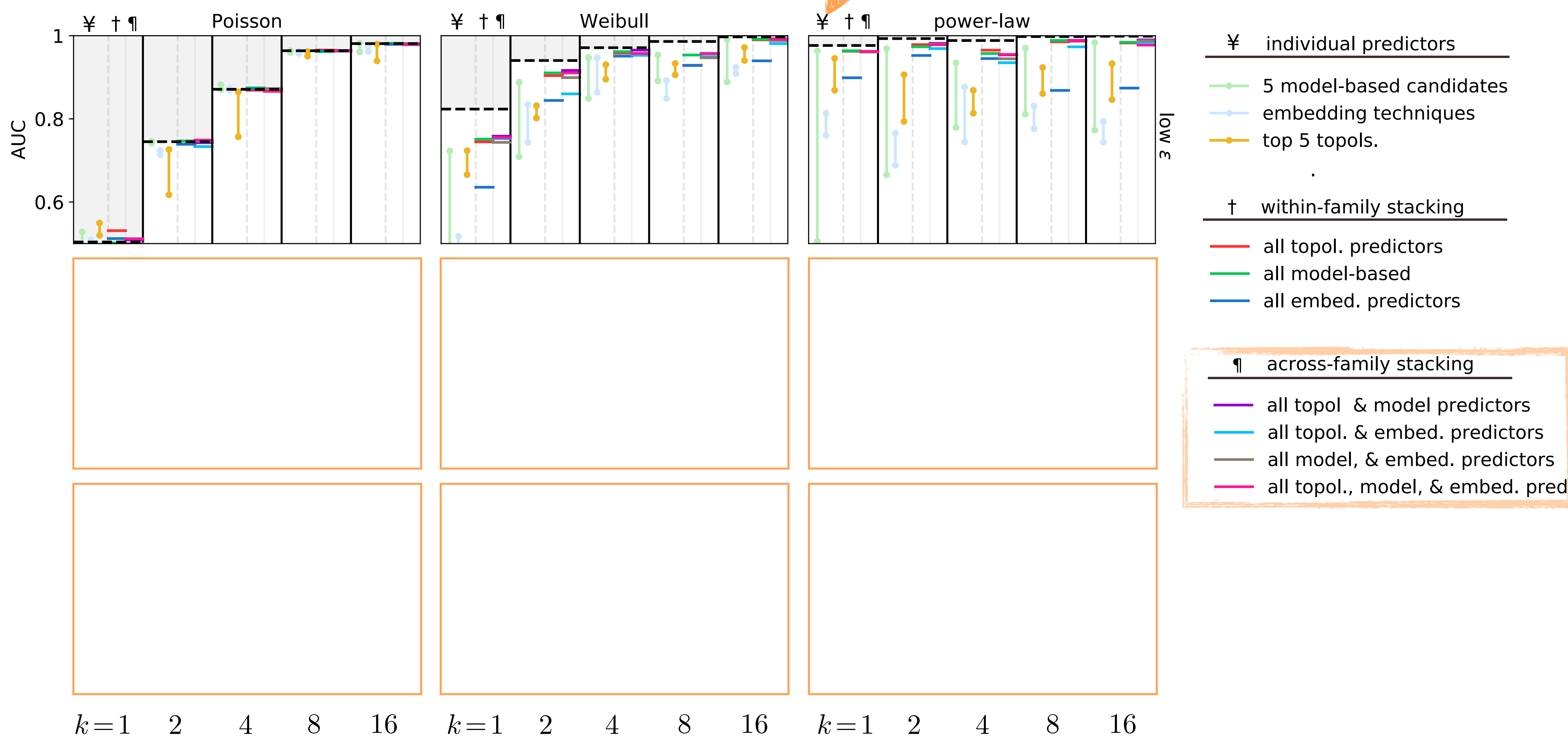
higher variance connectivity



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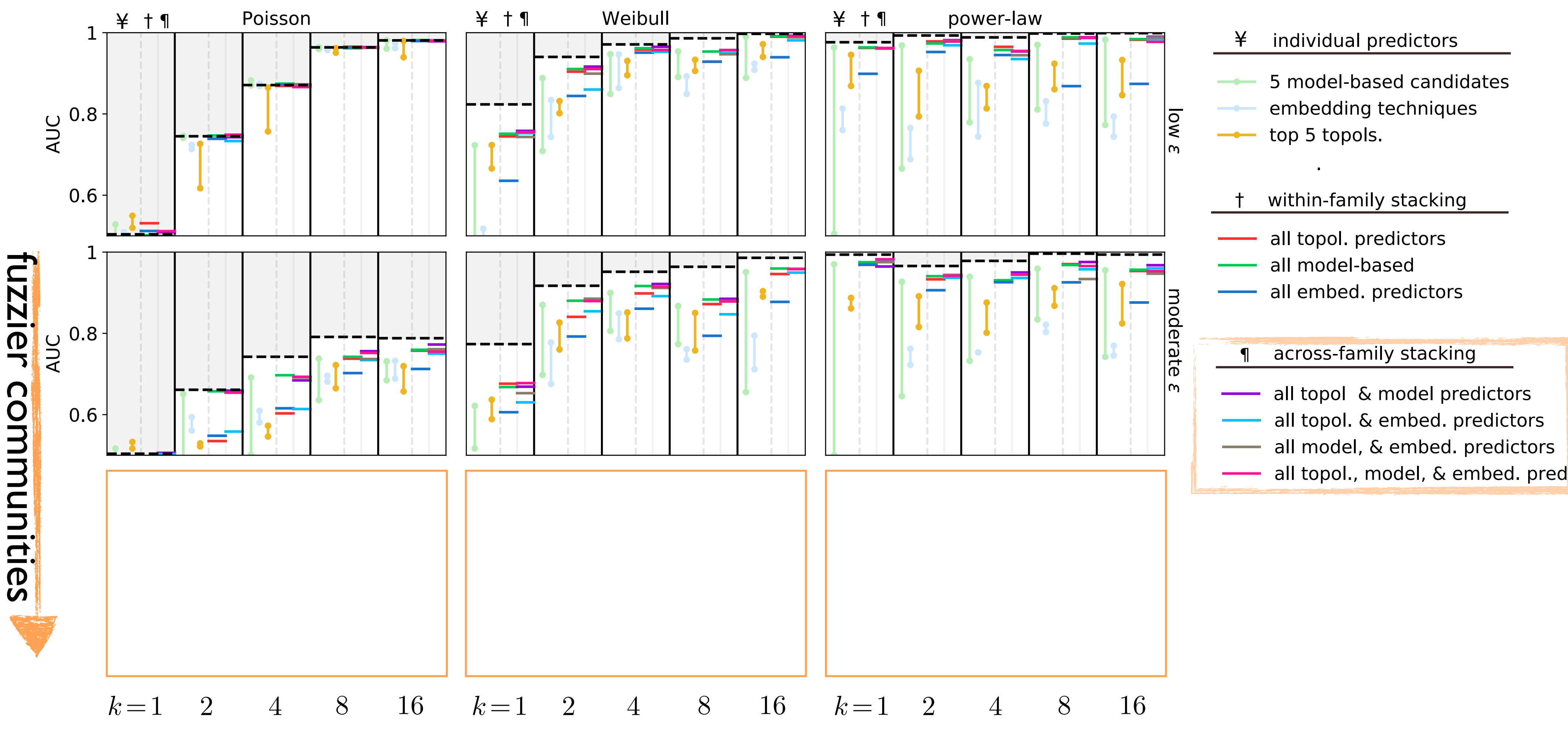

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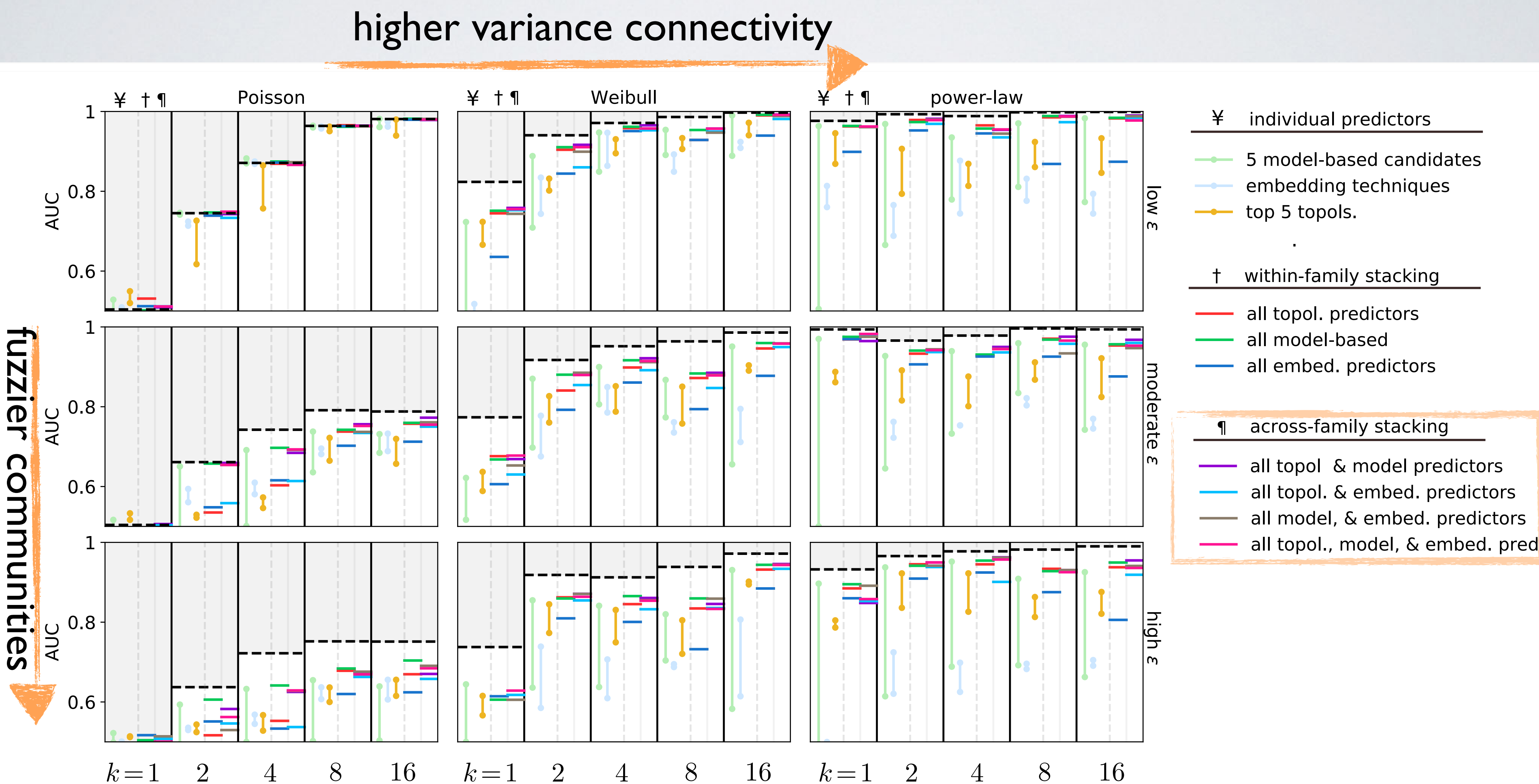

on synthetic data

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- fuzzier communities → harder link prediction
- more homogeneous degrees → harder link prediction
- less modular structure → harder link prediction
- performance differences → mismatch of model to data's structure
- **across methods, *stacking* best or nearly best**
- embedding methods (naively) perform poorly (overfitting?)
- supervised methods perform better than unsupervised (unsurprising)

on real data

- 550 structurally diverse networks from the CommunityFitNet corpus
- score by AUC on 20% holdout

stacked generalization nearly always the best, across domains

embeddings nearly always worst, across domains

* CommunityFitNet corpus : github.com/AGhasemian/CommunityFitNet

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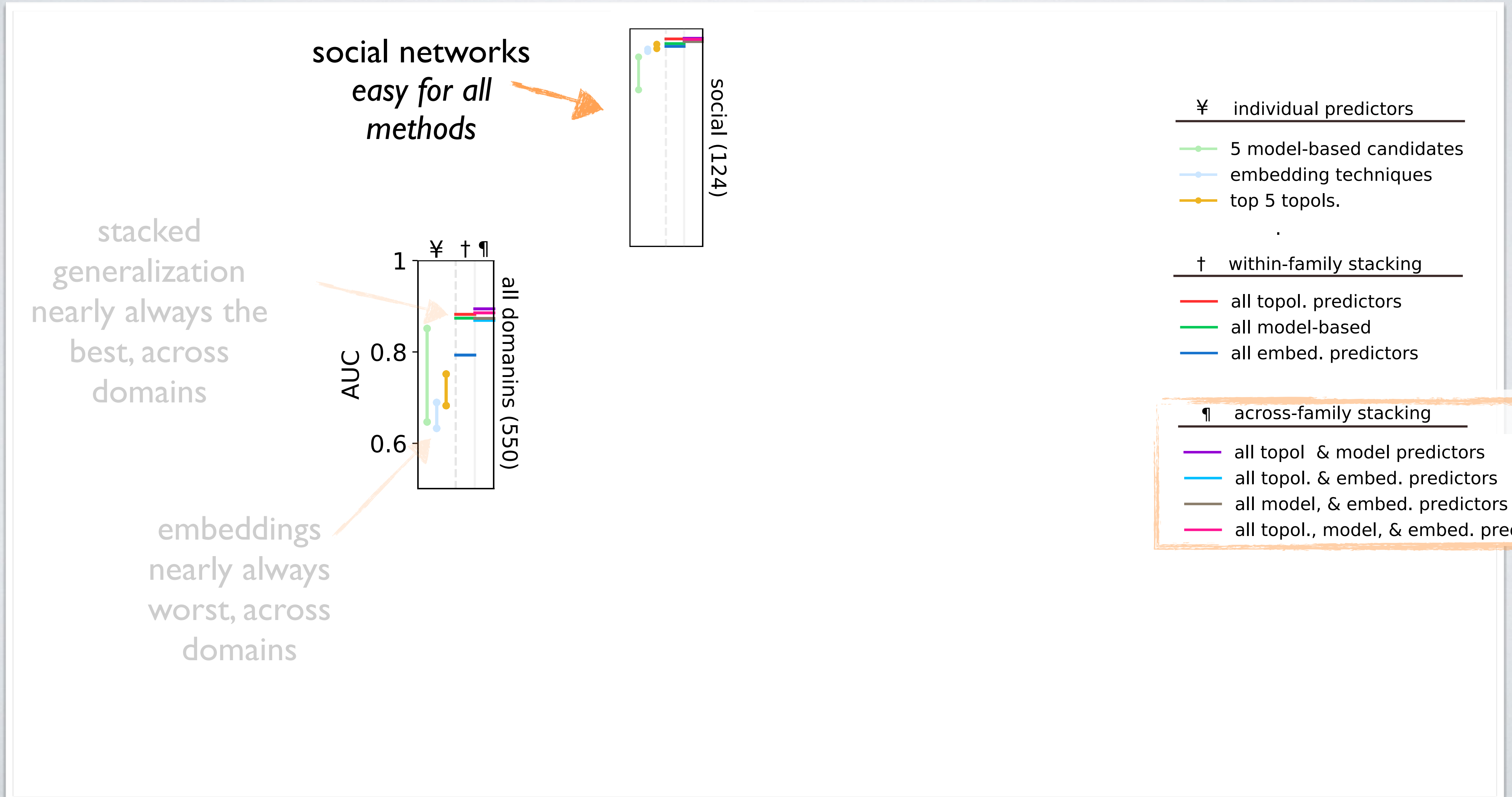

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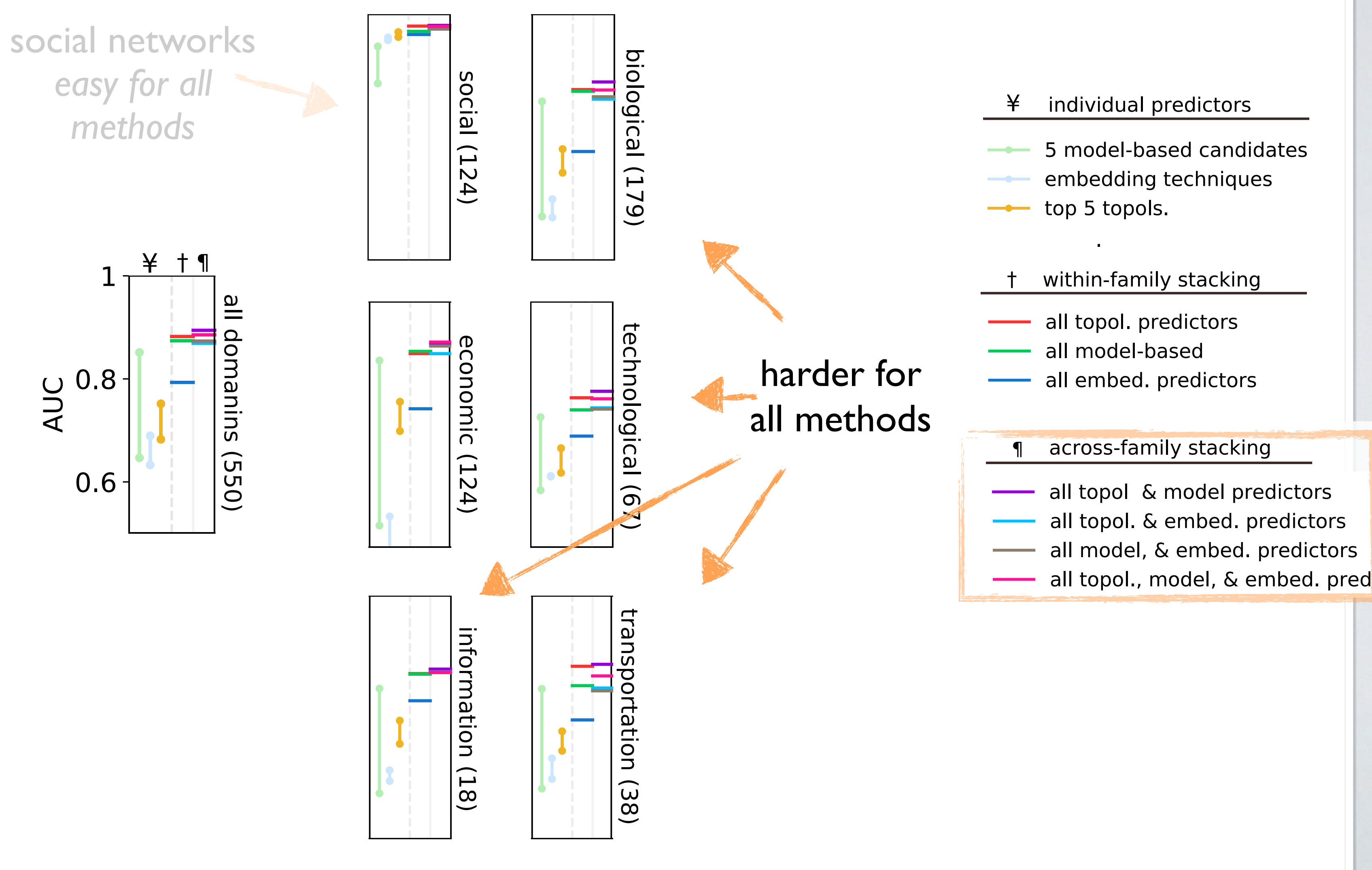

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- **across methods and domains, *stacking* best or nearly best**
- stacking advantage grows with network size (see paper)
- missing links in social networks are *easy* (all methods work well)
- hard domains → biological, technological, transportation, information

on real data

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- **across methods and domains, *stacking* best or nearly best**
- stacking advantage grows with network size (see paper)
- missing links in social networks are *easy* (all methods work well)
- hard domains → biological, technological, transportation, information
- only 25-30 features (models, topol.) sufficient for near-optimality
- state-of-the-art accuracy
- can train to optimize AUC or P/R

algorithm	AUC	precision	recall
mean model-based	0.75 ± 0.16	0.15 ± 0.24	0.24 ± 0.25
mean indiv. topol.	0.61 ± 0.14	0.09 ± 0.2	0.23 ± 0.27
mean indiv. topol. & model	0.64 ± 0.15	0.1 ± 0.21	0.23 ± 0.27
emd-DW	0.63 ± 0.23	0.11 ± 0.17	0.3 ± 0.29
emb-vgae	0.69 ± 0.19	0.15 ± 0.21	0.25 ± 0.23
all topol.	0.88 ± 0.1	0.31 ± 0.33	0.35 ± 0.29
all model-based	0.87 ± 0.1	0.25 ± 0.28	0.29 ± 0.22
all embed.	0.79 ± 0.14	0.18 ± 0.23	0.27 ± 0.23
all topol. & model	0.89 ± 0.09	0.31 ± 0.34	0.34 ± 0.28
all topol. & embed.	0.87 ± 0.11	0.27 ± 0.31	0.33 ± 0.25
all model & embed.	0.87 ± 0.11	0.23 ± 0.26	0.3 ± 0.23
all topol., model & embed.	0.89 ± 0.1	0.28 ± 0.31	0.34 ± 0.26

* mean AUC over 550 networks

conclusions and outlook

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- nearly all networks are incomplete — link prediction helps fill in the missing details
- 🥃 but, no link predictor is best across all networks (No Free Lunch)
- predictors make independent errors — *meta-learning* opportunity

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- nearly all networks are incomplete — link prediction helps fill in the missing details
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- predictors make independent errors — *meta-learning* opportunity

- *stacked generalization* combines many methods across settings — nearly always better than individual predictors + can incorporate new predictors as they emerge = state-of-the-art
- hits theoretical optimum across messy synthetic data — real-world performance possibly *nearly optimal*
- missing links in social networks *inherently* easy to recover; biological networks substantially harder

Stacking Models for Nearly Optimal Link Prediction in Complex Networks

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