MACIEJ BESTA, TORSTEN HOEFLER, ET AL.

Motif Prediction with Graph Neural Networks
Starting Point: Link Prediction
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Predicting links (edges)
Case 1: New Edges Appear (Dynamic Graphs)

Which links will appear?
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Which links will appear?

Why do we care?
Case 1: New Edges Appear (Dynamic Graphs)

Which links will appear?

Why do we care?

Predict future data
Case 2: Find Missing Data

Which links are missing?

Why do we care?
Case 2: Find Missing Data

Which links are missing?

Why do we care?
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Fixing missing data
Case 2: Find Missing Data

Which links are missing?

Why do we care?

Reduce experiment costs

Fixing missing data
Warmup: Link Prediction
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How to assess?
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$$s^{CN}_{u,v} = |\Gamma(u) \cap \Gamma(v)|$$
Warmup: Link Prediction

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\[
S_{u,v}^{CN} = |\Gamma(u) \cap \Gamma(v)|
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S_{u,v}^{Jaccard} = \frac{|\Gamma(u) \cap \Gamma(v)|}{|\Gamma(u) \cup \Gamma(v)|}
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Warmup: Link Prediction

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Warmup: Link Prediction

How to assess?

$$S^C_{u,v} = |\Gamma(u) \cap \Gamma(v)|$$

$$S^{Jaccard}_{u,v} = \frac{|\Gamma(u) \cap \Gamma(v)|}{|\Gamma(u) \cup \Gamma(v)|}$$
Warmup: Link Prediction

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\[ S_{u,v}^{\text{CN}} = |\Gamma(u) \cap \Gamma(v)| \]

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\[ S_{u,v}^{\text{Salton}} = \frac{|\Gamma(u) \cap \Gamma(v)|}{\sqrt{d_u d_v}} \]
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\[ S_{u,v}^{\text{AA}} = \sum_{z \in \Gamma(u) \cap \Gamma(v)} \frac{1}{\log d_z} \]

\[ S_{u,v}^{\text{HPI}} = \frac{|\Gamma(u) \cap \Gamma(v)|}{\min\{d_u, d_v\}} \]

\[ S_{u,v}^{\text{HDI}} = \frac{|\Gamma(u) \cap \Gamma(v)|}{\max\{d_u, d_v\}} \]

\[ S_{u,v}^{\text{RA}} = \sum_{z \in \Gamma(u) \cap \Gamma(v)} \frac{1}{d_z} \]

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\[ S_{u,v}^{\text{Sorensen}} = \frac{2|\Gamma(u) \cap \Gamma(v)|}{d_u + d_v} \]

\[ S_{u,v}^{\text{PAI}} = |\Gamma(u)||\Gamma(v)| = d_u d_v \]
Warmup: Link Prediction

How to assess?

One obtains a „score” $s(e) = s(u,v)$ for each (missing) link in a graph

$$s_{CN} = |\Gamma(u) \cap \Gamma(v)|$$

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### Warmup: Link Prediction

**How to assess?**

One obtains a „score“ $s(e) = s(u, v)$ for each (missing) link in a graph.

The higher the score, the more probable a given link $e$ is to appear in the graph.

<table>
<thead>
<tr>
<th>Method</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CN</strong></td>
<td>$s_{u,v}^{CN} =</td>
</tr>
<tr>
<td><strong>Jaccard</strong></td>
<td>$s_{u,v}^{J} = \frac{</td>
</tr>
<tr>
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Idea: Generalize Link Prediction to Motifs
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Motifs: small, recurring subgraphs (e.g. modelling molecules, gene interactions, groups of people)
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Motifs

Is this important?
Motifs

Is this important?

Network motifs: simple building blocks of complex networks
R Milo, S Shen-Orr, S Itzkovitz, N Kashtan... - ..., 2002 - science.sciencemag.org
Complex networks are studied across many fields of science. To uncover their structural design principles, we defined "network motifs," patterns of interconnections occurring in complex networks at numbers that are significantly higher than those in randomized ...

Network motifs: theory and experimental approaches
U Alon - Nature reviews Genetics, 2007 - nature.com
Transcription regulation networks control the expression of genes. The transcription networks of well-studied microorganisms appear to be made up of a small set of recurring regulation patterns, called network motifs. The same network motifs have recently been ...
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Is this important?

A lot of work into motifs exists, recent renewed interest under the theme „Higher-order network organization“

Seeing a graph through the perspective of motifs instead of edges ("higher order")

Network motifs: simple building blocks of complex networks

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How to generalize to motifs?

**General vision**: assign some score to motifs (make them comparable)

Motifs with higher scores are more probable
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...but there are so many differences to link prediction!
**Idea: Generalize Link Prediction**

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Link prediction is well understood for, well, links (scores assigned to links, similarity based methods, etc.)

Motifs with higher scores are more probable

How to generalize to motifs?

**General vision**: assign some score to motifs (make them comparable)

...but there are so many differences to link prediction!

Let’s go over them [1] ...
Difference 1: There May Be Many Potential New Motifs for a Fixed Vertex Set

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Link prediction:

A link is either there or not there

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Motif prediction:

How to consider such diversity of possible patterns in score functions?

Difference 2: Incoming Motifs May Have Existing Edge

Link prediction:

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A link to be predicted does not exist

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Already exists

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Already exists

How to consider such edges in the score functions?

Difference 2: Incoming Motifs May Have Existing Edge

Link prediction:

A link to be predicted does not exist

Motif prediction:

Example: some existing relationships in a group of people

How to consider such edges in the score functions?

$S(\ )$?

Difference 3: There May Be “Deal-Breaker” Edges

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Link prediction:

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We don’t want these links! (i.e., these links appearing would make it impossible for a motif in question to appear)

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Example: chemical bonds

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How to consider such edges in the score functions?

Example: chemical bonds

Difference 3: There May Be “Deal-Breaker” Edges

**Link prediction:**

No such effect (a link to be predicted is never a "deal breaker")

**Motif prediction:**

We don’t want these links! (i.e., these links appearing would make it impossible for a motif in question to appear)

How to consider such edges in the score functions?

Example: chemical bonds

Difference 4: Motif Prediction Query May Depend on Vertex Labeling

Link prediction:

Motif prediction:

Difference 4: Motif Prediction Query May Depend on Vertex Labeling

Link prediction:

Motif prediction:

We want this:

Difference 4: Motif Prediction Query May Depend on Vertex Labeling

Link prediction:

Motif prediction:

We want this:

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We want this:

...but not this:

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No such effect (not enough room with a single link)

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How to formulate motif prediction, considering all these differences?

Motif Prediction Score Functions

Starting Simple: Motif Scores Based on Independent Links

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A motif: \( M = (V_M, E_M) \)

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Motif edges that do not yet exist

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Motif edges that do not yet exist

Motif edges that already exist

\[ s_\perp(M) = \prod_{e \in E_M,N} s(e) \]

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\( s(e) \) is any link prediction score which outputs into \([0, 1]\) (e.g., Jaccard)

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Motif Prediction Score Functions

Starting Simple: Motif Scores Based on Independent Links

For edges that already exist, we set \( s(e) = 1 \) (i.e., we assume that a motif is more likely to appear if the edges that participate in that motif are also more likely)

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$\in [0, 1]$ by construction

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Example heuristic for the Jaccard score $s(e)$ for links:

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Example heuristic for the Jaccard score \( s(e) \) for links:

\[
s_{\perp}(M)^J = \prod_{e_{u,v} \in E_M, \mathcal{N}} \frac{|N_u \cap N_v|}{|N_u \cup N_v|}
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Motif Prediction Score Functions

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Example heuristic for the Jaccard score \( s(e) \) for links:

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s(M) = f(s(e)) = \langle w, s(e) \rangle
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Example heuristic for the Jaccard score \( s(e) \) for links:

\[ s(M) = f(s(e)) = \langle w, s(e) \rangle \]

\( s(M) \) is a convex combination of the vector of link prediction scores \( s(e) \)

Motif Prediction Score Functions

What if the arrival of some (motif) links impacts the chances for other motif links to appear?

Adding correlation between links

The weight vector (incorporates user’s domain knowledge)

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Example heuristic for the Jaccard score \( s(e) \) for links:

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What if the arrival of some (motif) links reduces, or even prevents, motif’s appearance?

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\[ E^*_M = E_M \]

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A deal-breaker edge that does not exist (i.e., it might arrive later):

\[ s^*_i(e) = -s_i(e) \]

The weight vector (incorporates user’s domain knowledge)

\[ s^*(M) = f(s^*(e)) = \max(0, \langle w, s^*(e) \rangle) \]

A motif:

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A deal-breaker edge that does not exist (i.e., it might arrive later):

$$s^*_i(e) = -s_i(e)$$

A deal-breaker edge that does already exist:

$$s^*(e) = 0$$

A motif:

$$M = (V_M, E_M)$$

$$E_M = E_{M,\mathcal{N}} \cup E_{M,\mathcal{E}}$$

$$E^*_M \equiv E_M \cup \overline{E_{M,\mathcal{D}}}$$

Motif edges

Deal-breaker edges

Motif Prediction Score Functions

What if the arrival of some (motif) links reduces, or even prevents, motif’s appearance?

Incorporating deal-breaker links

The weight vector (incorporates user’s domain knowledge)

\[ s^*(M) = f(s^*(e)) = \max(0, \langle w, s^*(e) \rangle) \]

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Another formulation (perhaps more intuitive):

\[ s^*_\perp(M) = \prod_{e \in E_M} s(e) \cdot \prod_{e \in \overline{E_M},\mathcal{D}} (1 - s(e)) \]

Motif Prediction Score Functions

A motif:

$$M = (V_M, E_M)$$

$$E_M = E_{M,N} \cup E_{M,E}$$

$$E^*_M = \overline{E_{M,D}} \cup E_{M,N}$$

Incorporating deal-breaker edges

$$s^*(M) = f(s^*(e)) = \max(0, \langle w, s^*(e) \rangle)$$

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Motif Prediction Score Functions

A motif: $M = (V_M, E_M)$

The weight vector (incorporates user's domain knowledge)

Deal-breaker edges that do not exist (i.e., it might arrive later):

$[1] \text{M. Besta et al.: “Motif prediction with graph neural networks”, KDD'22}$

Motif edges

Deal-breaker edges

Another formulation (perhaps more intuitive):

A deal-breaker edge that does already exist:

Check the paper [1] for details about heuristics (based on pairwise Jaccard, Common Neighbors, and Adamic-Adar scores)

$s^*(M) = f(s^*(e)) = \max(0, \langle w, s^*(e) \rangle)$

These are all heuristics... but recent results for learning-enhanced link prediction [2] post a question: can we use learning for motif prediction as well?

$s^*_\perp(M) = \prod_{e \in E_M} s(e) \cdot \prod_{e \in \overline{E}_{M,\mathcal{D}}} (1 - s(e))$

The graph structure may be arbitrary, maybe one could arrive at better heuristics by learning?

How does deep learning work?
The graph structure may be arbitrary, maybe one could arrive at better heuristics by **learning**?

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Samples
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How does deep learning work?

- **Samples**
- **Learning a heuristic**

\[ f(x) \]
The graph structure may be arbitrary, maybe one could arrive at better heuristics by learning?

How does deep learning work?

The animation borrowed from T. Hoefler

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<td>Truck</td>
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How does deep learning work?

The animation borrowed from T. Hoefer
Motif Prediction: Deep Learning Formulation

A motif: \( M = (V_M, E_M) \)
Motif Prediction: Deep Learning Formulation

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**Goal:** predict this motif \( M \):
Motif Prediction: Deep Learning Formulation

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A motif: \[ M = (V_M, E_M) \]

Goal: predict this motif M:

A given fixed set of vertices:
Motif Prediction: Deep Learning Formulation

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Positive samples
Motif Prediction: Deep Learning Formulation

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The neighborhood of the sampled vertex set

A "positive" sample for the neural network architecture

Goal: predict this motif \( M \):

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Positive samples
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The neighborhood of the sampled vertex set

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Positive samples

Negative samples
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Goal: predict this motif \( M \):

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Positive samples

Negative samples
Motif Prediction: Deep Learning Formulation

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A given fixed set of vertices:

A "positive" sample for the neural network architecture

Positive samples

The neighborhood of the sampled vertex set

A "negative" sample for the neural network architecture

Negative samples

A motif: \( M = (V_M, E_M) \)
Motif Prediction: Deep Learning Formulation
Motif Prediction: Deep Learning Formulation

layer-wise weight update

f(x)

Cat 0.54
Dog 0.28
Airplane 0.07
Horse 0.04
Bicycle 0.33
Truck 0.02

Cat 1.00
Dog 0.00
Airplane 0.00
Horse 0.00
Bicycle 0.00
Truck 0.00
Motif Prediction: Deep Learning Formulation

A given fixed set of vertices:

f(x)

layer-wise weight update

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Cat
Dog
Airplane
Horse
Bicycle
Truck

1.00
0.00
0.00
0.00
0.00
0.00
Motif Prediction: Deep Learning Formulation

A given fixed set of vertices: f(x)

Will a k-clique appear or not?

layer-wise weight update
Motif Prediction: Deep Learning Formulation

The samples are used to train a neural network model called Deep Graph Convolutional Neural Network (DGCNN) [1]

A given fixed set of vertices:

f(x)

Layer-wise weight update

Will a k-clique appear or not?

SEAM Architecture (learning from Subgraphs, Embeddings and Attributes for Motif prediction)
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1. Specify vertex set in a motif to be predicted
   Details: §4.2

2. Specify motif edges $E_M$ and dealbreaker edges $E_{M,D}$
   All edge classes are explained in detail in Table 1 and Figure 3

Details: §4.2
SEAM Architecture (learning from Subgraphs, Embeddings and Attributes for Motif prediction)

1. Specify vertex set in a motif to be predicted
   Details: §4.2
   $V_M$
   Input graph

2. Specify motif edges $E_M$ and dealbreaker edges $E_{M,D}$
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3. Find positive & negative samples $G_P$, $G_n$
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   Negative sample (instance that differs from motif $M$)
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   - Positive sample (instance of motif $M$)
   - Negative sample (instance that differs from motif $M$)

4. Extract subgraphs around samples
   (here, $h = 1$)
   1-hop neighbors
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5. Construct node embeddings
   Details: §4.5
   Use Node2Vec / DeepWalk
   - (1.2 0 2.3 ... )
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   Details: §4.6, §4.7

- Inner label (1 0 0 1 ...)
- Outer label (1 2 2 3 ...)

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   Inner label $(1 0 0 1 ...)$
   Outer label $(1 2 2 3 ...)$
   Inner labels of vertices in a subgraph

7. Create final feature matrix
   Details: §4.6
   $(1 0 0 1 ...)$
   $(1 2 2 3 ...)$
   $(1.2 0 2.3 ...)$
   Outer labels of vertices in neighborhood
   Node embeddings
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   Details: §4.5

6. Label nodes in subgraphs
   Details: §4.6

7. Create final feature matrix
   Details: §4.6

8. Training and inference with a GNN
   Details: §4.3, §4.8

- Inner labels of vertices in a subgraph
- Outer labels of vertices in neighborhood
- Node embeddings

- Input features of extracted subgraphs
- Distribute the features of each vertex to its neighbors
- Sort vertices based on their importance in the subgraph
- Use DGCNN

- Binary classification: will a given motif M appear?
- Multi-classification: Which of given motifs will appear?

- Loss function
Evaluation: considered motifs & scenarios

$k$-stars

Sparse  Dense
Evaluation: considered motifs & scenarios

$k$-stars  sparse clusters  $\ldots$  dense clusters  $k$-cliques

Sparse  $\Rightarrow$ Dense
Evaluation: considered motifs & scenarios (transductive, inductive)
Evaluation: considered motifs & scenarios (transductive, inductive)

Pick motif X in graph A

Train for predicting new instances of motif X in graph A
Evaluation: considered motifs & scenarios (transductive, inductive)

Pick motifs $X, Y, \ldots$ in graph $A$  \quad \Rightarrow \quad \text{Train for predicting new instances of motifs $X, Y, \ldots$ in graph $A$}
Evaluation: considered motifs & scenarios (transductive, inductive)

Pick motifs
X, Y, ...
in graphs
A, B, ...

Train for predicting
new instances
of motifs X, Y, ...
in graphs
A, B, ...

27
### Evaluation

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**SEAM**: learning from Subgraphs, Embeddings and Attributes for Motif prediction
### Evaluation

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<td>55.78 ± 0.74</td>
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**SEAM**: learning from Subgraphs, Embeddings and Attributes for Motif prediction

„db“ – with deal-breaker edges


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### Attr: learning from Subgraphs, Embeddings and Attributes for Motif prediction

**CN**: Common Neighbors, **AA**: Adamic-Adar, **SEAL** [2]: Link Prediction using GNNs

**Mul, Min, Avg**: different variants (i.e., how link scores are aggregated to form motif scores)


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- "db" – with deal-breaker edges
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<td>90.00 ± 1.84</td>
<td>91.53 ± 1.53</td>
<td>93.06 ± 0.61</td>
<td>97.26 ± 0.23</td>
<td>98.90 ± 0.18</td>
<td>83.81 ± 0.53</td>
<td>87.56 ± 0.79</td>
<td>88.59 ± 1.51</td>
</tr>
</tbody>
</table>

**Evaluation**

“db” – with deal-breaker edges

Evaluation

With correlation

No correlation

CN: Common Neighbors, AA: Adamic-Adar, SEAL [2]: Link Prediction using GNNs

Mul, Min, Avg: different variants (i.e., how link scores are aggregated to form motif scores)


Much more results and sensitivity analyses in the paper 😊
Thank you for your attention