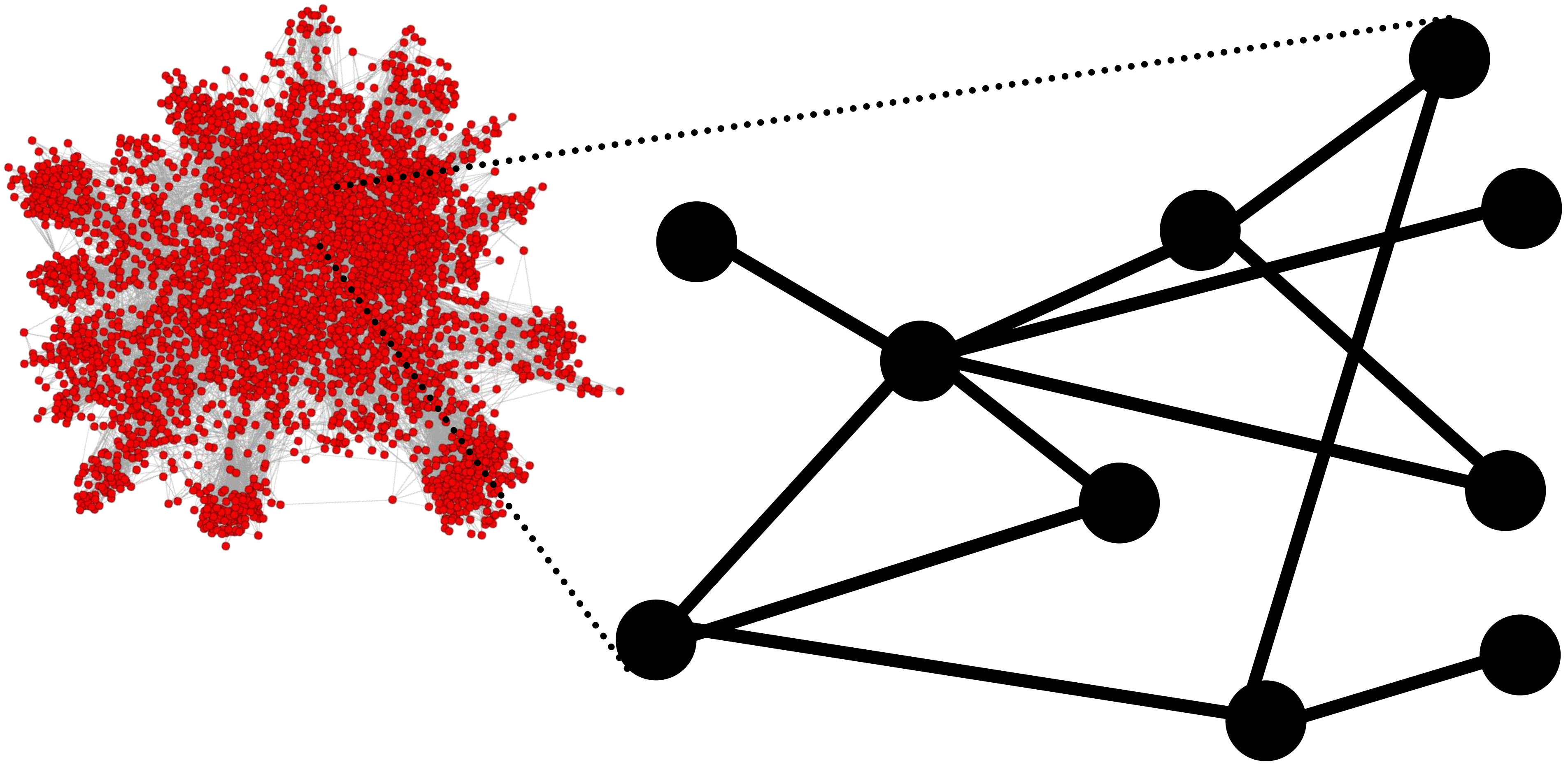
MACIEJ BESTA, TORSTEN HOEFLER, ET AL.

Motif Prediction with Graph Neural Networks

Starting Point: Link Prediction



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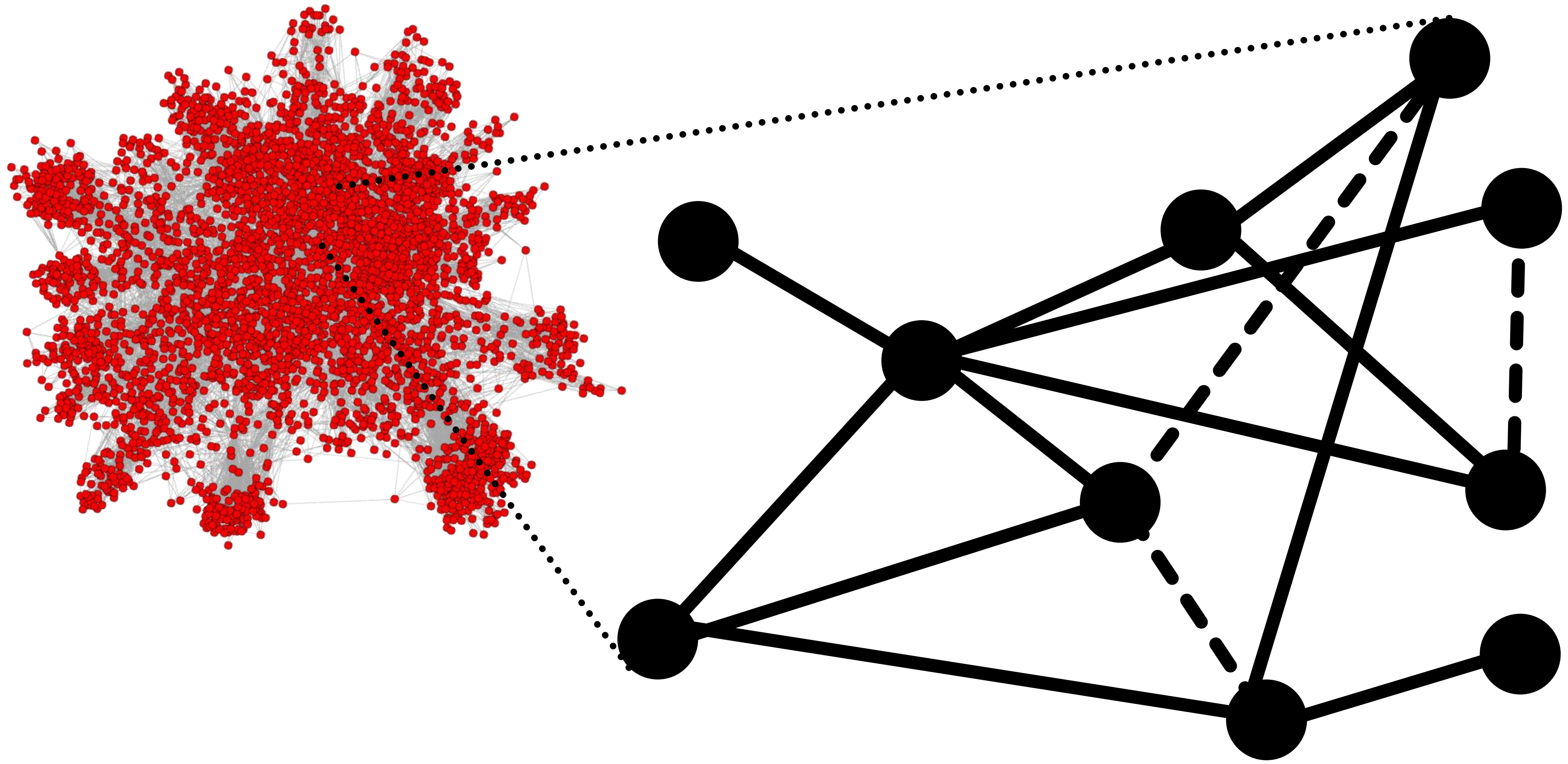

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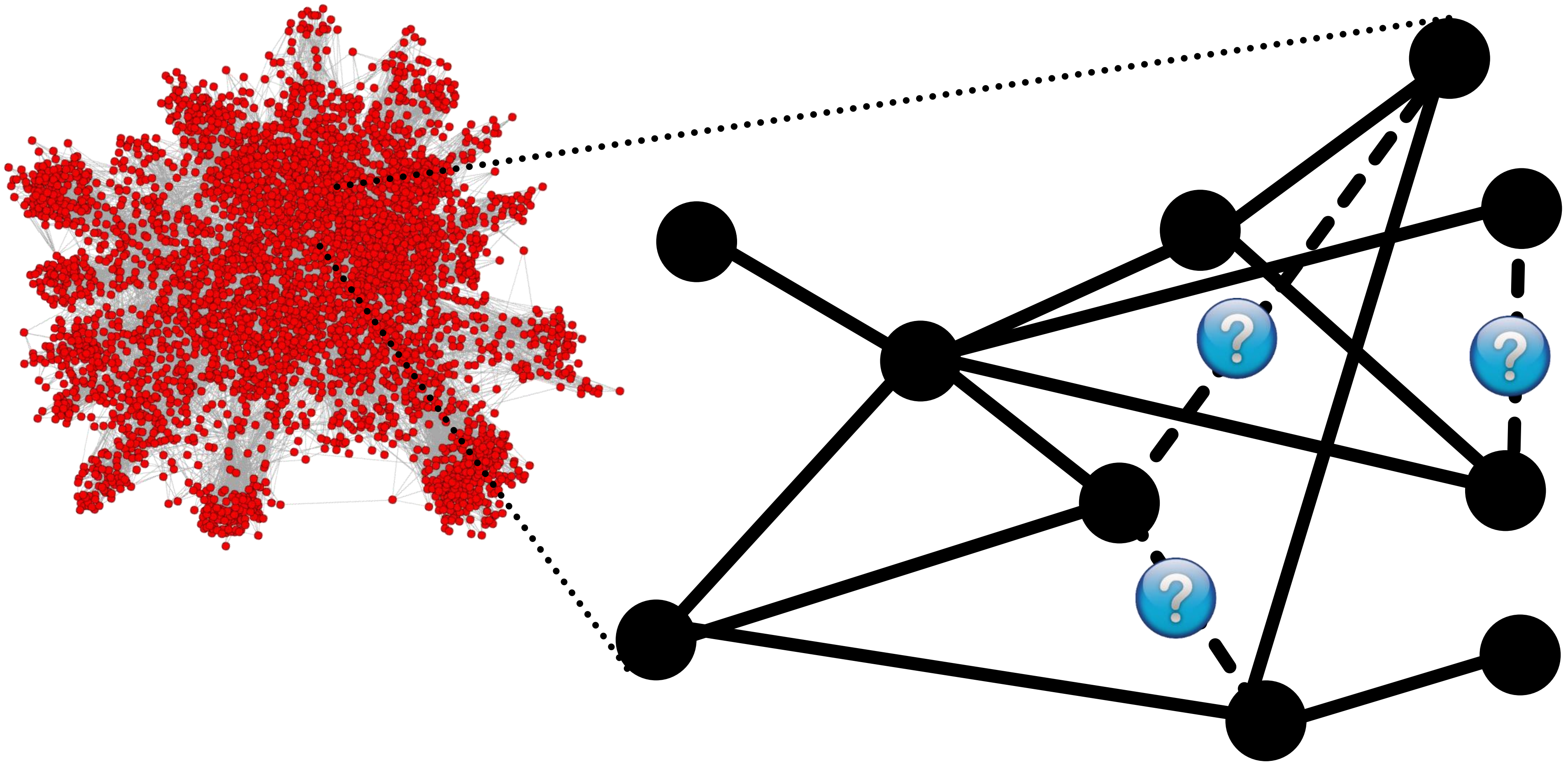

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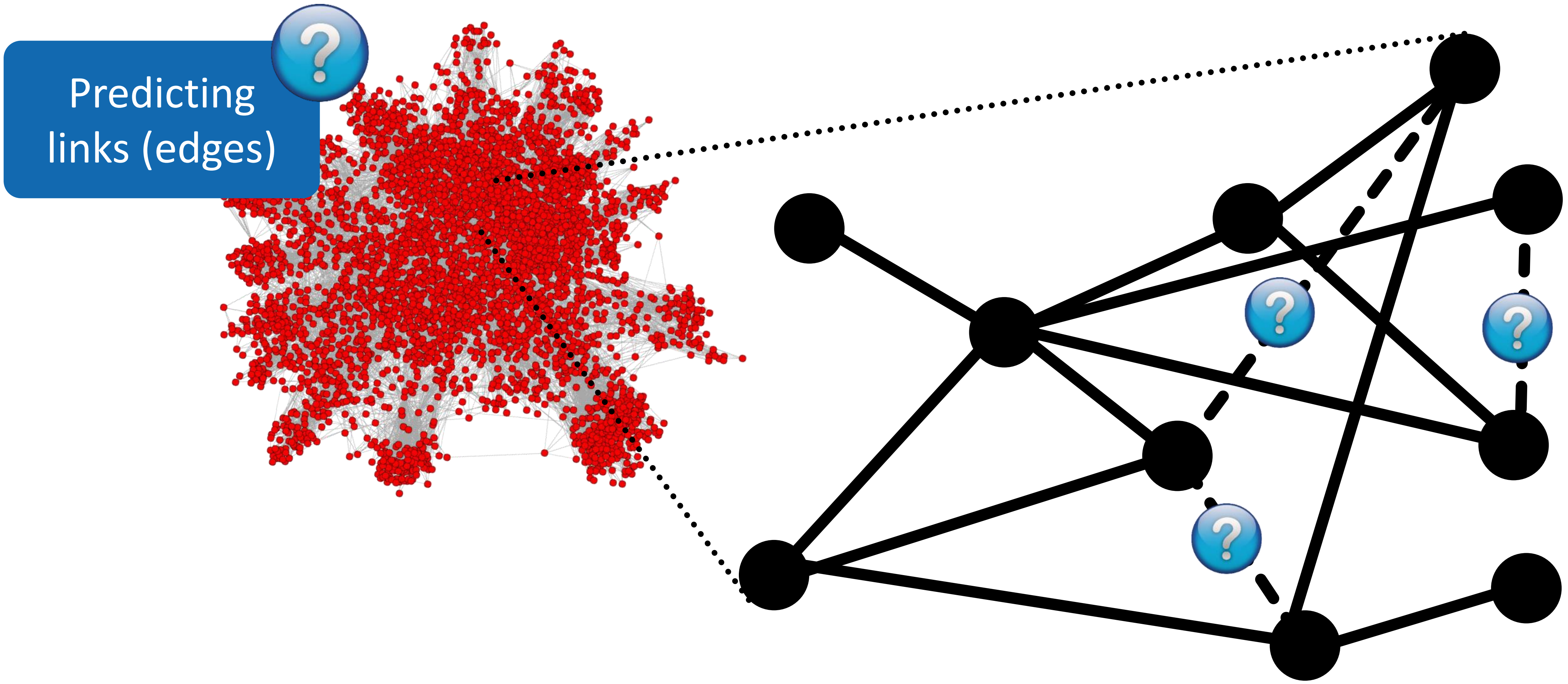
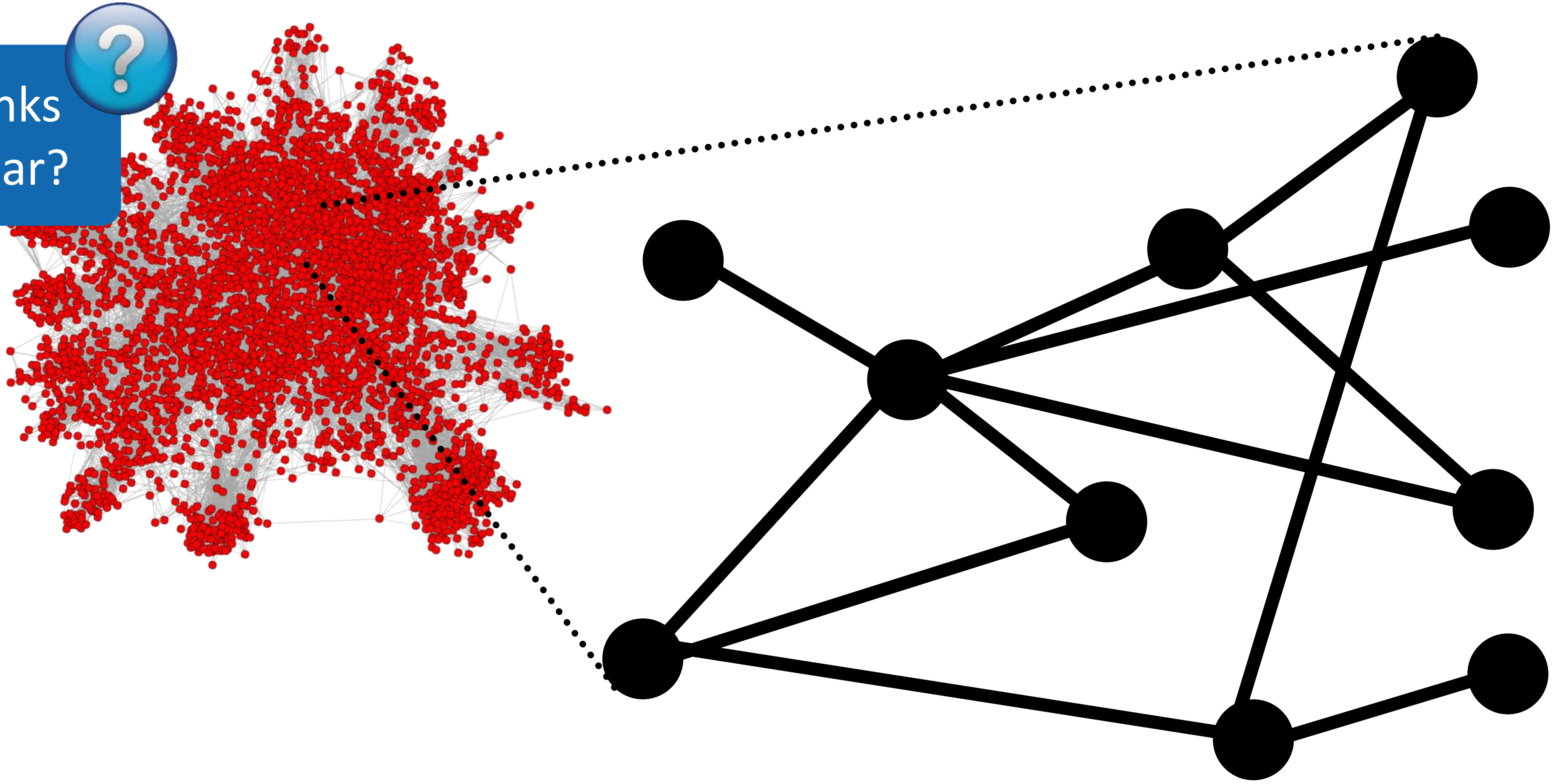


Case 1: New Edges Appear (Dynamic Graphs)

Which links will appear?



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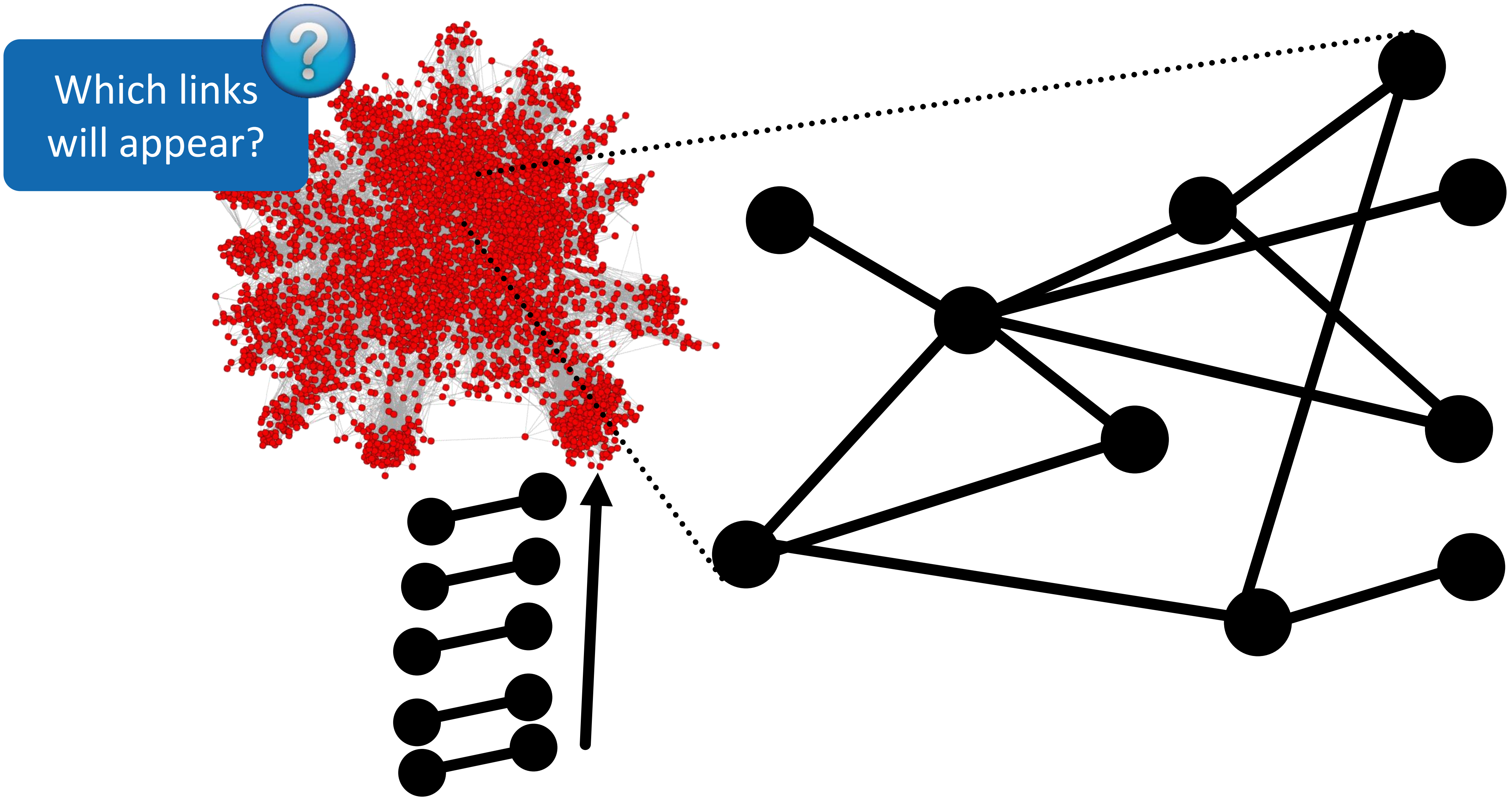

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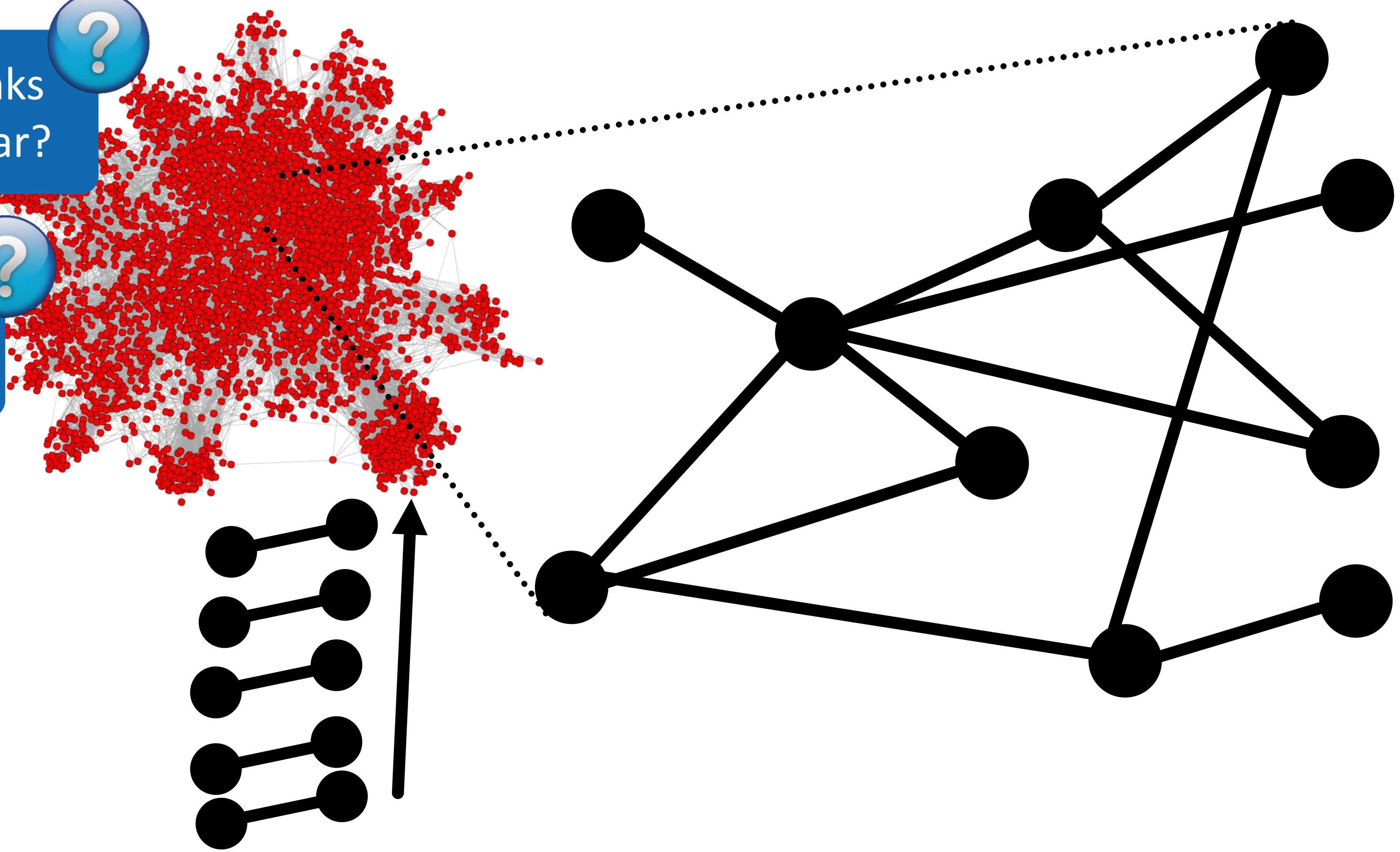

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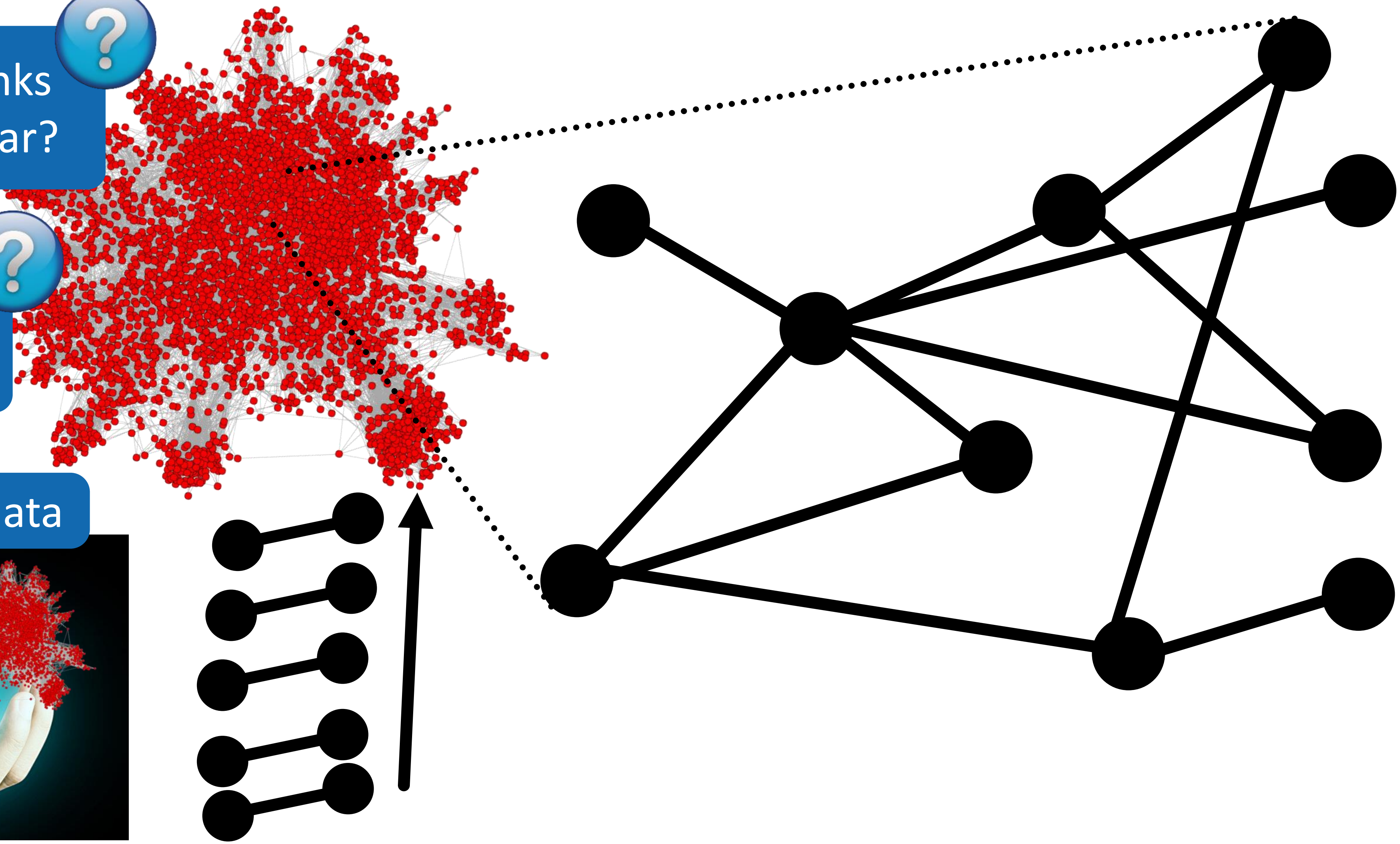
Predict future data



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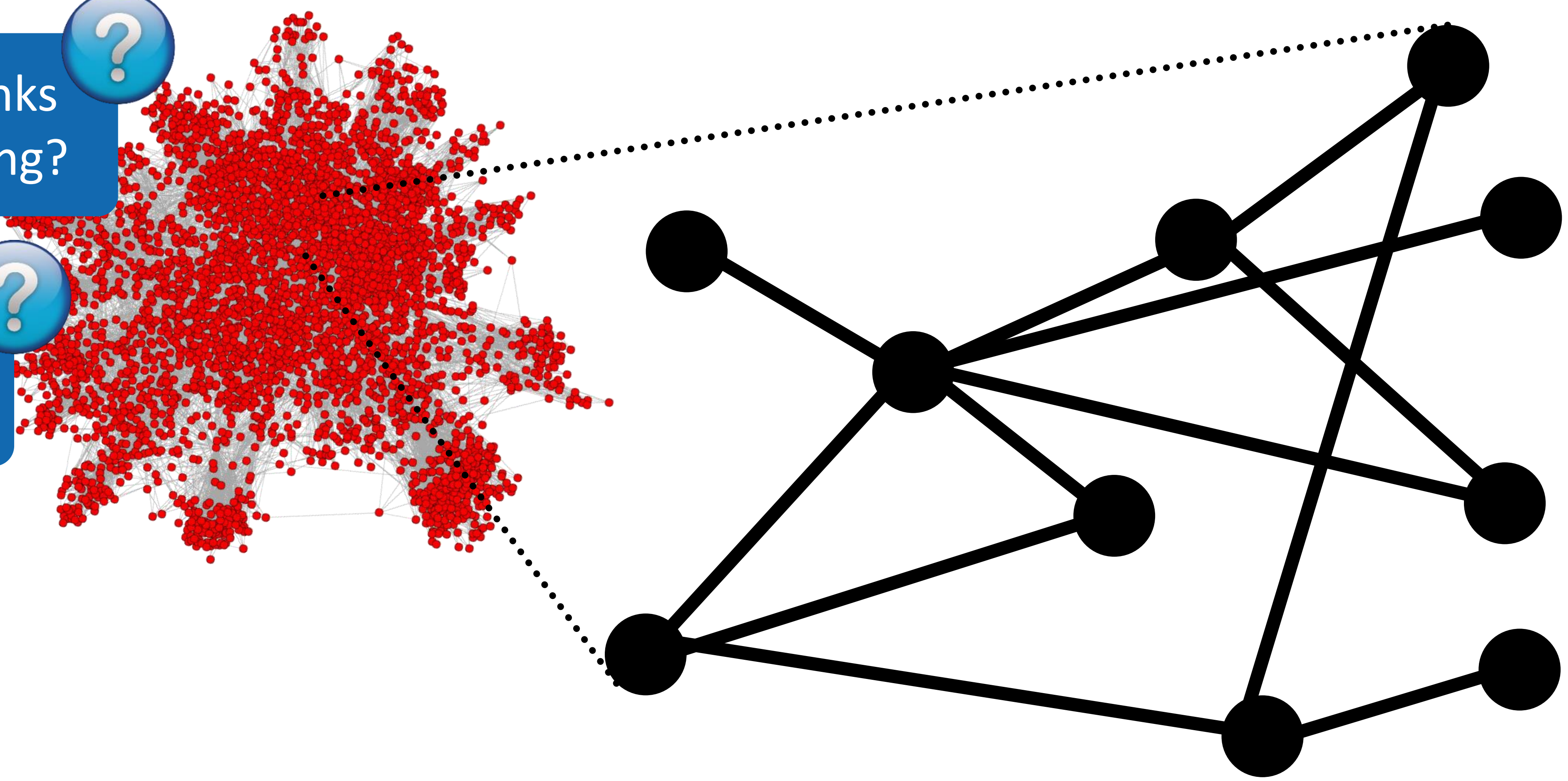

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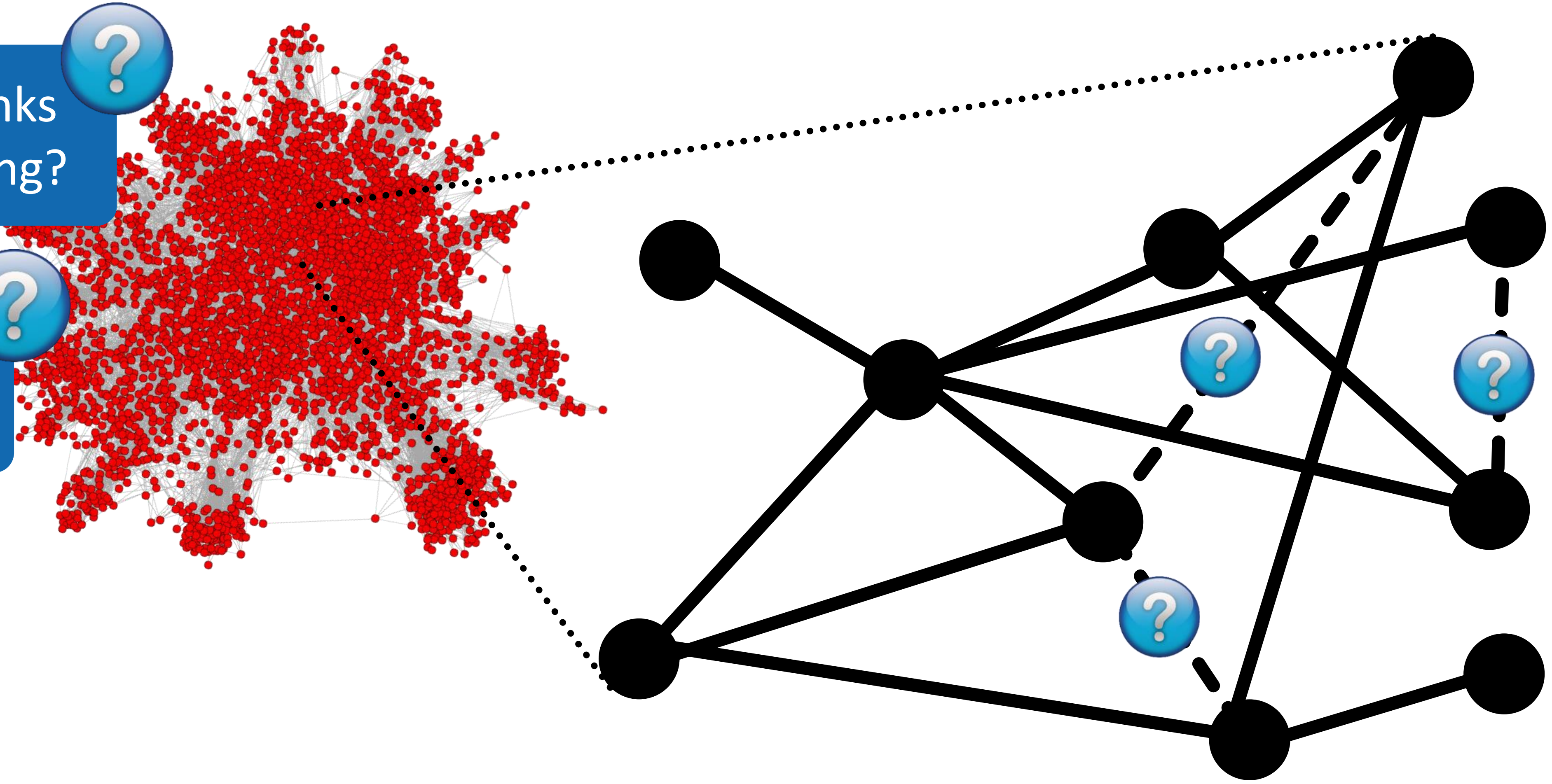

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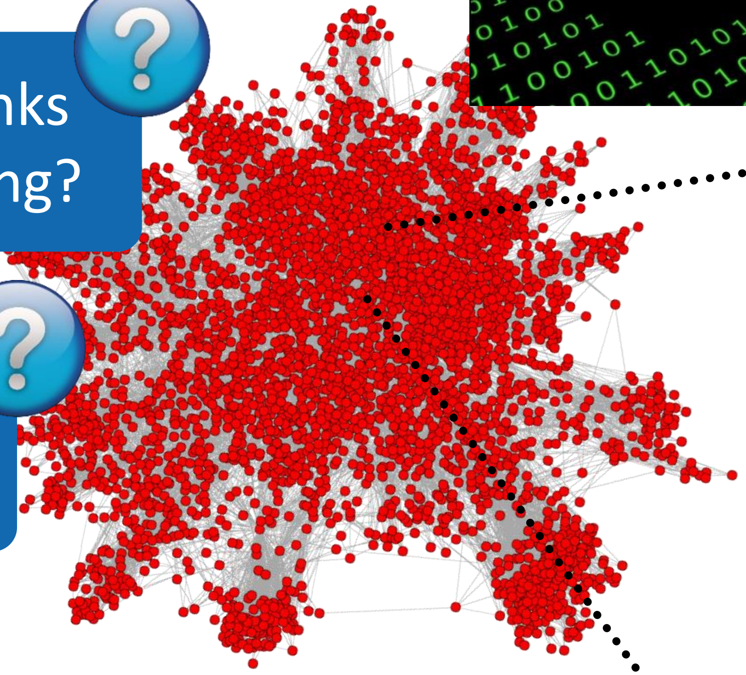

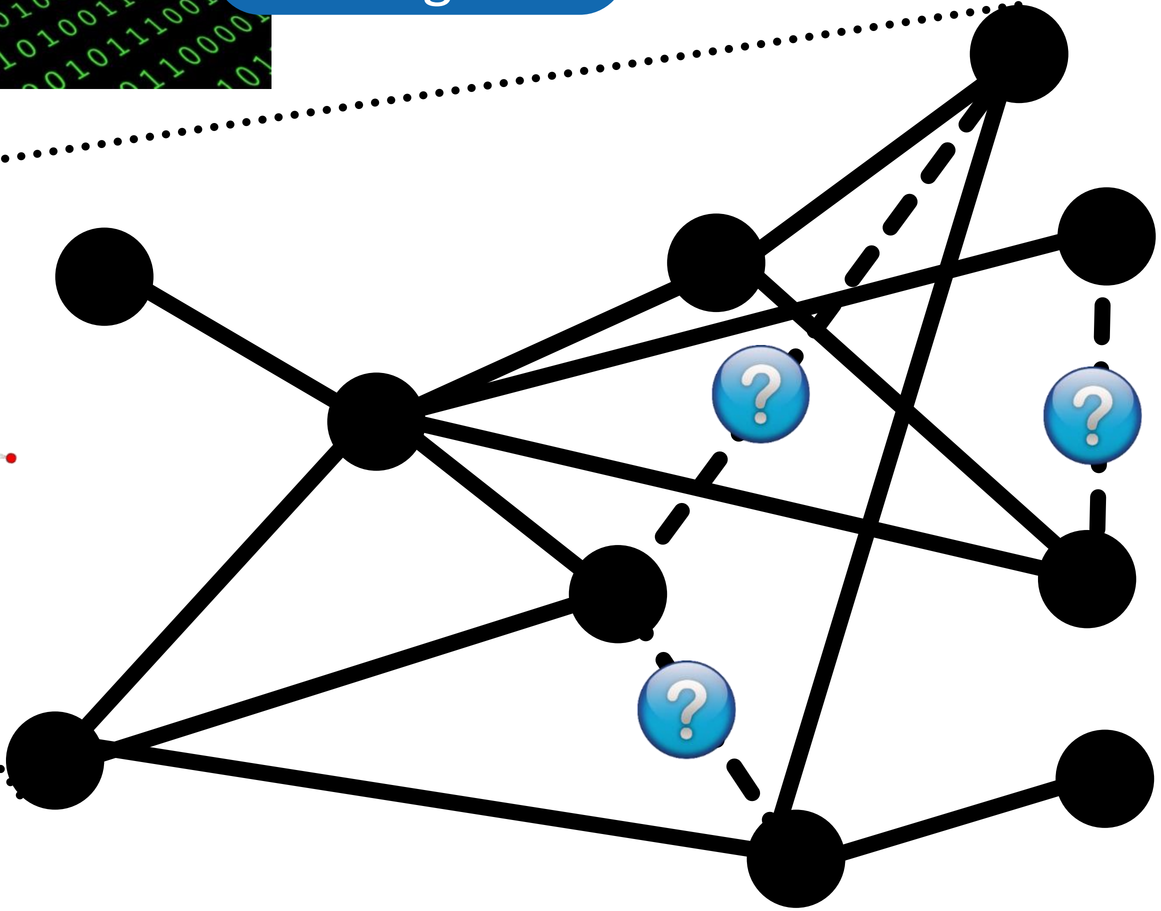

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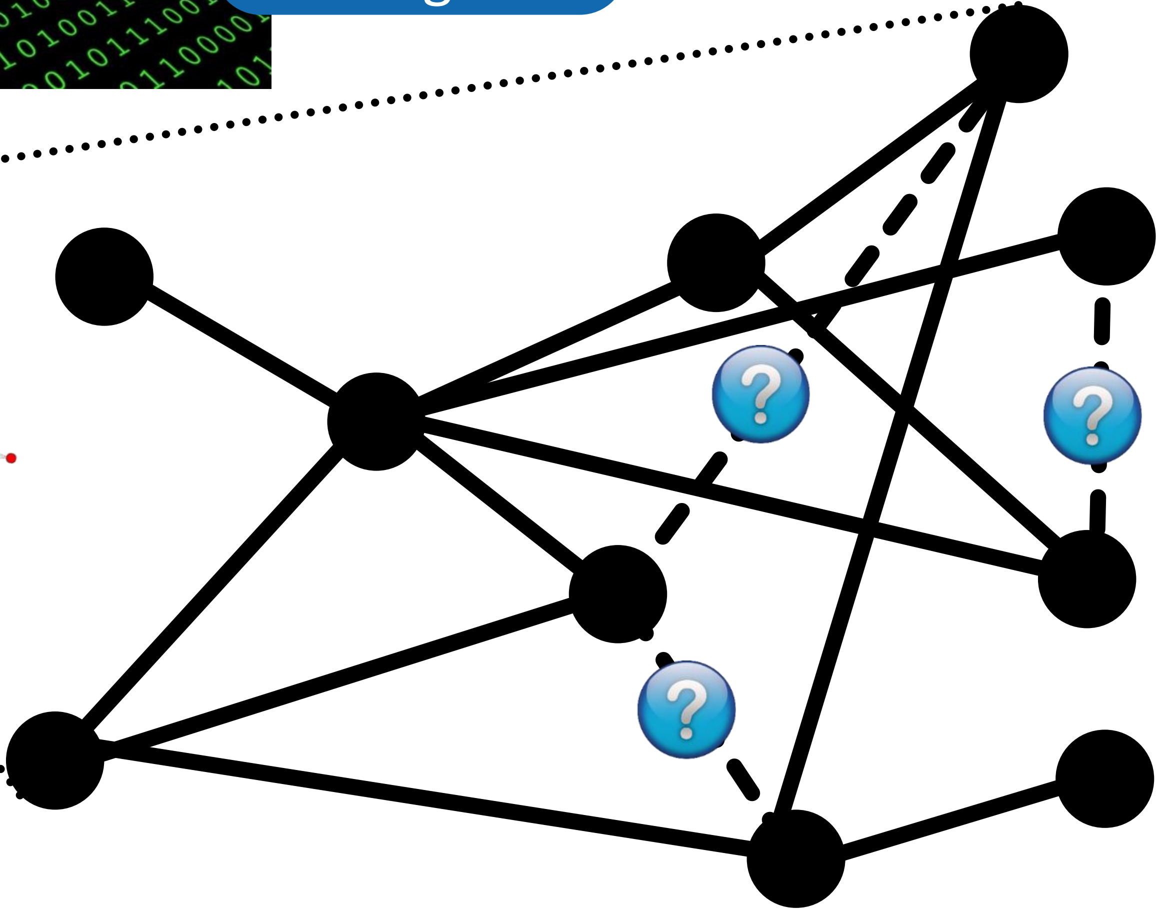
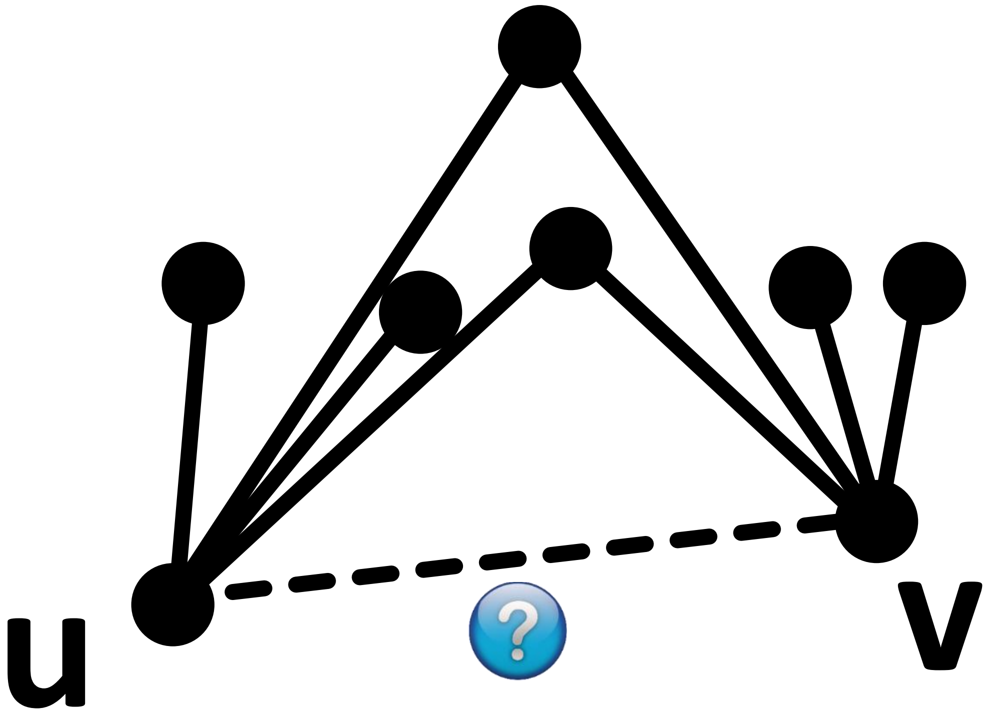


Reduce experiment costs

Warmup: Link Prediction



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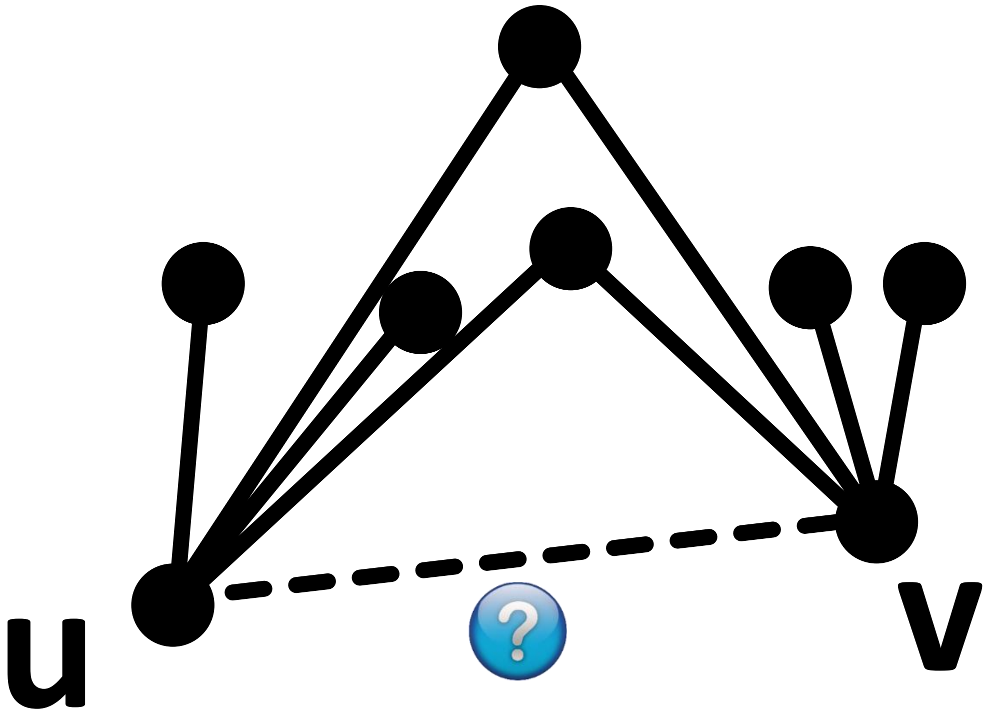

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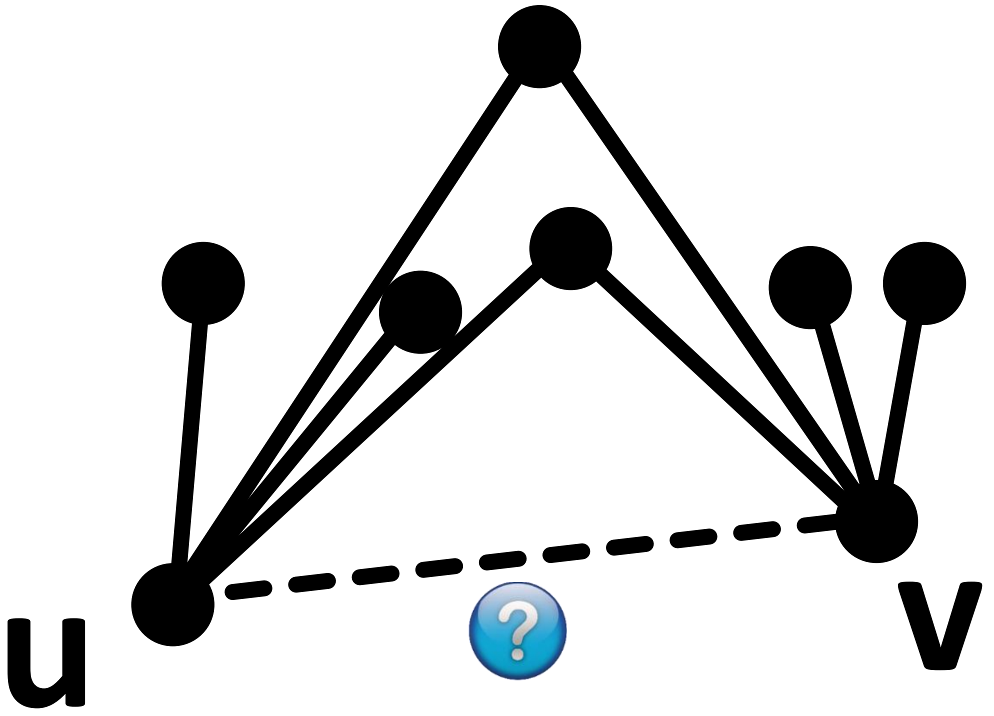

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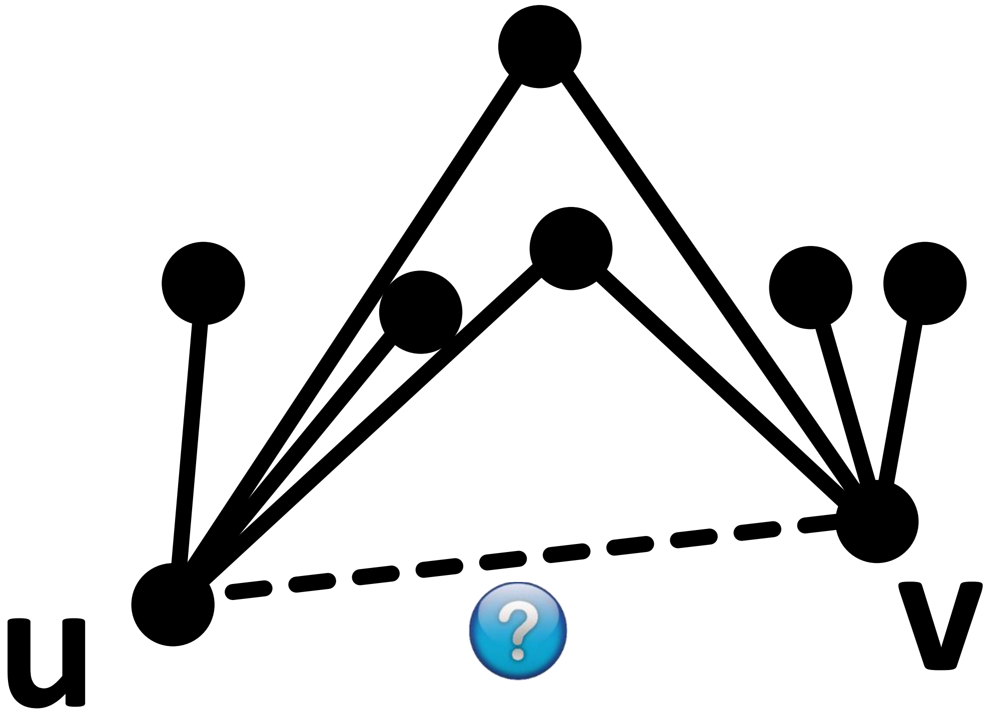

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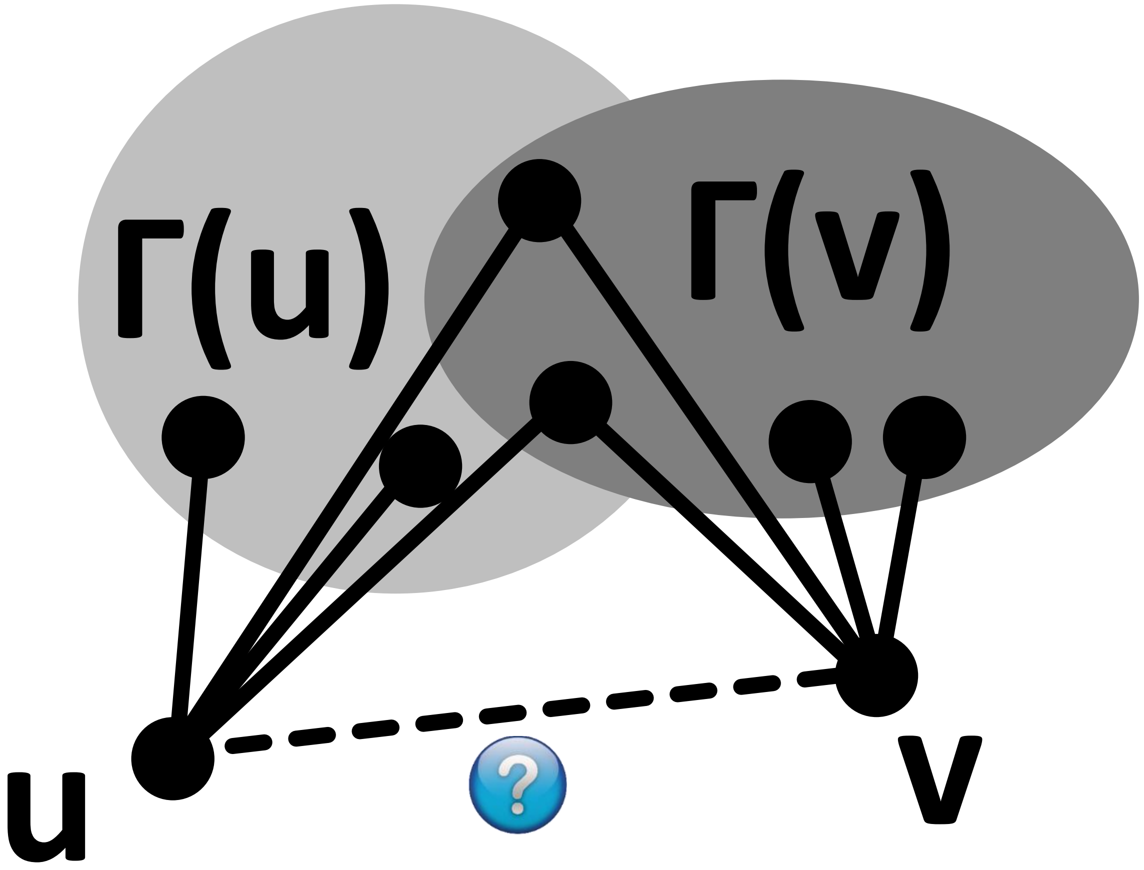

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One obtains a „score" s(e) = s(u,v) **for each (missing) link in a graph**

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

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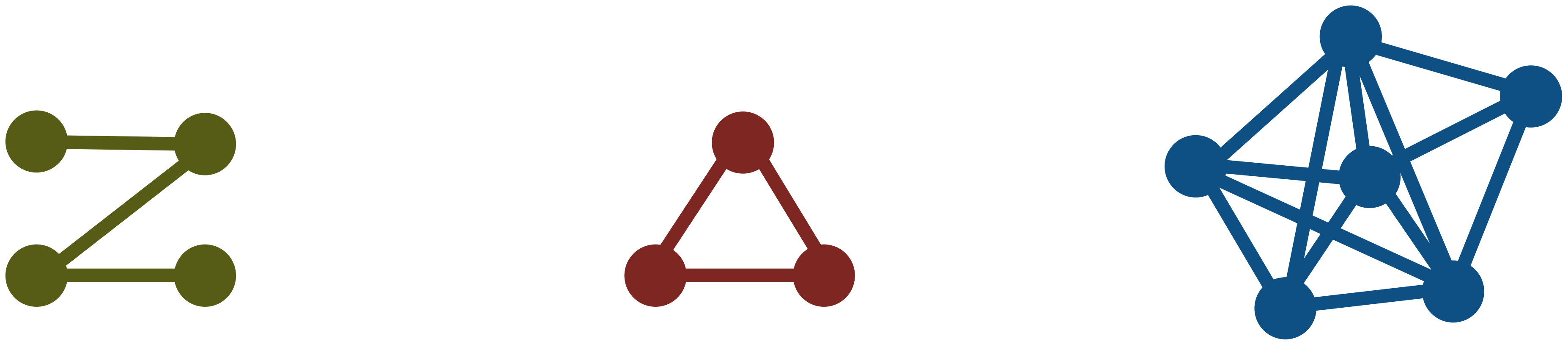

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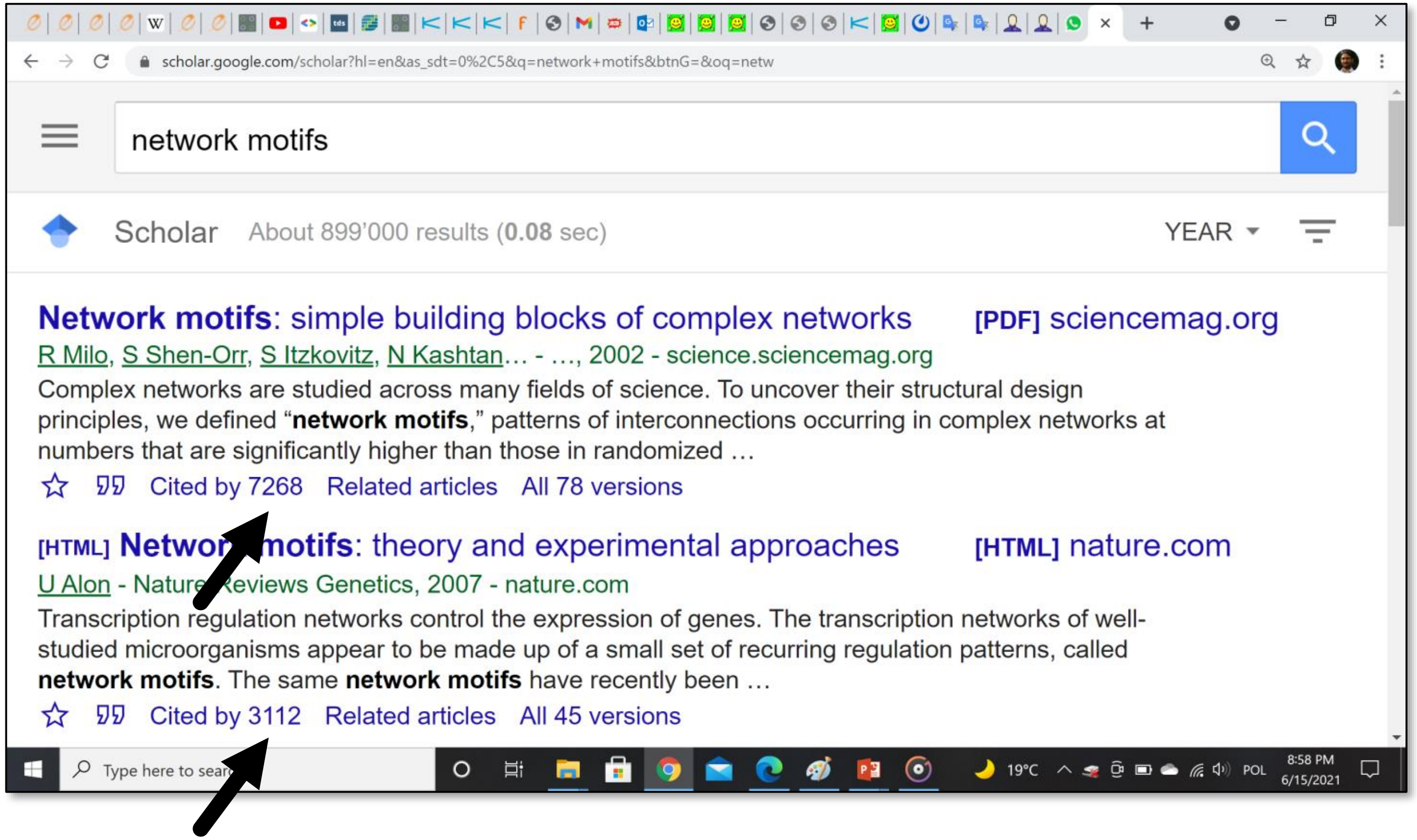

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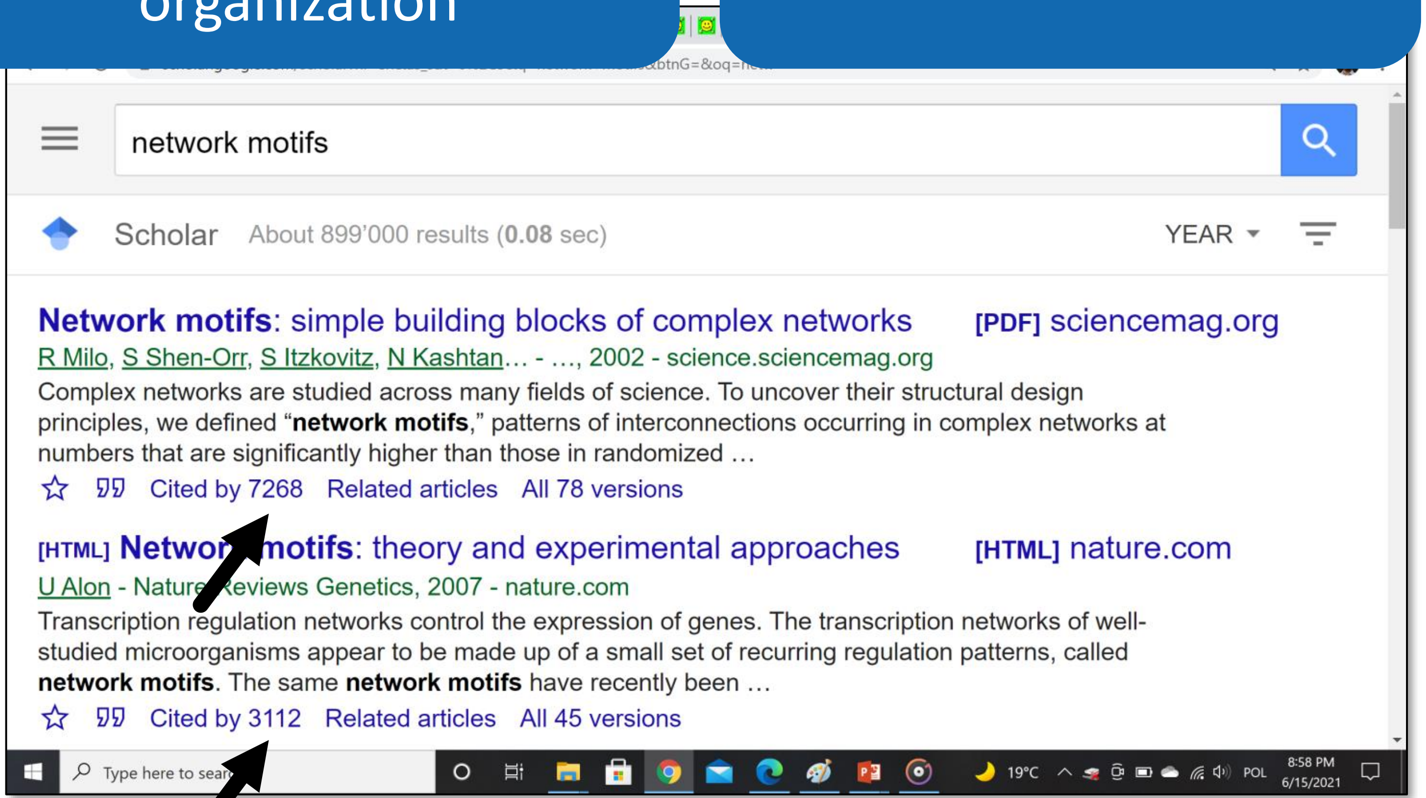
A lot of work into motifs exists, recent renewed interest under the theme „Higher-order network organization"

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



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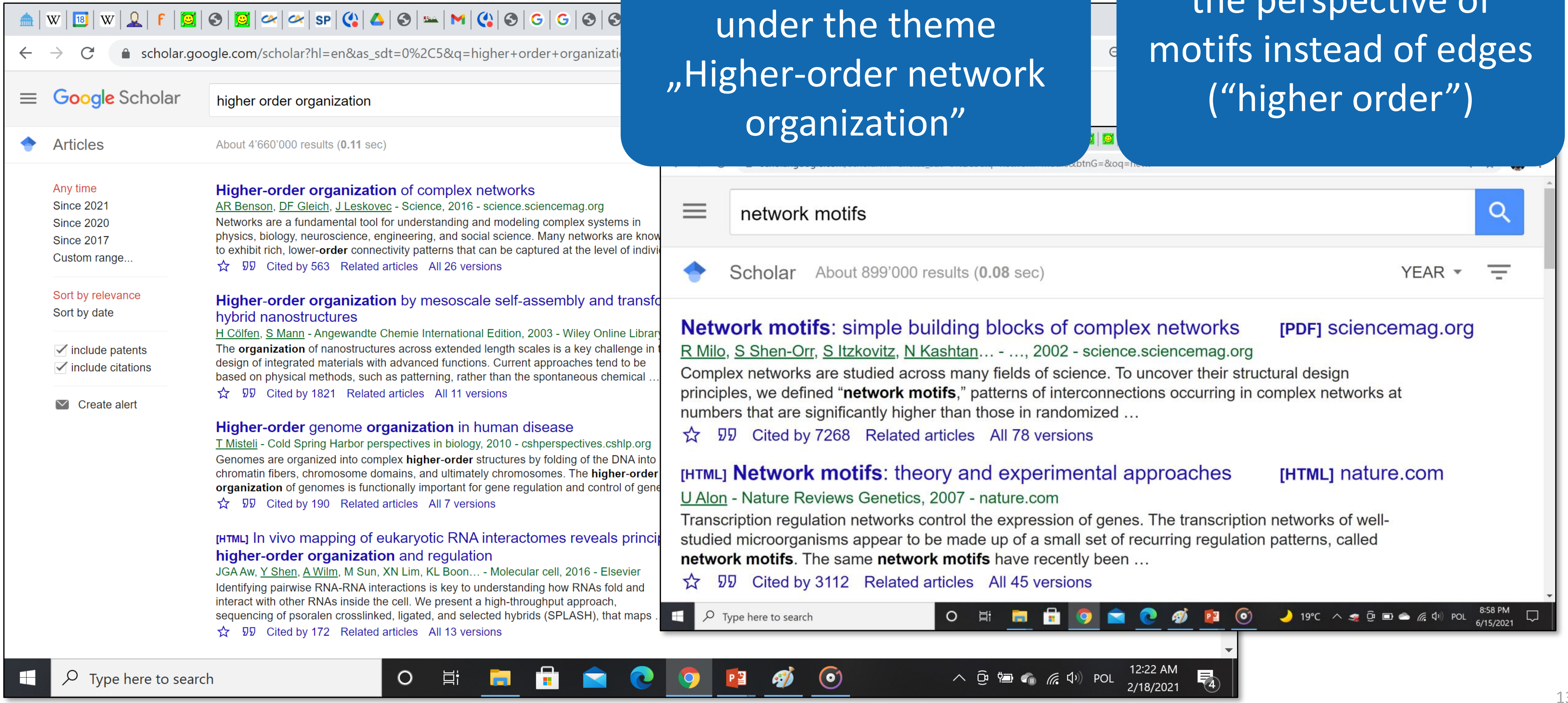

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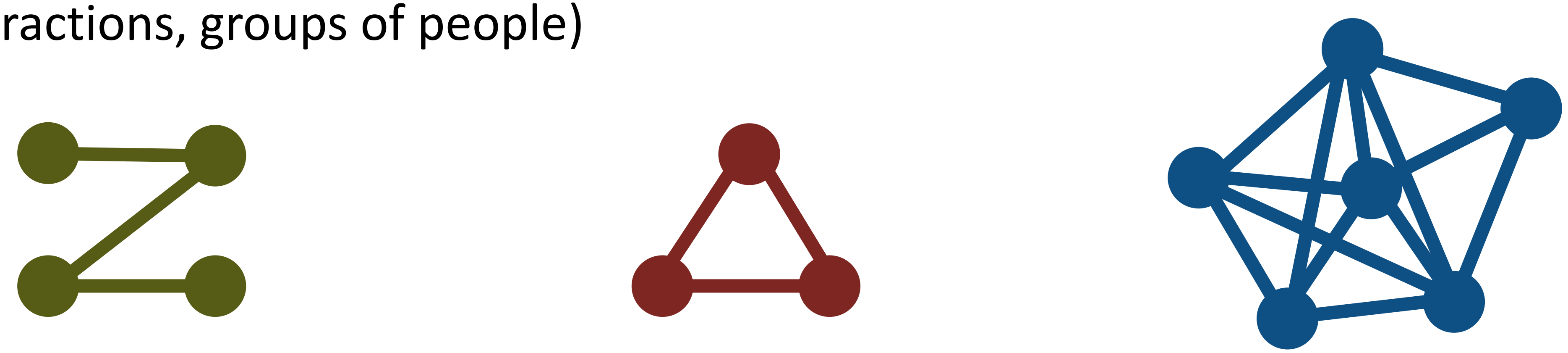

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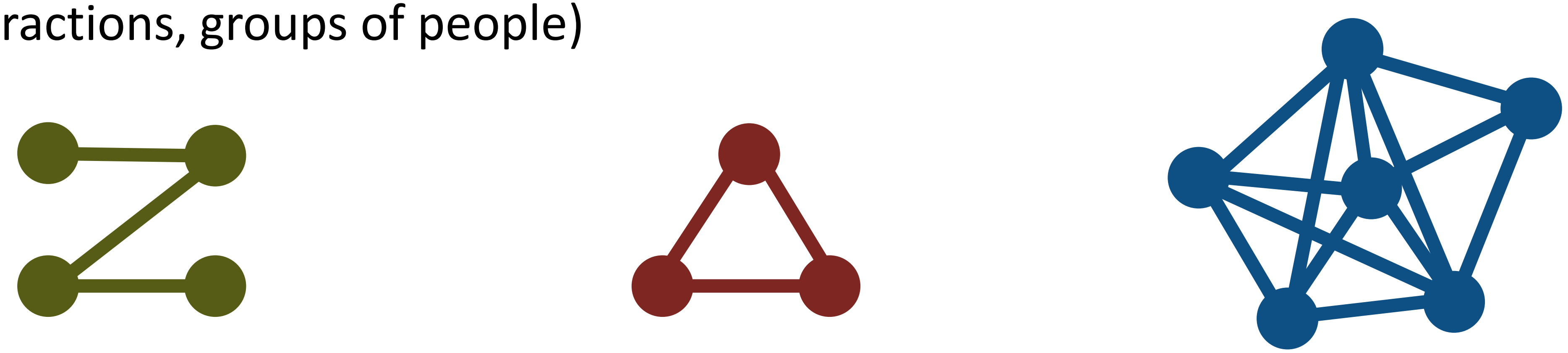

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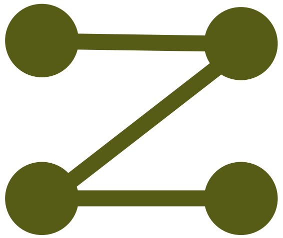

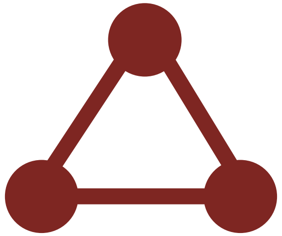

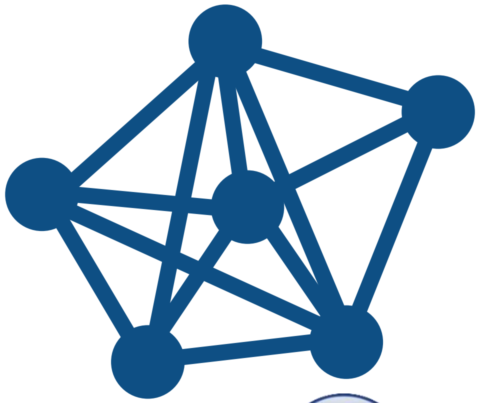

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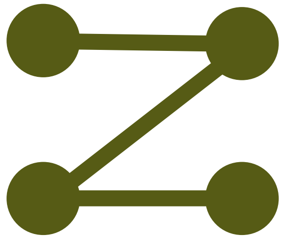

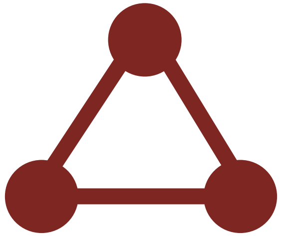

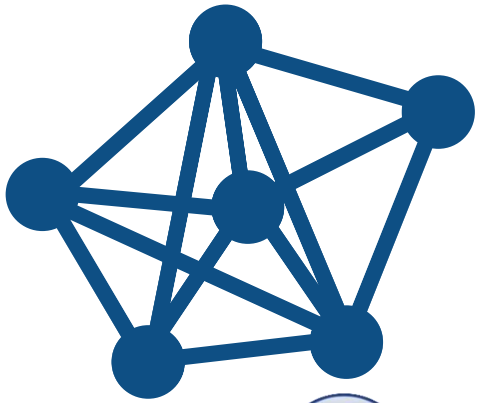

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General vision: assign some score to motifs (make them comparable)

Motifs with higher scores are more probable

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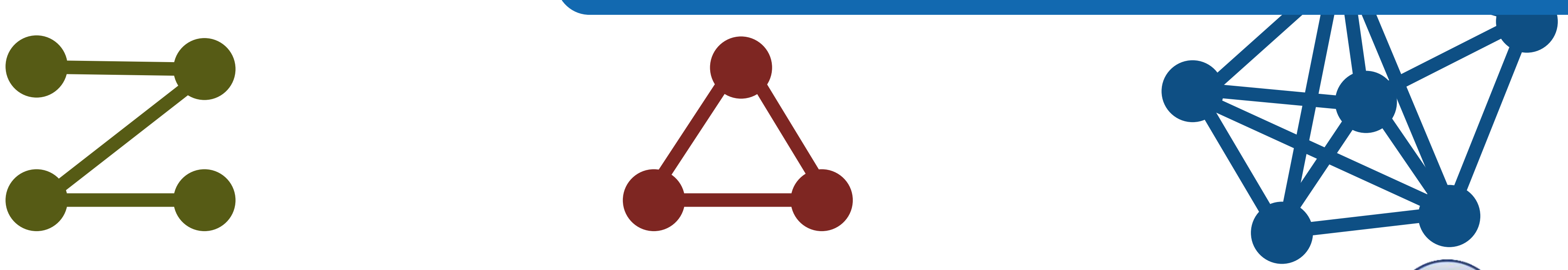

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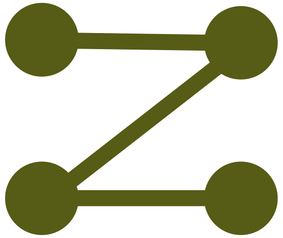

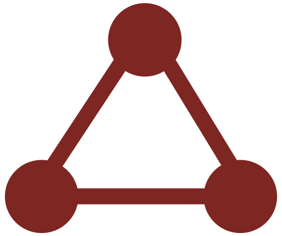

Let's go over them [1] ...

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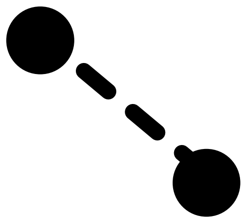

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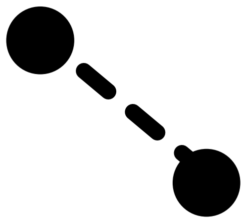

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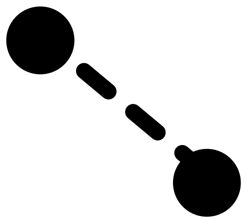

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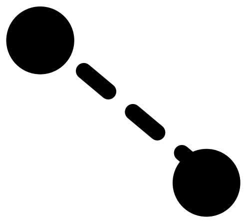

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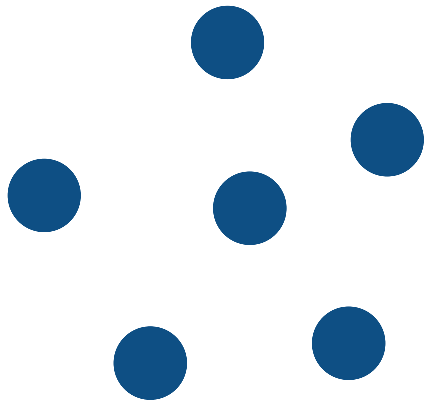

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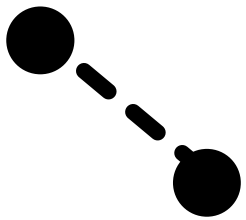

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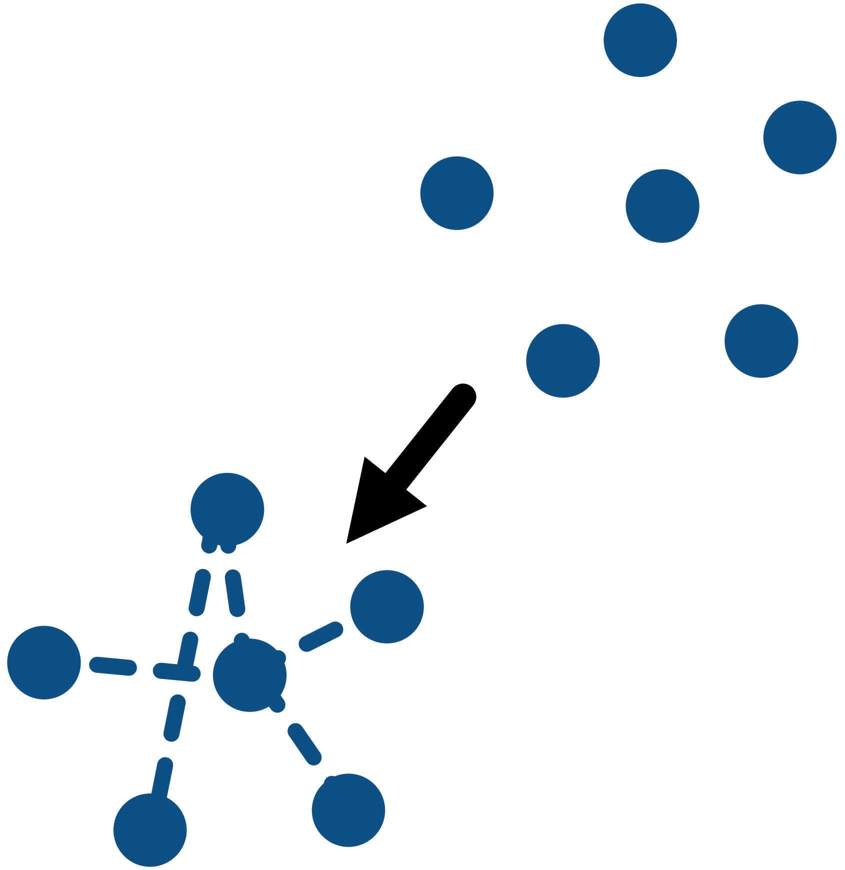

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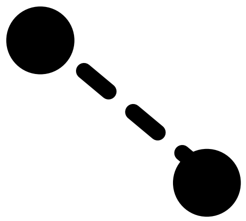

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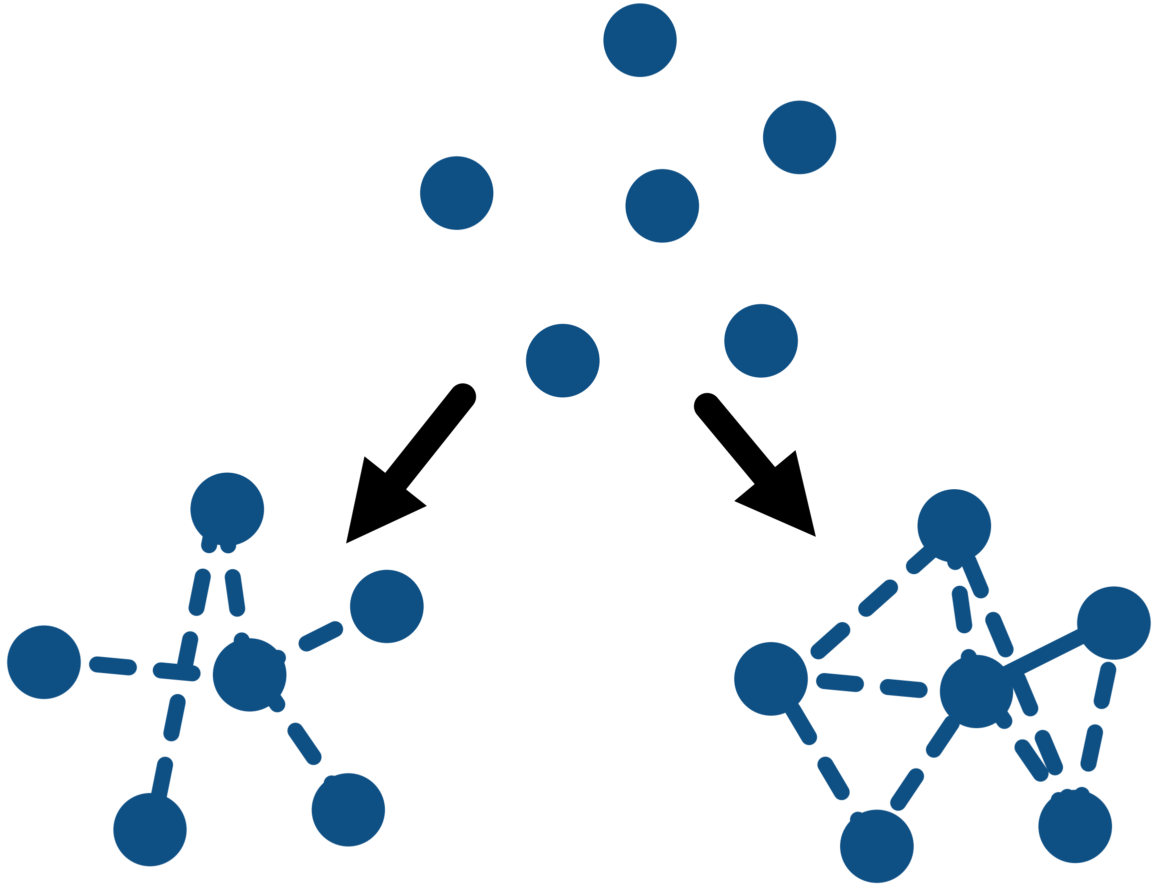

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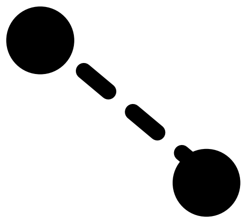

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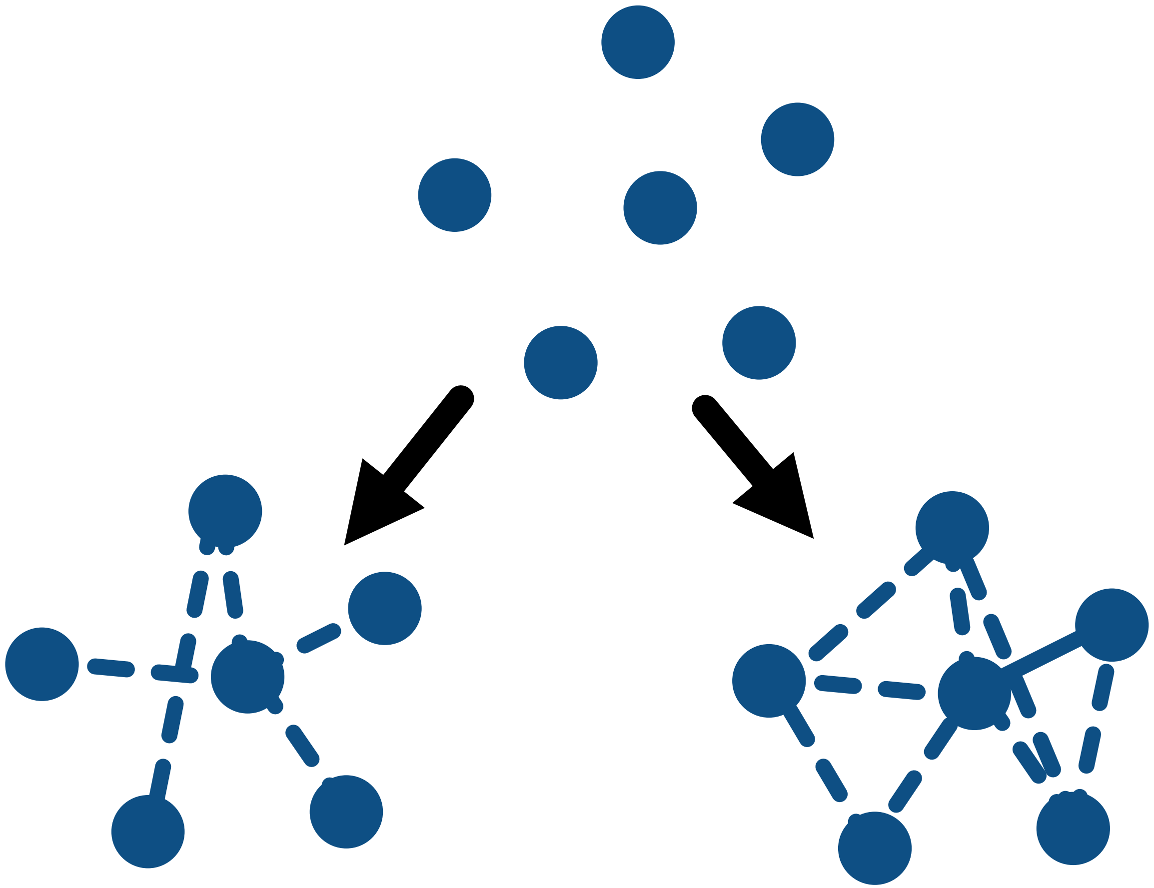

How to consider such diversity of possible patterns in score functions?

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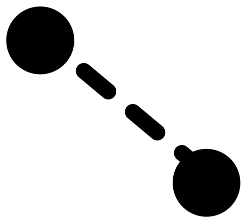

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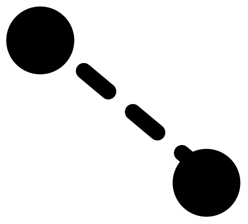

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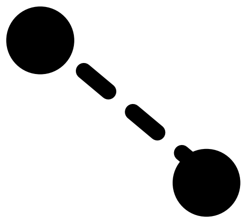

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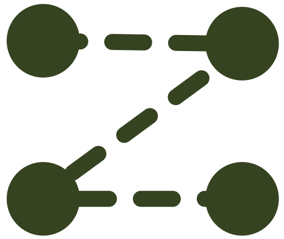

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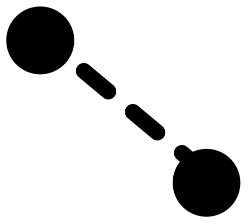
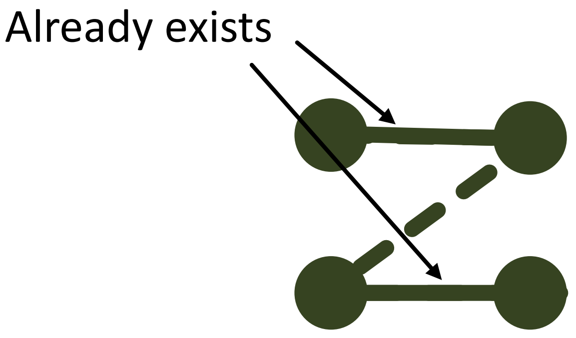


A link to be predicted does not exist

Motif prediction:



[1] M. Besta et al.: "Motif prediction with graph neural networks", KDD'22

Difference 2: Incoming Motifs May Have Existing Edge

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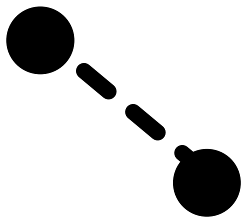

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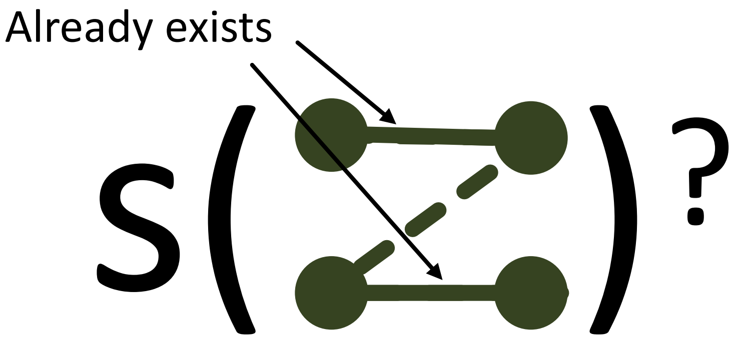

How to consider such edges in the score functions?

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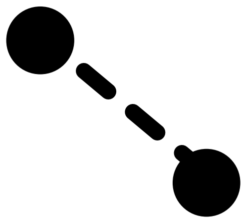

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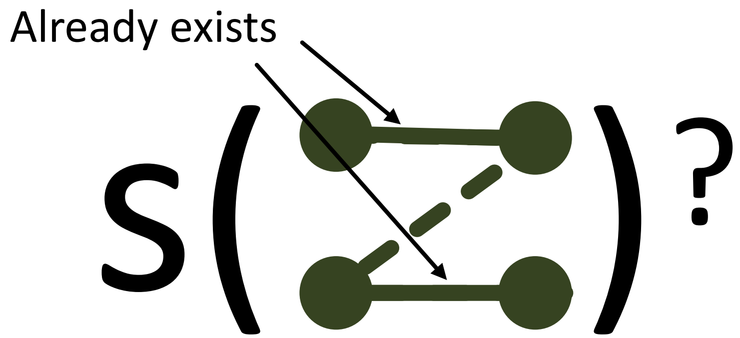

How to consider such edges in the score functions?

Example: some existing relationships in a group of people

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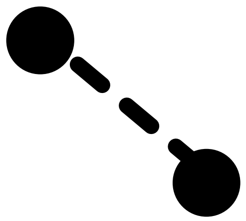
Difference 3: There May Be "Deal-Breaker" Edges

Link prediction:



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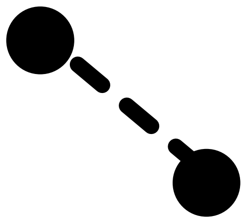

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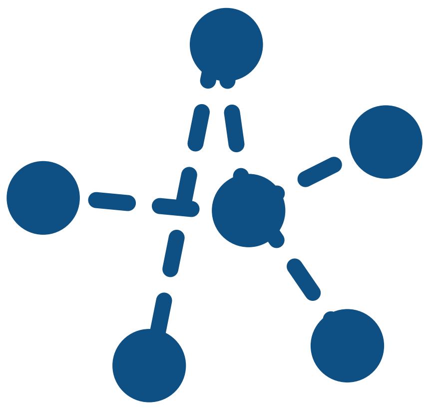

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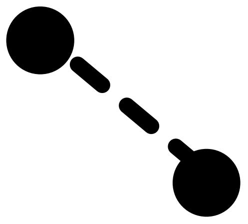
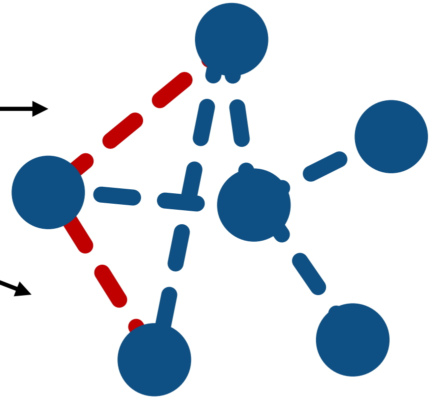


Motif prediction:

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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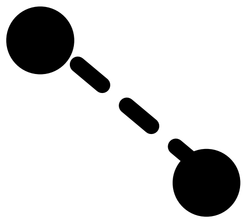

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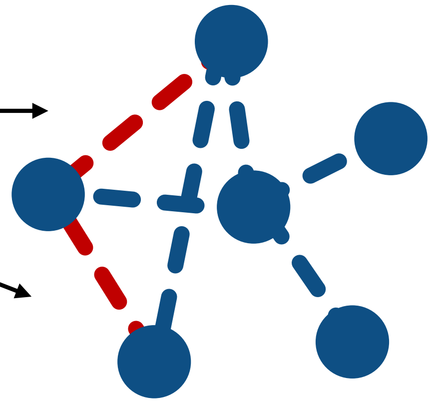

Example:
chemical bonds

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

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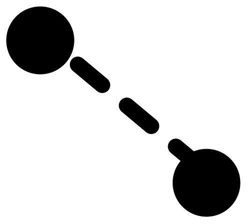

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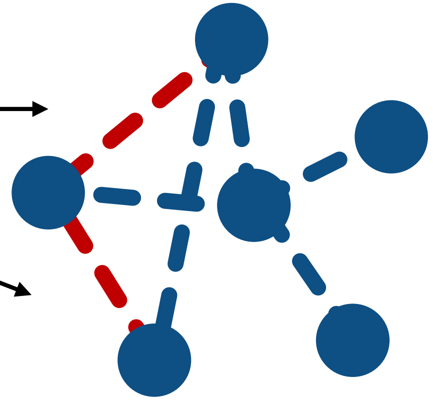

How to consider such edges in the score functions?

Example: chemical bonds

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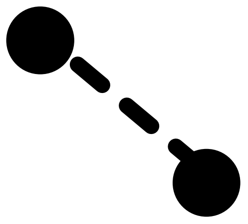
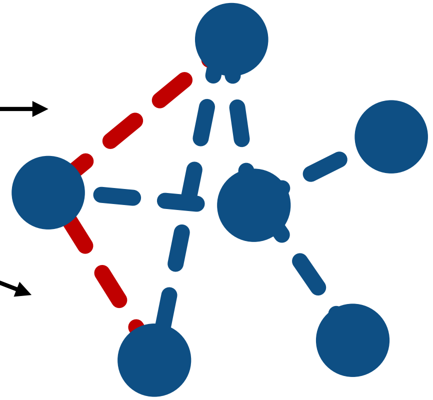


No such effect (a link to be predicted is never a „deal breaker")

Motif prediction:

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



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Difference 4: Motif Prediction Query May Depend on Vertex Labeling

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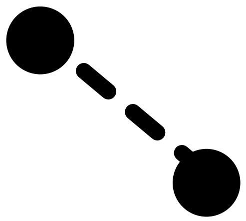

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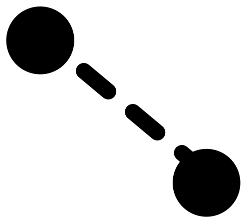

Motif prediction:

We want **this**:

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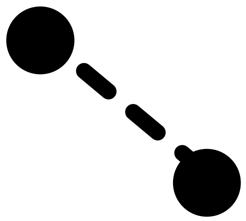

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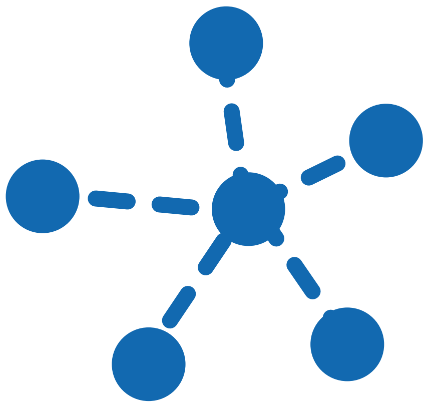

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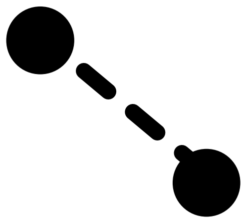

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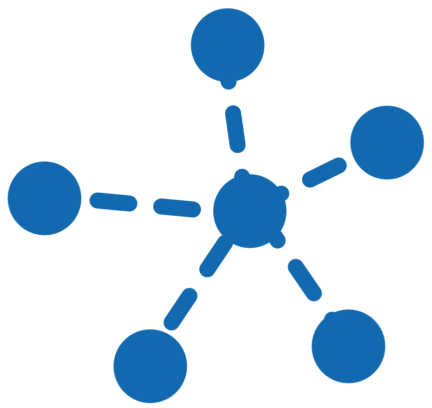
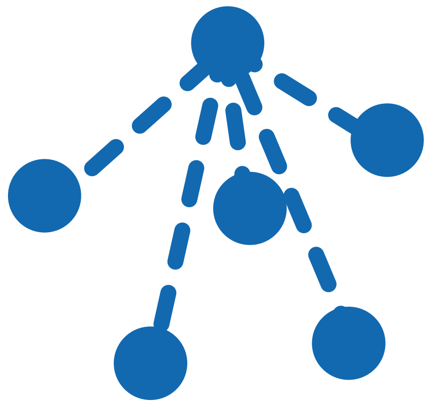


...but **not** this:



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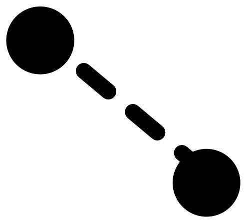

No such effect (not enough room with a single link)

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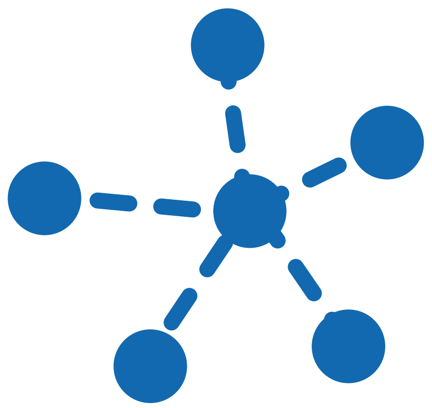

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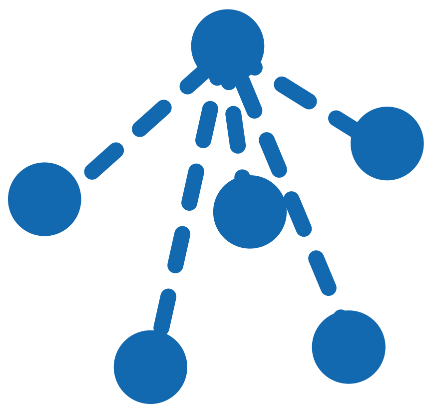

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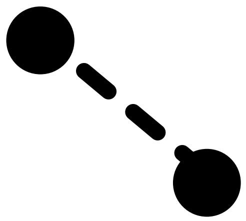

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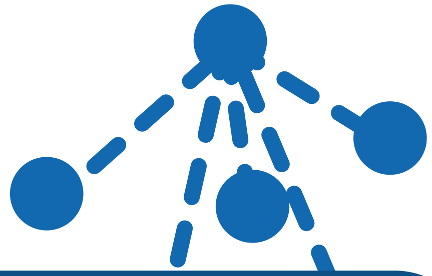

How to formulate motif prediction, considering all these differences?

[1] M. Besta et al.: "Motif prediction with graph neural networks", KDD'22

Motif Prediction Score Functions

Starting Simple: Motif Scores Based on Independent Links

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Motif Prediction Score Functions

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

Starting Simple: Motif Scores Based on Independent Links

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

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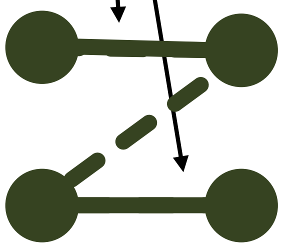

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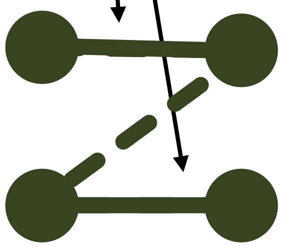

$$s_\perp(M) = \prod_{e \in E_{M,\mathcal{N}}} s(e)$$

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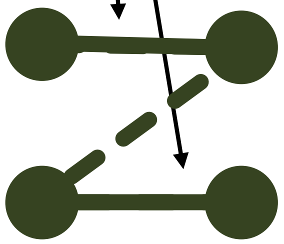

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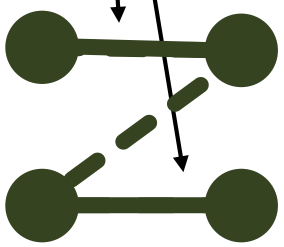
s(e) is any link prediction score which outputs into [0, 1] (e.g., Jaccard)



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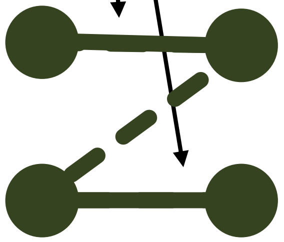

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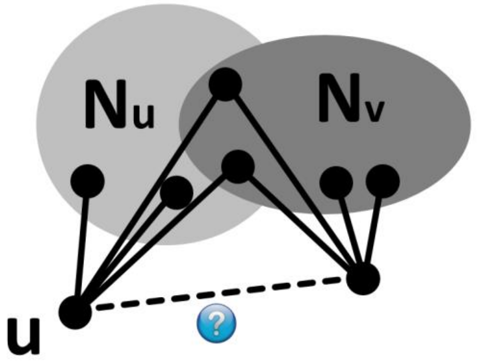

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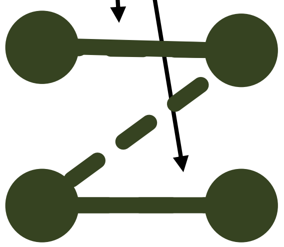

Starting Simple: Motif Scores Based on Independent Links

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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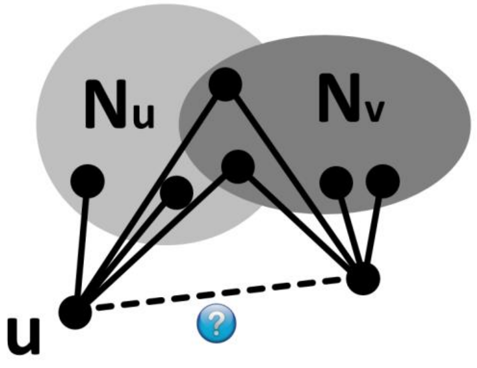

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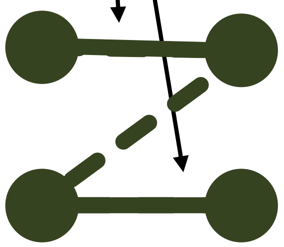

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For edges that already exist, we set s(e) = 1 (i.e., we assume that a motif is more likely to appear if the edges that participate in that motif are also more likely)

$$s_\perp(M) = \prod_{e \in E_{M,\mathcal{N}}} s(e)$$

∈ [0, 1] by construction

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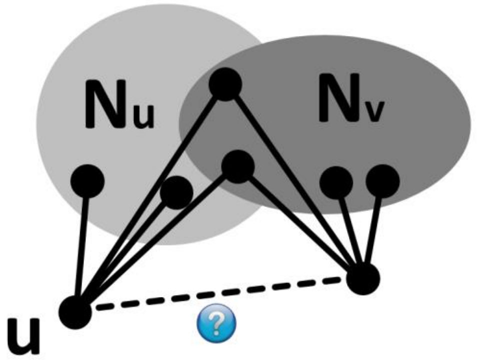

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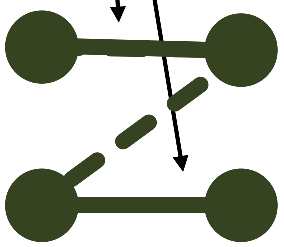
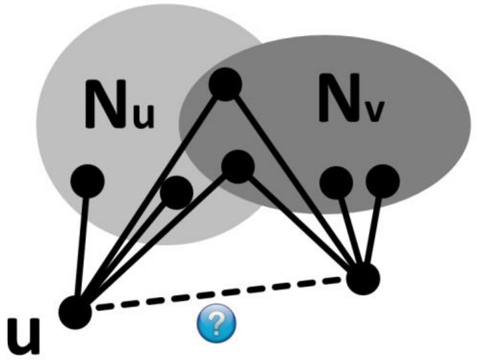


Example heuristic for the Jaccard score s(e) for links:



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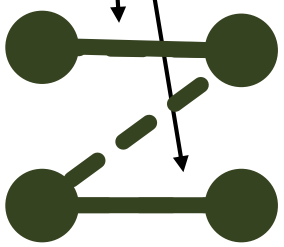
Starting Simple: Motif Scores Based on Independent Links

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

Motif edges that do **not** yet exist

Motif edges that **already** exist



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)

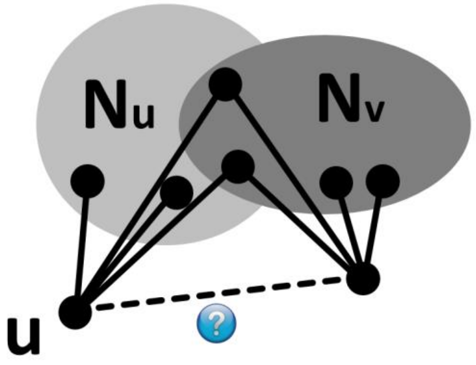
$$s_{\perp}(M) = \prod_{e \in E_{M,\mathcal{N}}} s(e)$$

∈ [0, 1] by construction

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

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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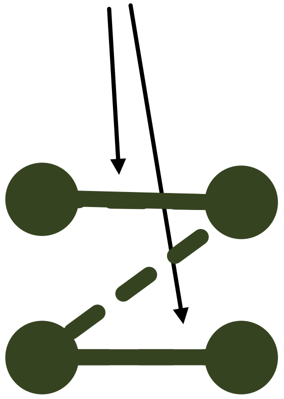
Motif edges that do **not** yet exist

Motif edges that **already** exist



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Motif Prediction Score Functions

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

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

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

Motif edges that do **not** yet exist

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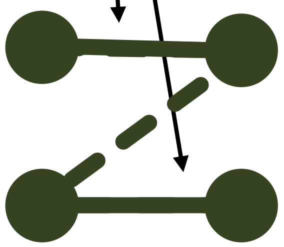

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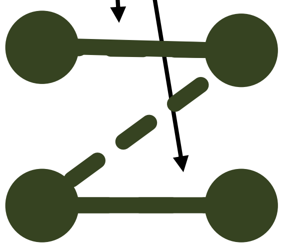
Motif edges that do **not** yet exist

Motif edges that **already** exist

Adding correlation between links



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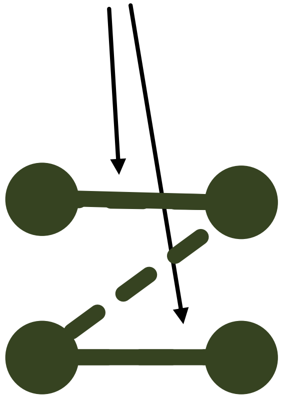

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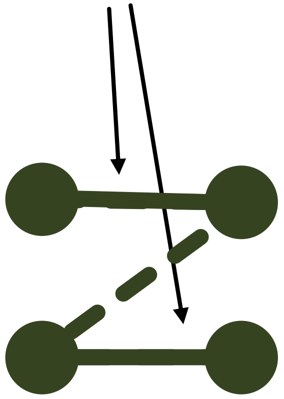

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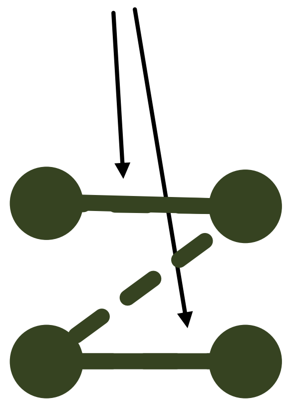

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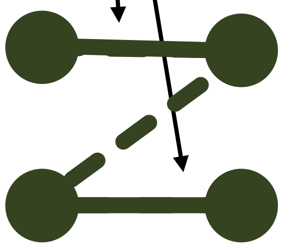

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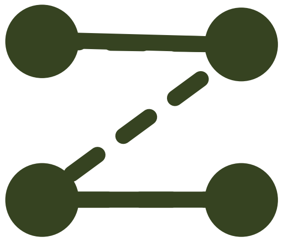

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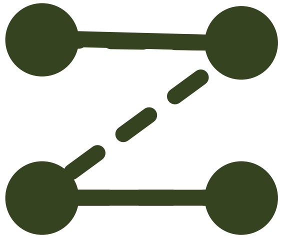

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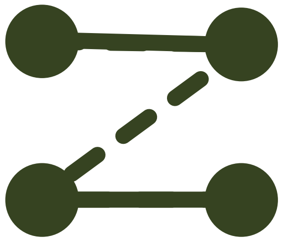

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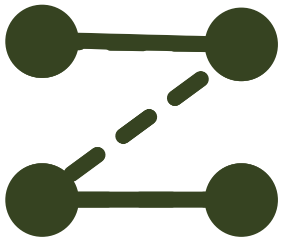

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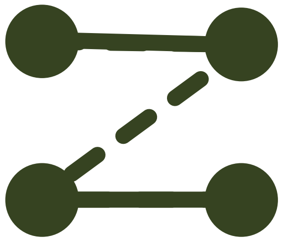

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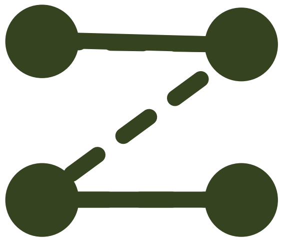

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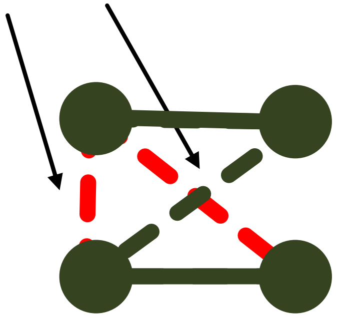

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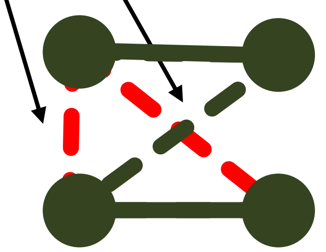

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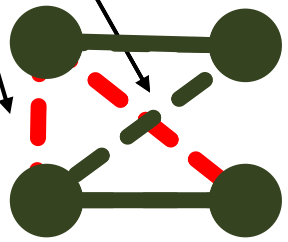

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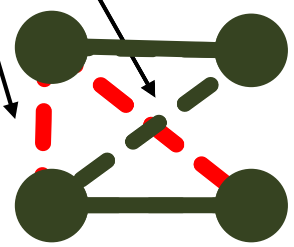

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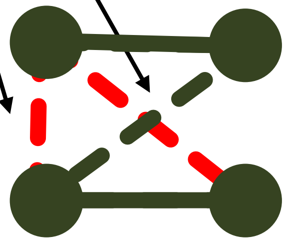

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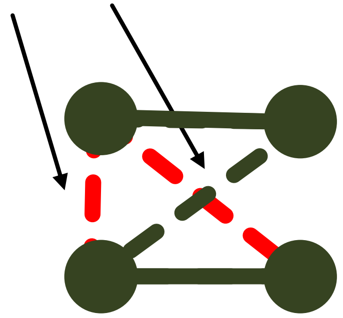

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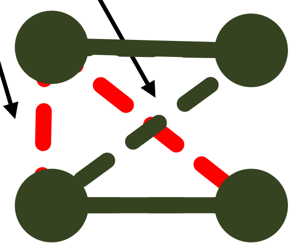

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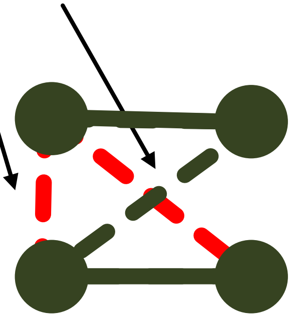

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[1] M. Besta et al.: "Motif prediction with graph neural networks", KDD'22

[2] M. Zhang et al.: "Link Prediction Based on Graph Neural Networks", NeurIPS'18

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How does deep learning work?

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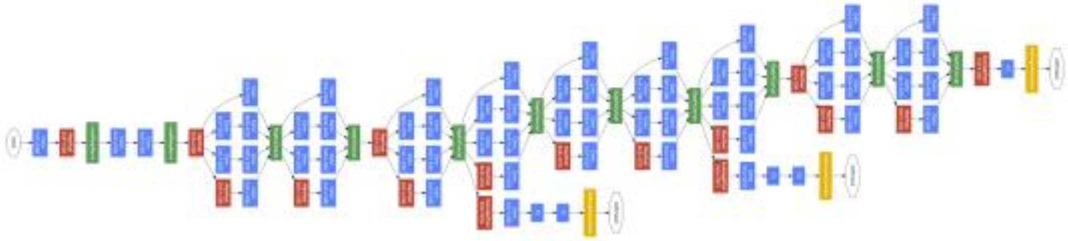

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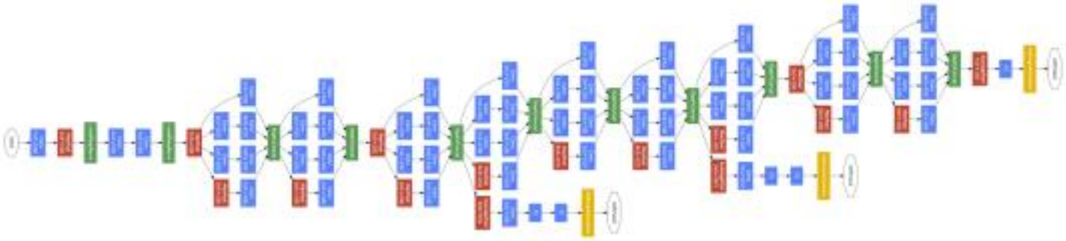

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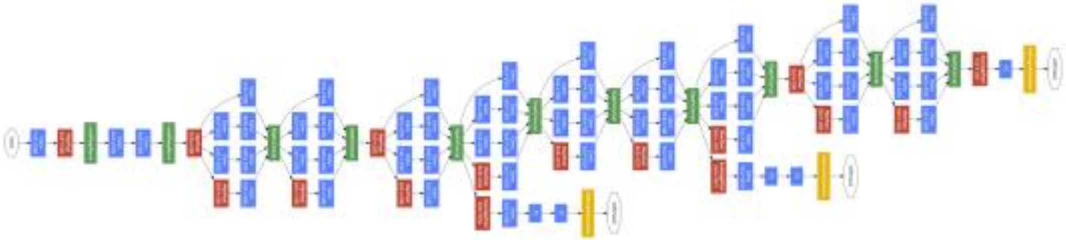

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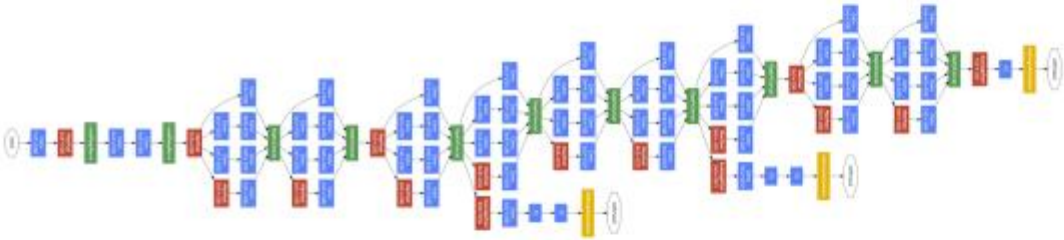

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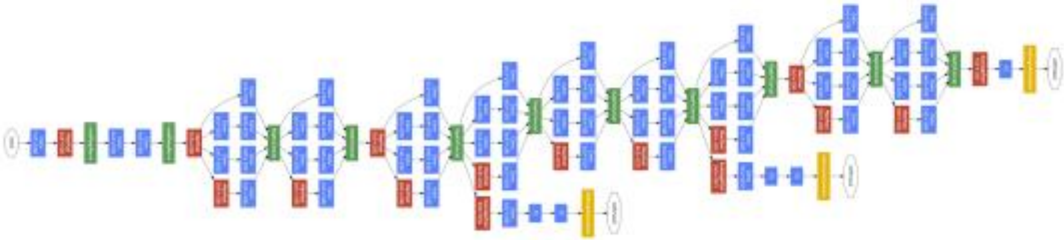

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Dog	0.28
Airplane	0.07
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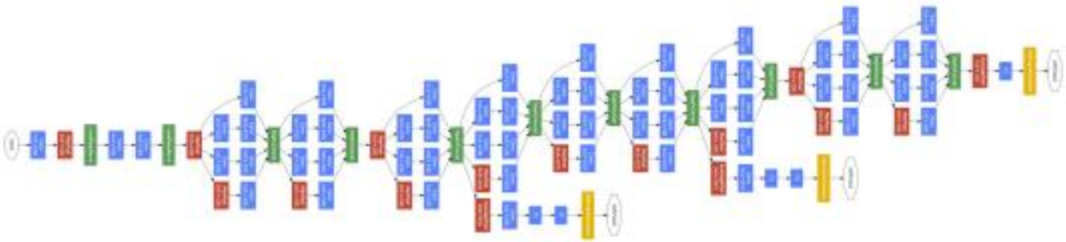

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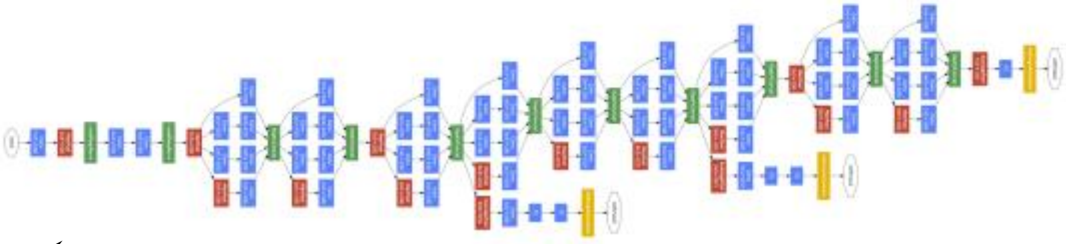

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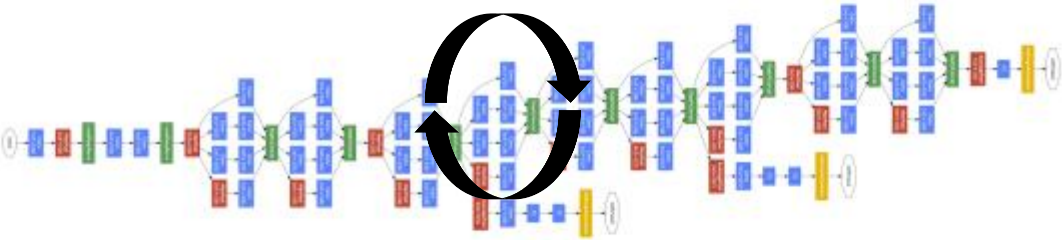

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Motif Prediction: Deep Learning Formulation

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

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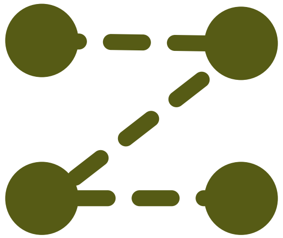
Goal: predict this motif M:



Motif Prediction: Deep Learning Formulation

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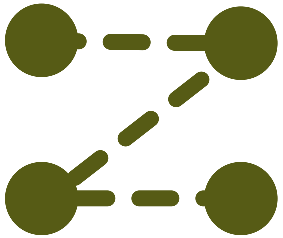

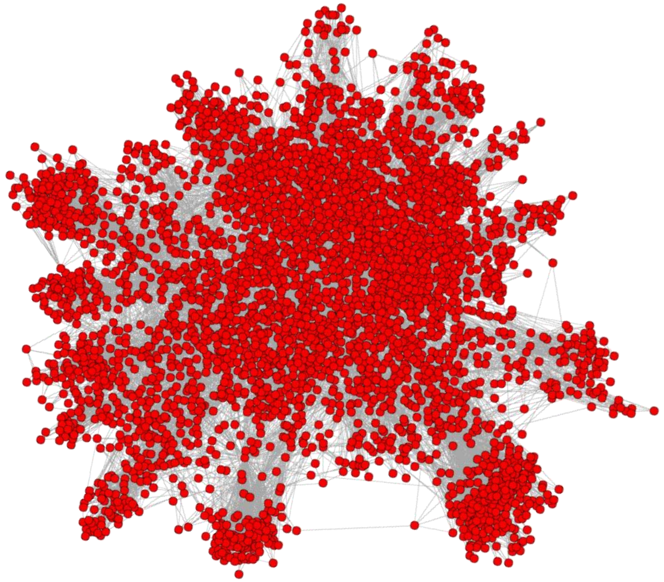

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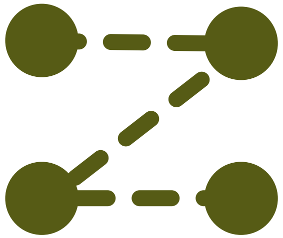
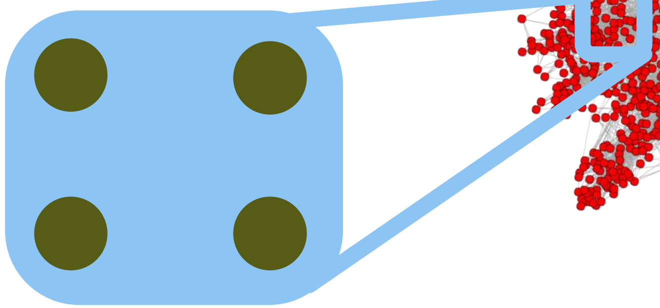
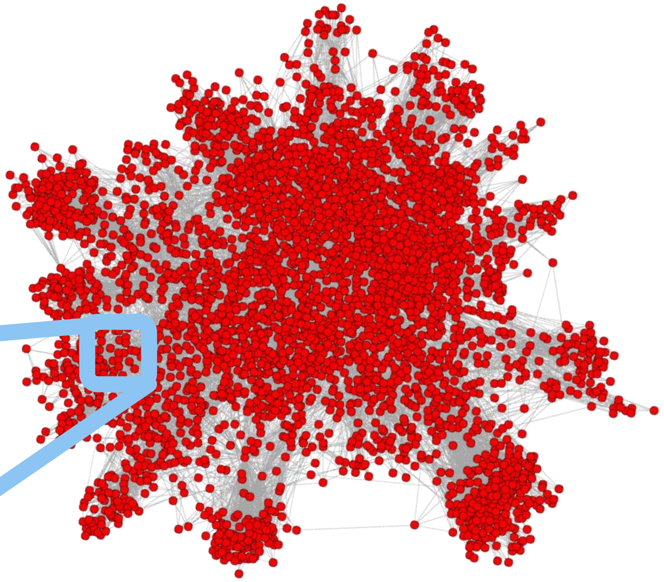


A given fixed set of vertices:





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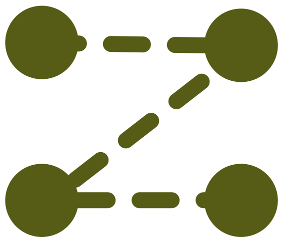
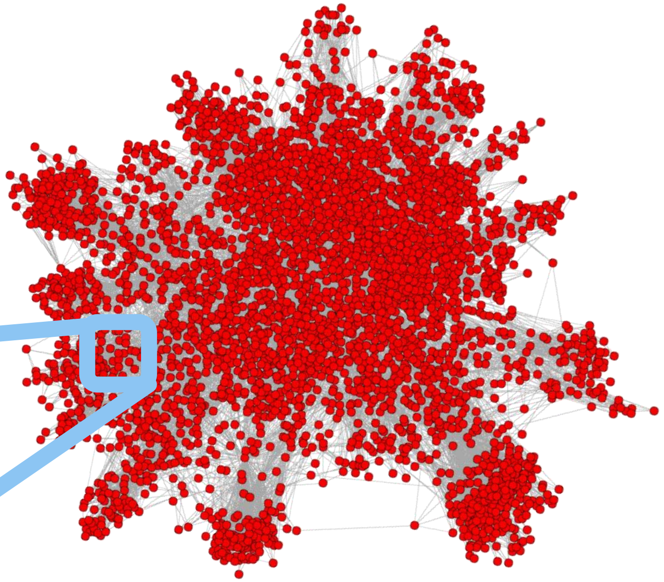


Positive samples



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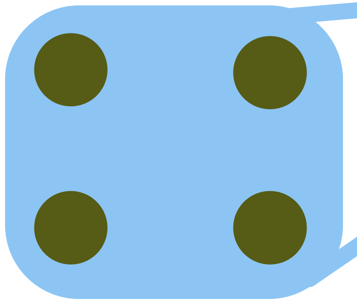

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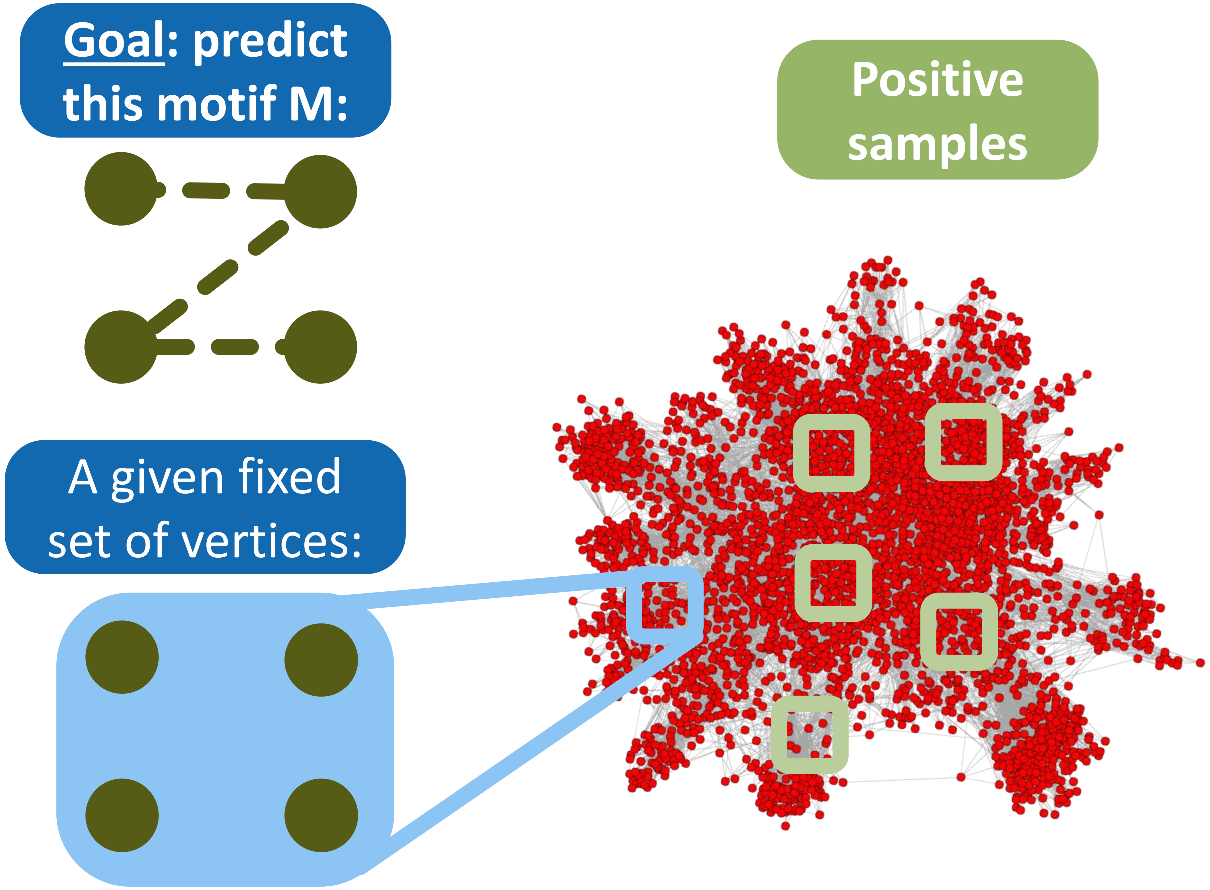

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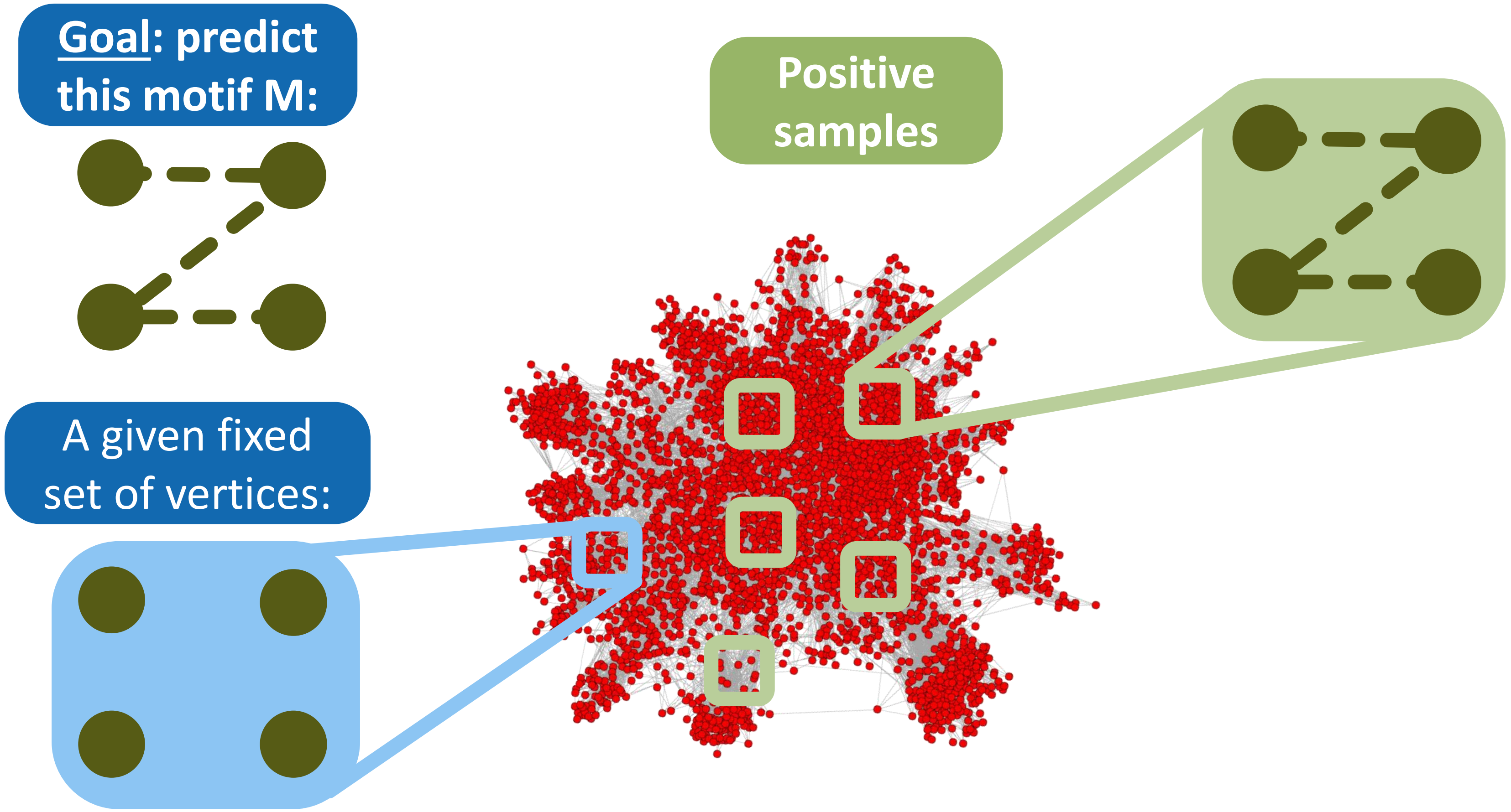

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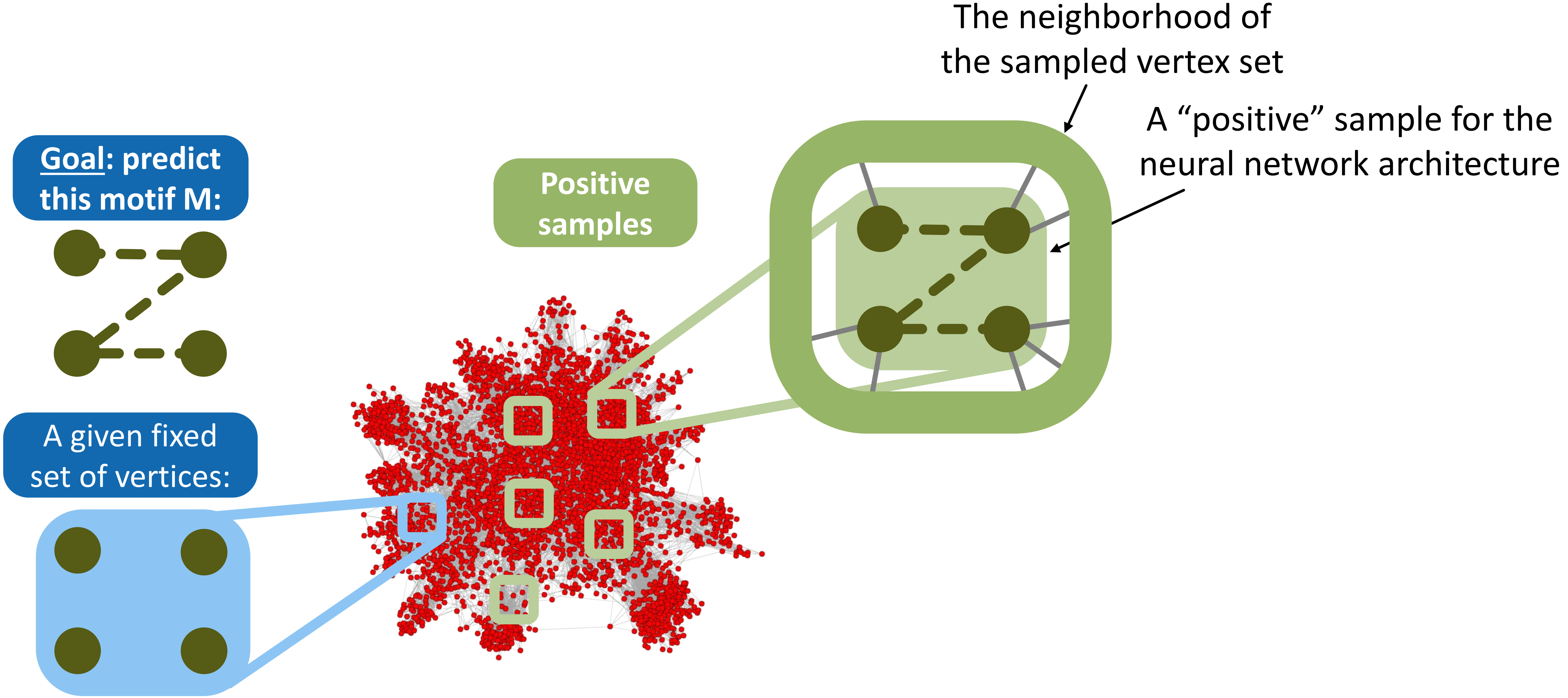

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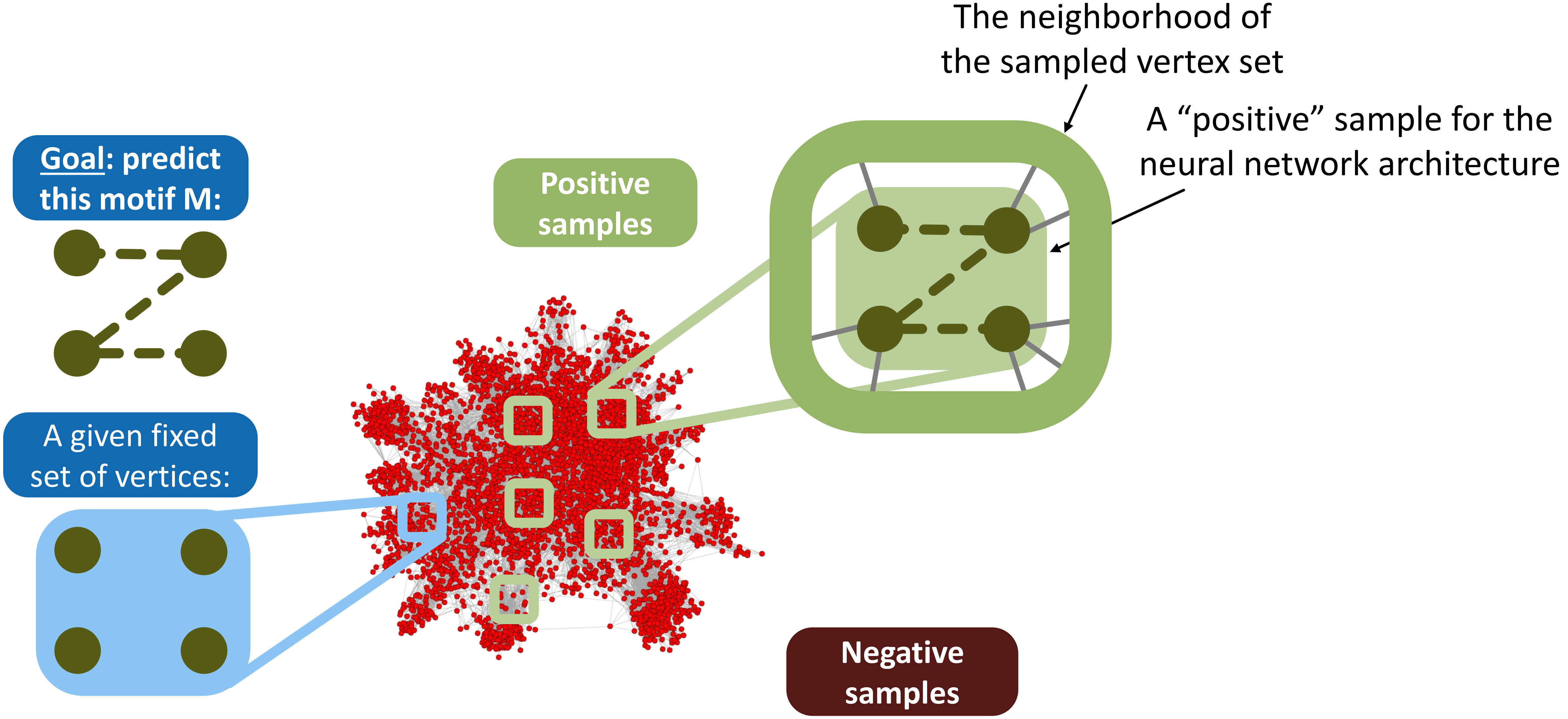

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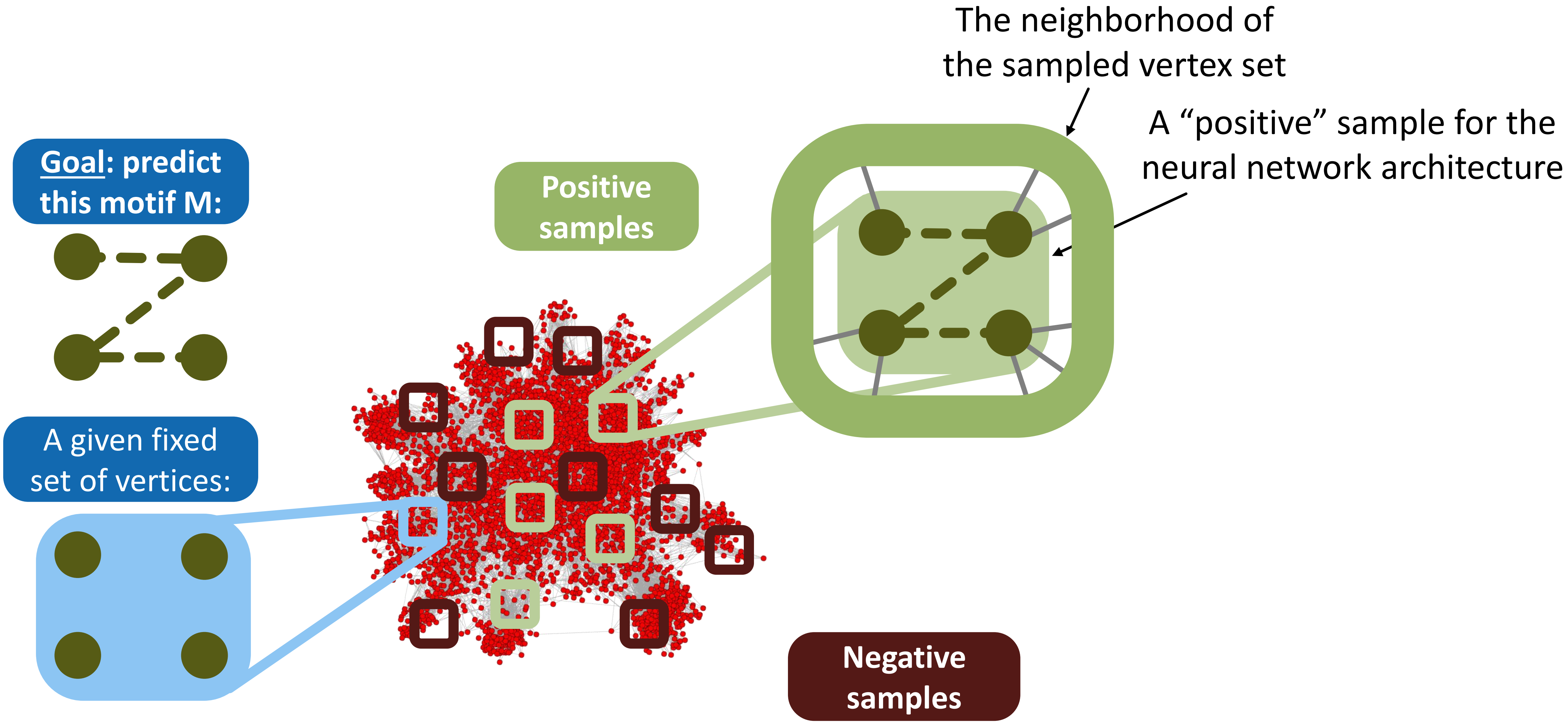

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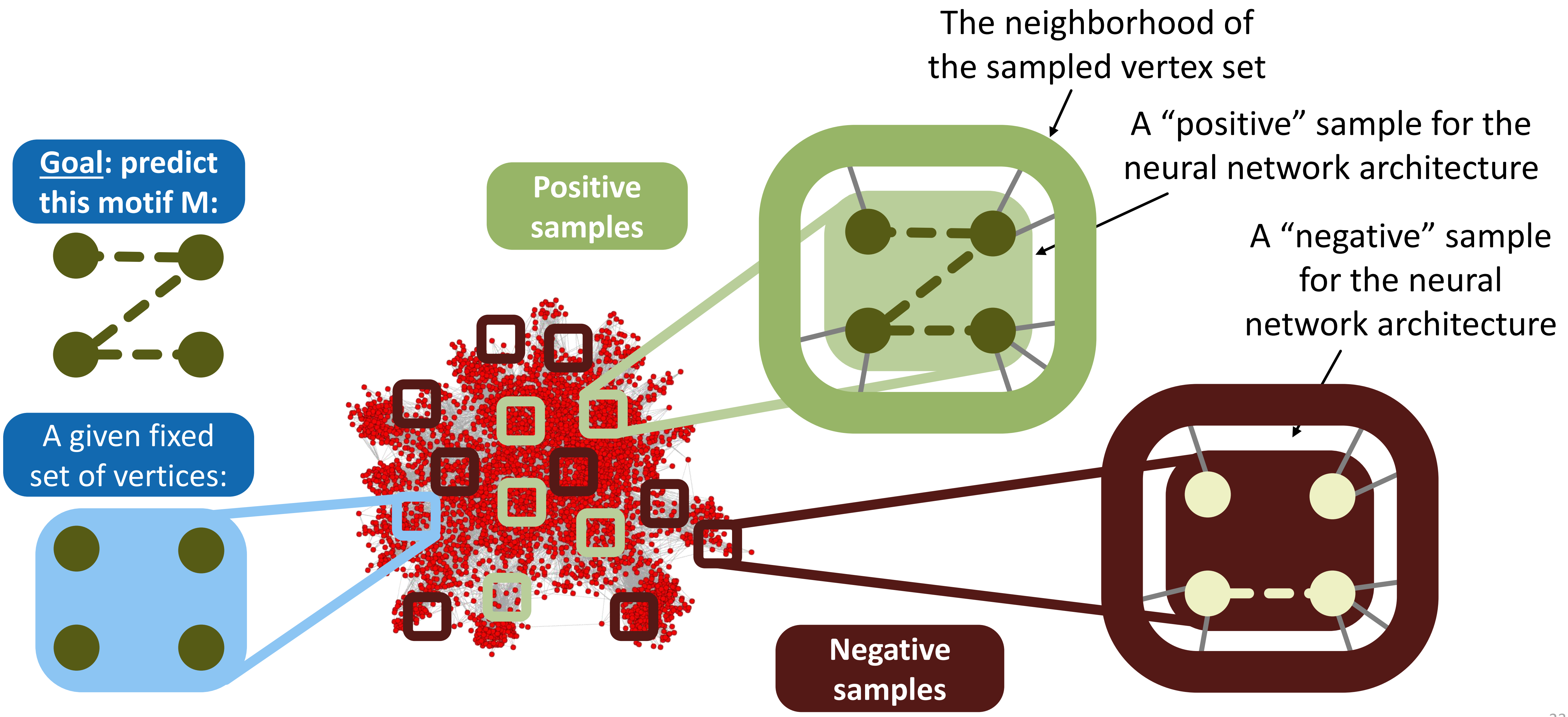
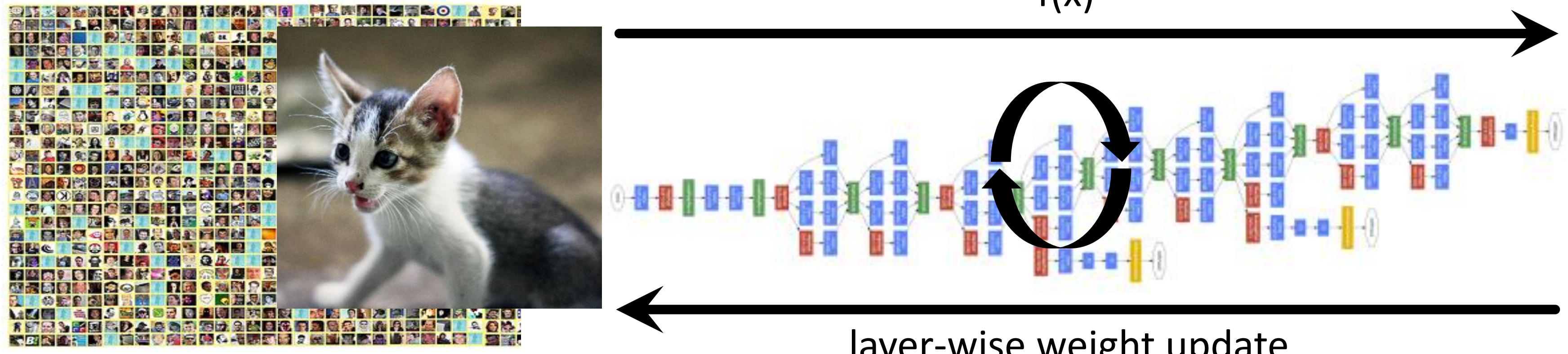
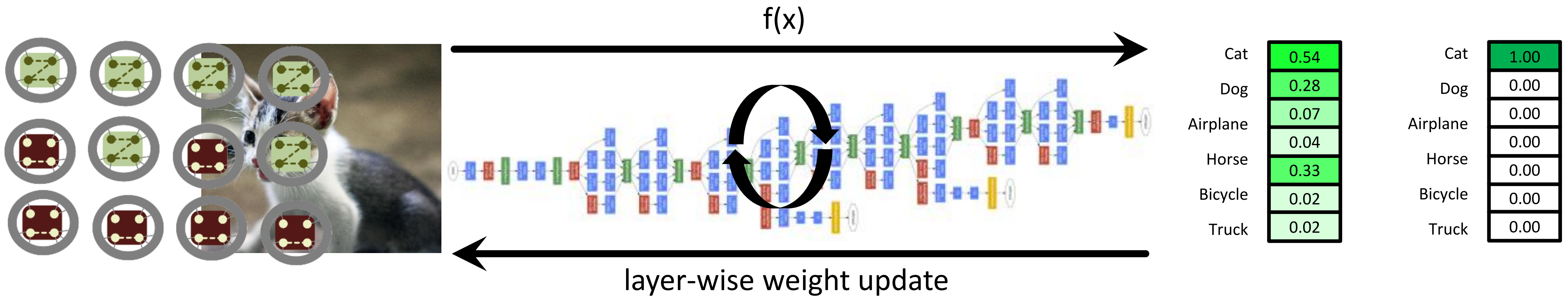


Motif Prediction: Deep Learning Formulation



Cat	0.54	1.00
Dog	0.28	0.00
Airplane	0.07	0.00
	0.04	0.00
Horse	0.33	0.00
Bicycle	0.02	0.00
Truck	0.02	0.00

Motif Prediction: Deep Learning Formulation



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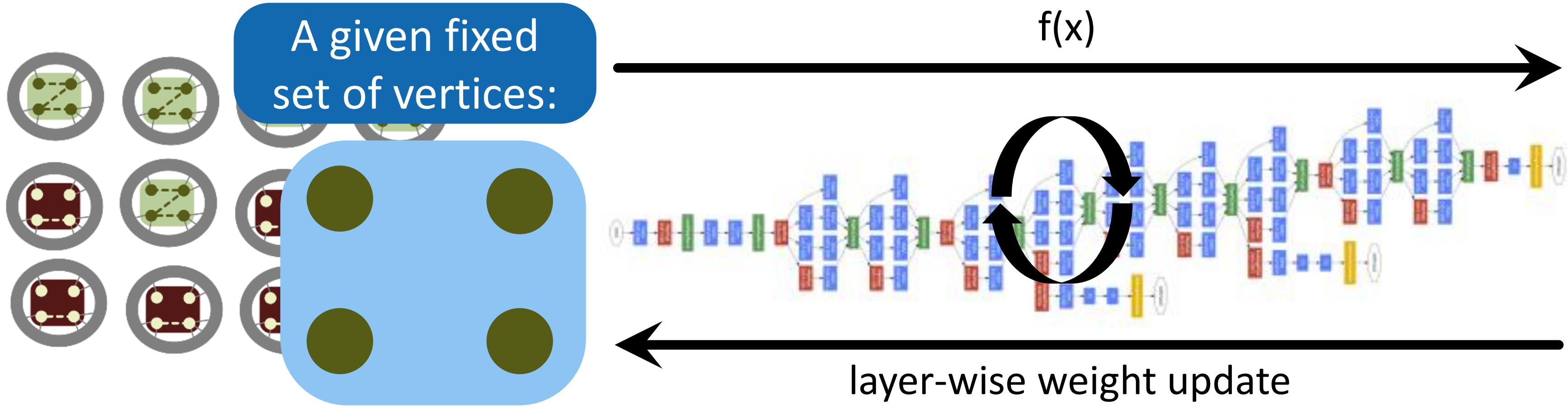

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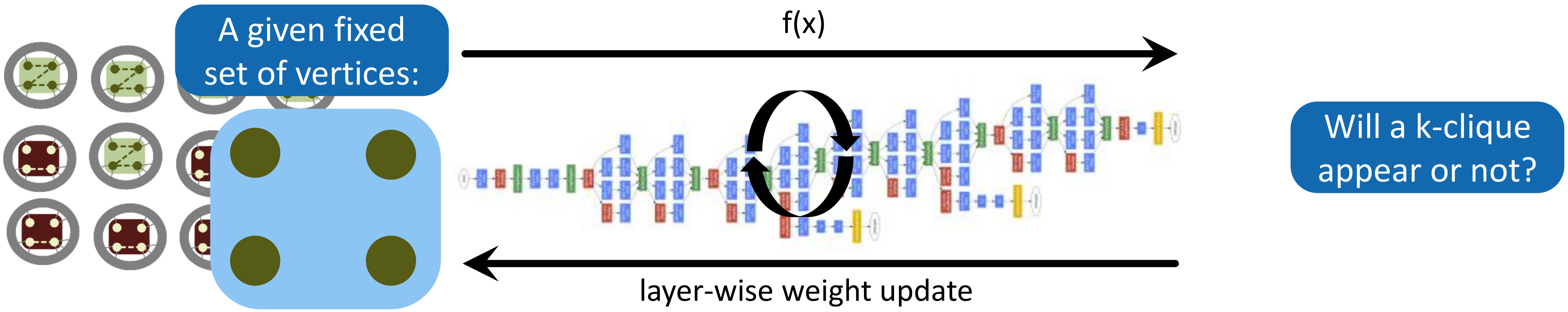
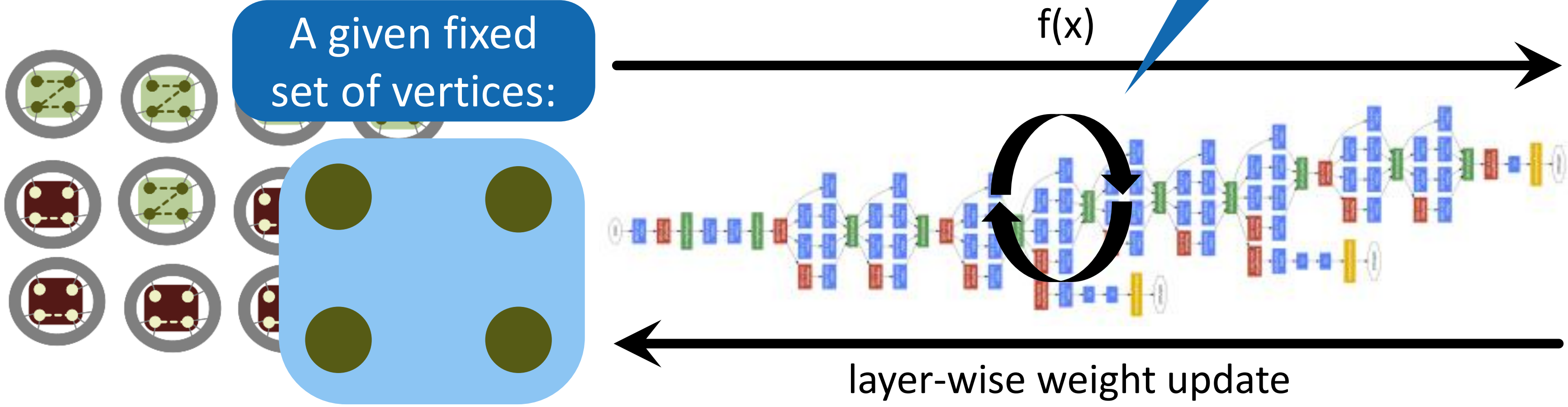


Motif Prediction: Deep Learning Formulation

[1] M. Zhan et al. 2018. An end-to-end deep learning architecture for graph classification. AAAI Conference on Artificial Intelligence

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

A given fixed set of vertices:



Will a k-clique appear or not?

SEAM Architecture (learning from Subgraphs, Embeddings and Attributes for Motif prediction)

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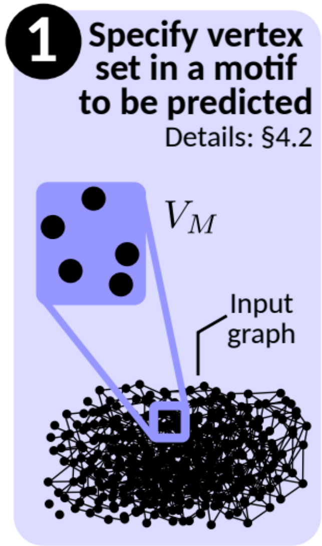

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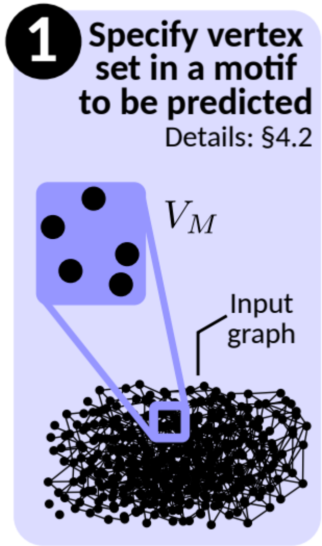

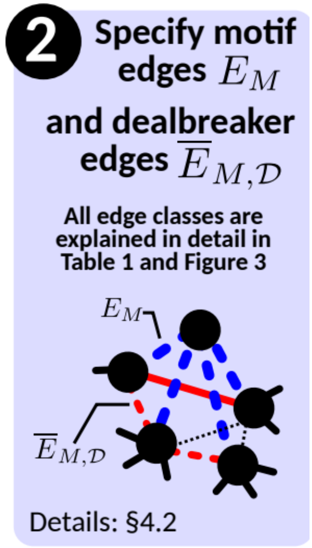

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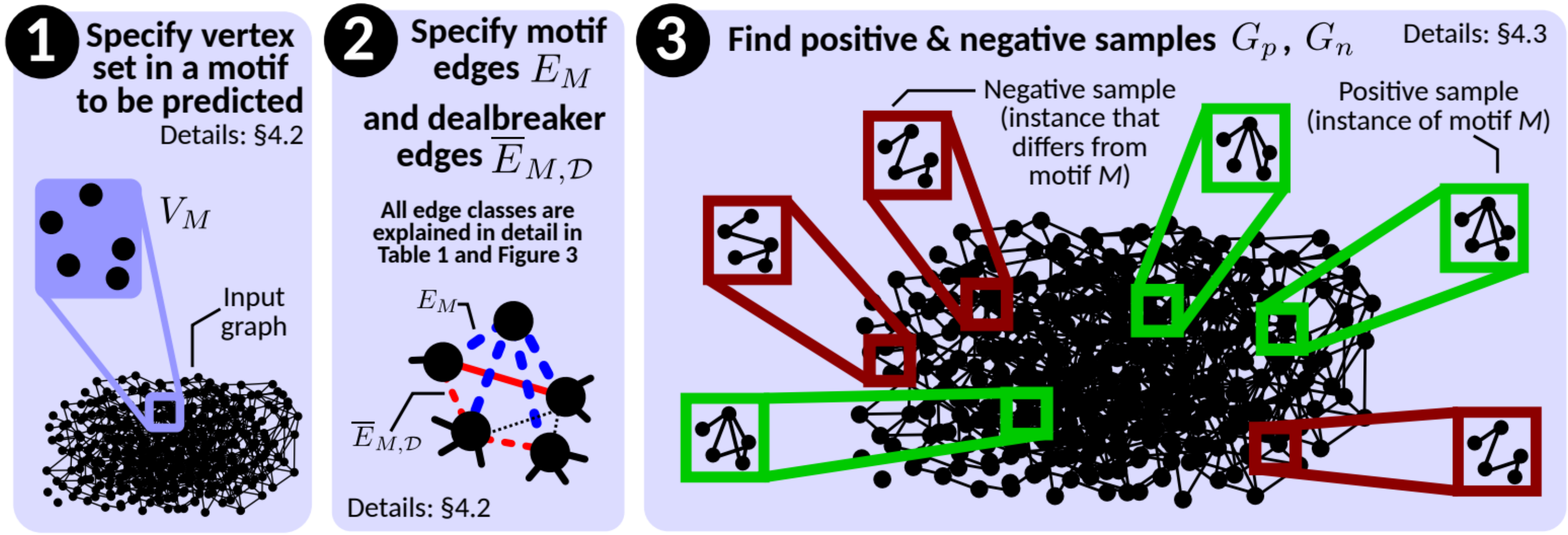

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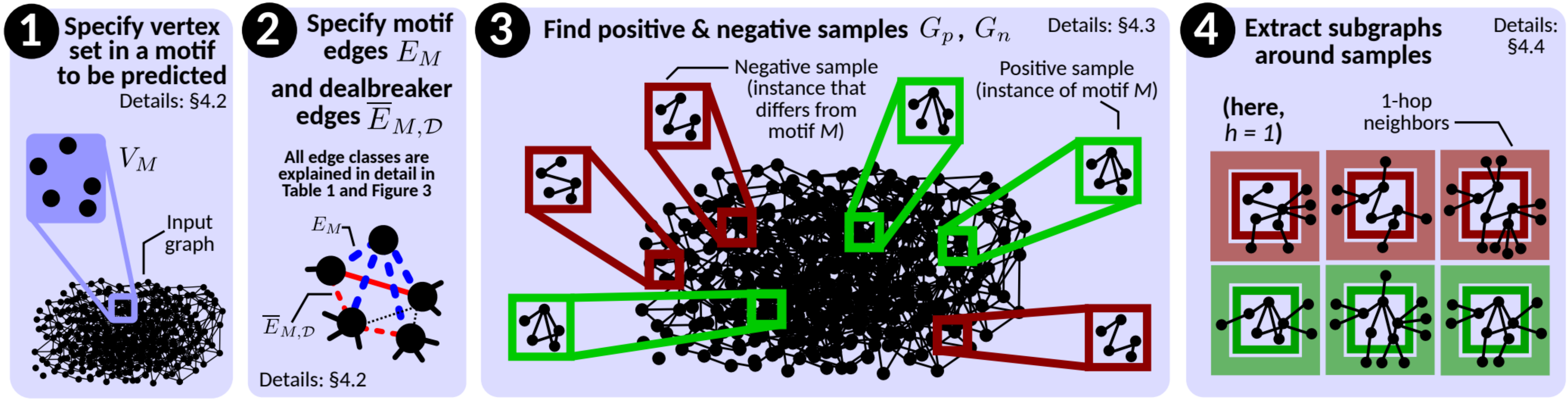

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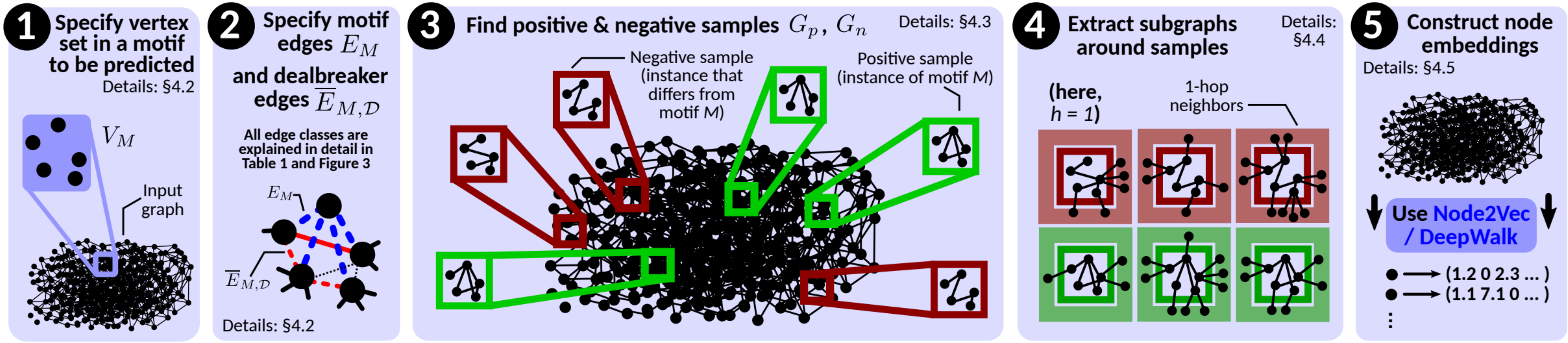

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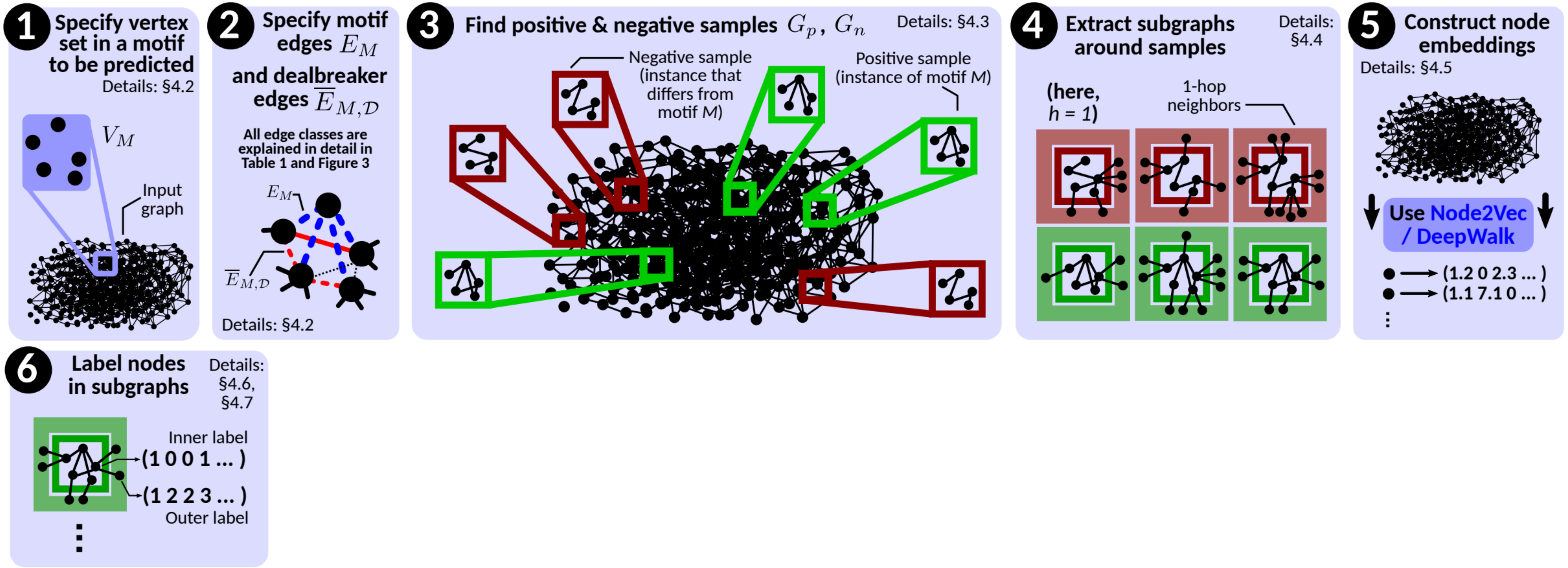

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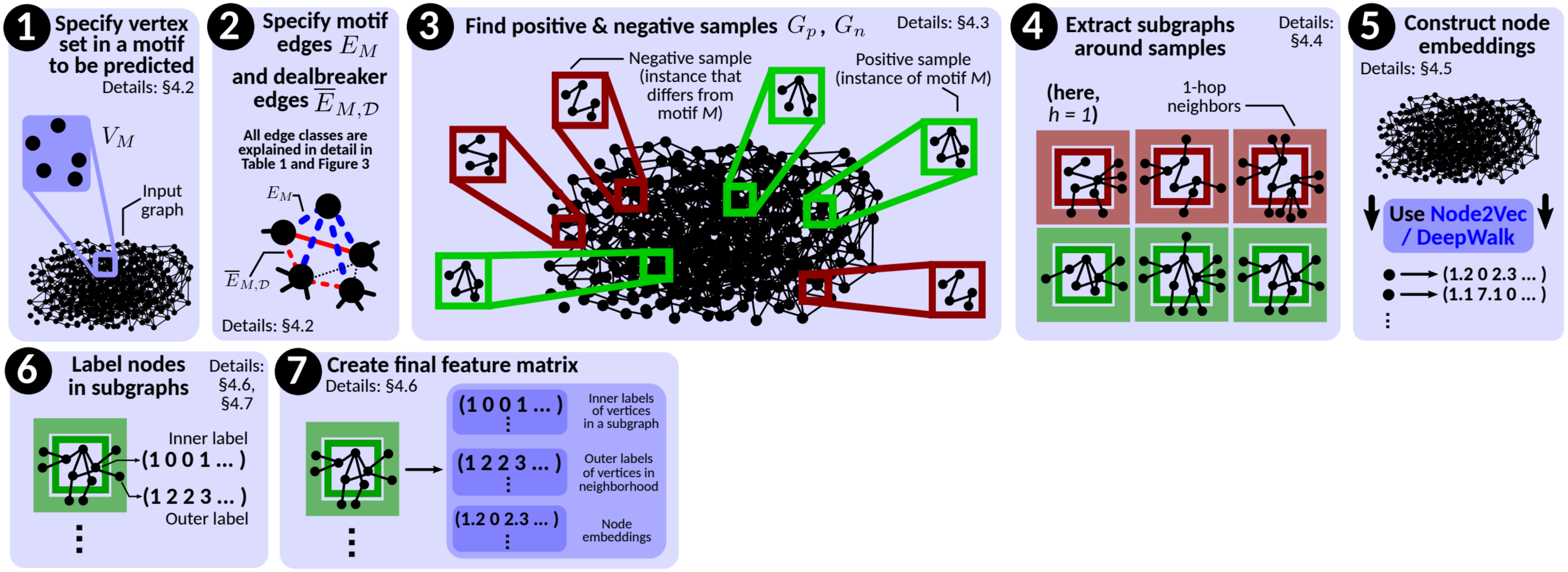

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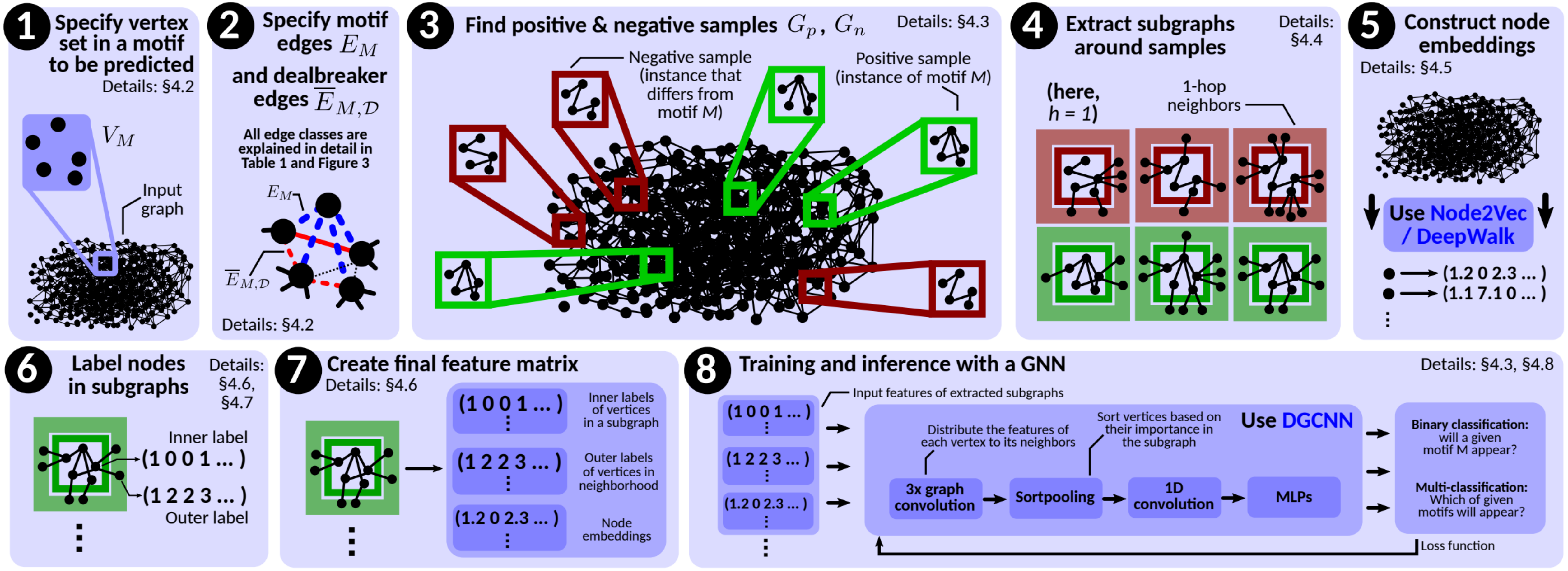

Evaluation: considered motifs & scenarios

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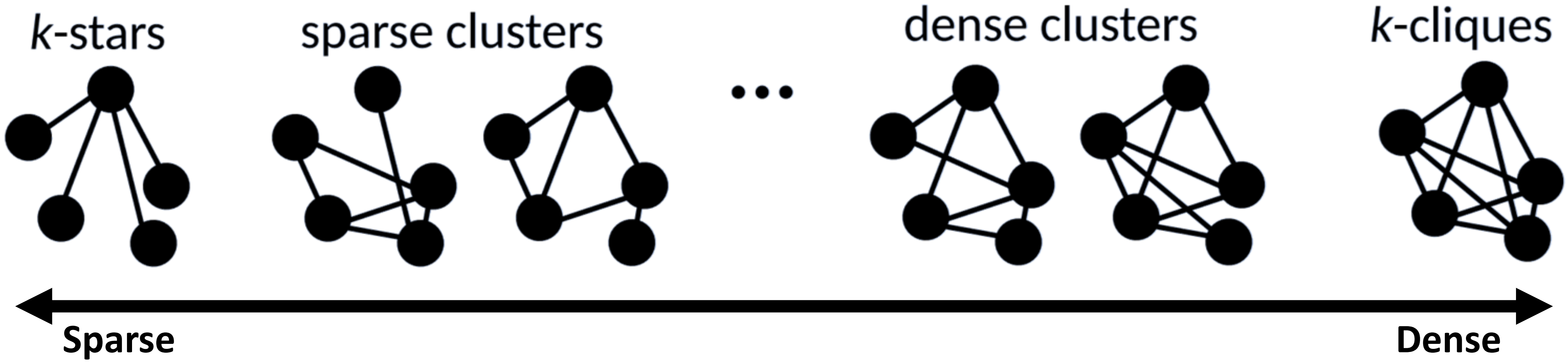

Evaluation: considered motifs & scenarios (transductive, inductive)

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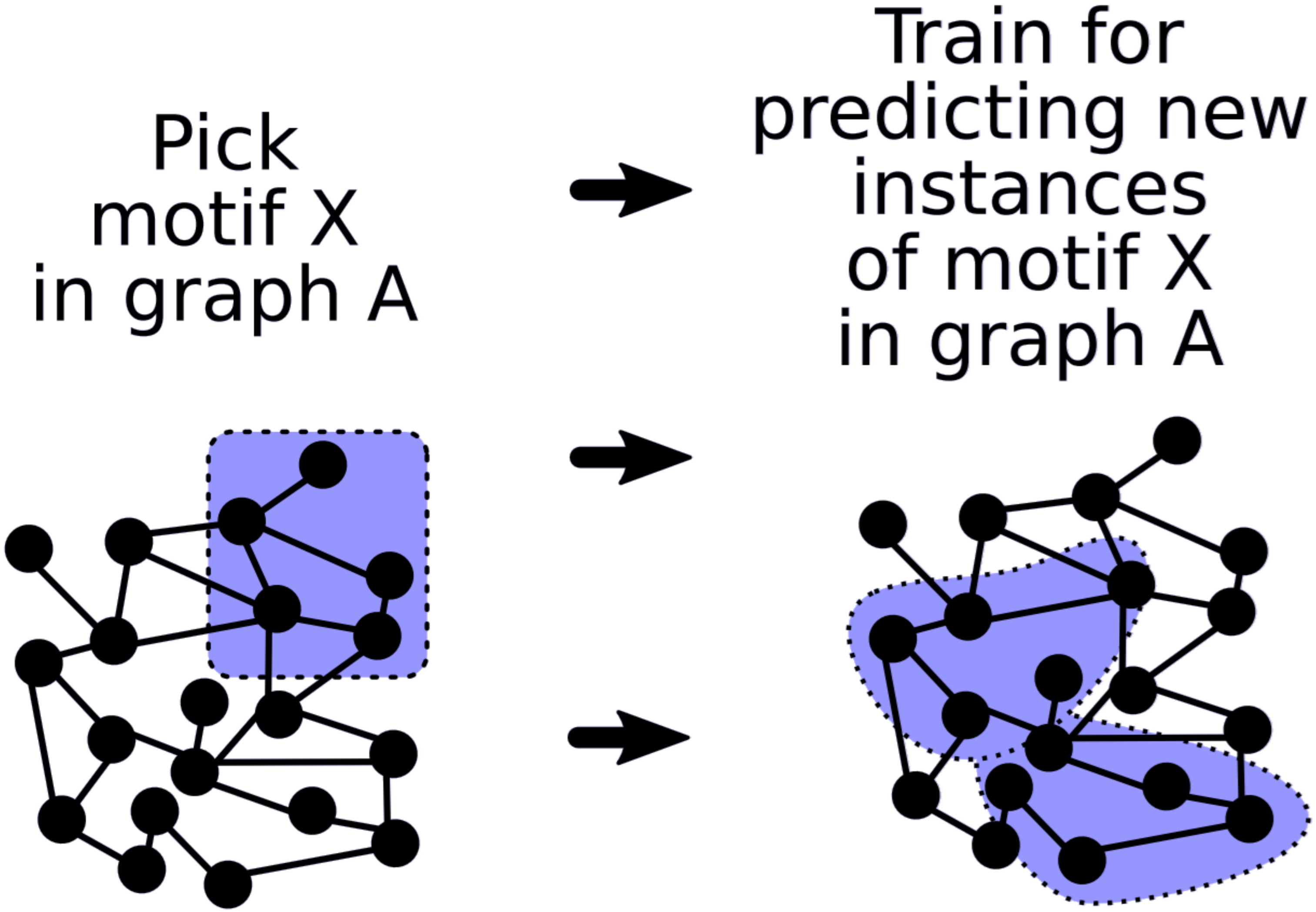
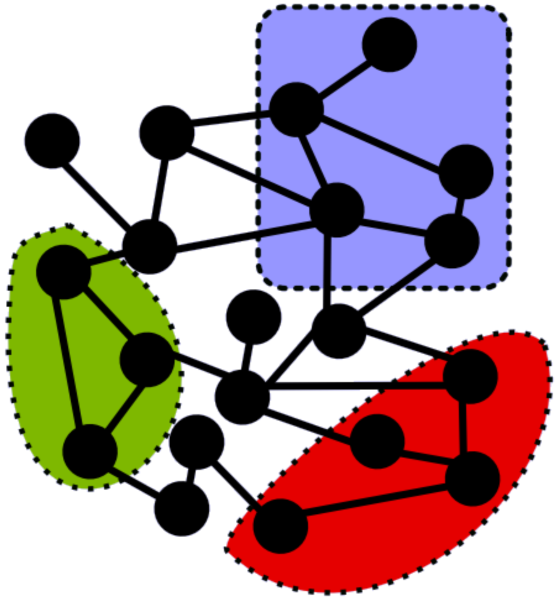
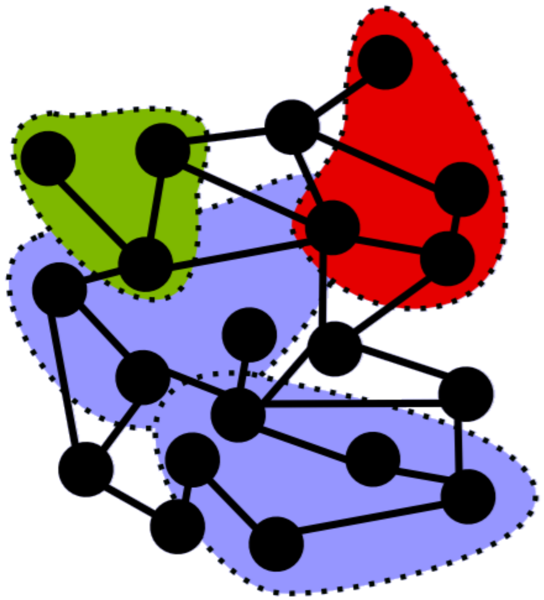


Evaluation: considered motifs & scenarios (transductive, inductive)

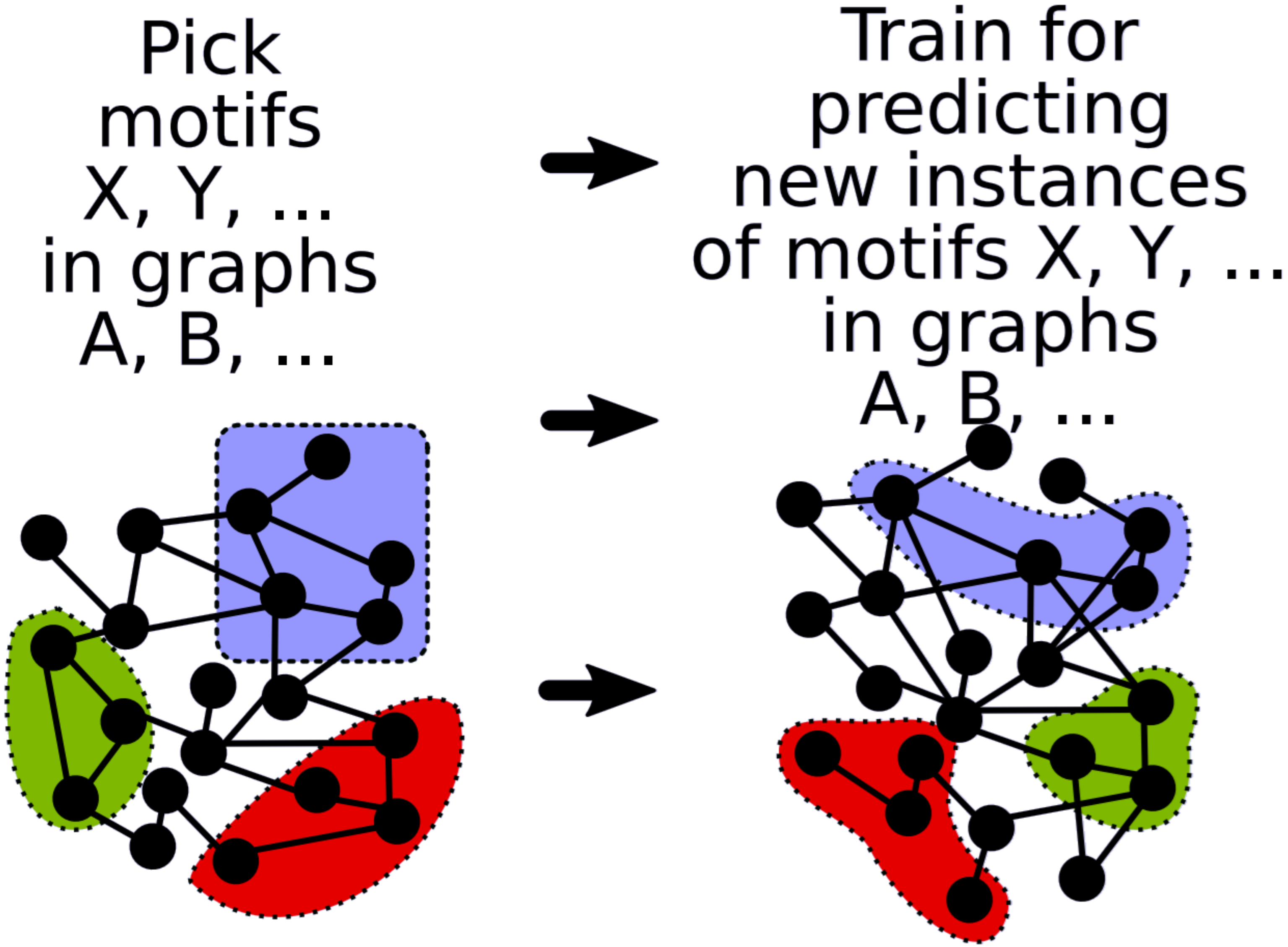
Pick motifs X, Y, ... in graph A

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





Evaluation: considered motifs & scenarios (transductive, inductive)



Evaluation

	3-star	5-star	7-star	3-clique	5-clique	7-clique	3-db-star	5-db-star	7-db-star
CN (Mul)	49.99 ± 0.45	49.78 ± 0.39	50.19 ± 0.47	50.13 ± 0.65	50.37 ± 0.79	51.55 ± 0.32	52.93 ± 0.61	55.42 ± 0.58	54.81 ± 0.58
CN (Min)	49.98 ± 0.33	49.72 ± 0.49	50.26 ± 0.59	50.35 ± 0.27	50.48 ± 0.32	51.77 ± 0.40	52.99 ± 0.75	54.75 ± 0.48	54.60 ± 0.85
CN (Avg)	49.76 ± 0.32	49.50 ± 0.64	50.18 ± 0.64	50.28 ± 0.51	50.91 ± 0.35	51.70 ± 0.59	53.32 ± 0.35	54.93 ± 0.77	54.20 ± 0.68
AA (Mul)	63.05 ± 0.71	62.09 ± 0.57	60.67 ± 0.95	54.95 ± 0.92	51.25 ± 0.63	51.40 ± 0.68	53.92 ± 0.52	55.15 ± 0.77	54.93 ± 0.61
AA (Min)	63.34 ± 0.68	62.81 ± 0.80	61.59 ± 0.94	54.81 ± 0.77	51.26 ± 0.38	51.60 ± 0.68	54.15 ± 0.89	54.59 ± 0.65	54.94 ± 0.27
AA (Avg)	63.96 ± 0.68	63.66 ± 0.48	62.71 ± 0.52	55.78 ± 0.74	51.28 ± 0.55	51.79 ± 0.62	54.52 ± 0.57	55.20 ± 0.53	54.55 ± 0.39
Jaccard (Mul)	67.17 ± 0.92	62.01 ± 0.72	59.71 ± 0.93	69.62 ± 1.09	57.60 ± 0.73	52.75 ± 0.97	51.75 ± 1.10	51.68 ± 0.85	50.93 ± 0.64
Jaccard (Min)	69.20 ± 0.80	67.11 ± 0.46	65.24 ± 0.80	73.88 ± 0.88	63.36 ± 1.17	56.50 ± 0.94	52.30 ± 0.54	51.86 ± 0.77	50.87 ± 0.53
Jaccard (Avg)	70.12 ± 0.78	68.59 ± 0.71	68.69 ± 0.77	75.35 ± 0.60	67.93 ± 0.87	61.22 ± 1.11	51.76 ± 0.91	49.74 ± 0.75	47.66 ± 0.58
SEAL (Mul)	76.68 ± 0.61	74.00 ± 0.50	71.80 ± 0.95	76.25 ± 1.90	63.66 ± 4.01	59.48 ± 4.87	68.53 ± 0.88	67.49 ± 1.27	67.88 ± 1.43
SEAL (Min)	77.15 ± 0.43	74.62 ± 0.55	73.11 ± 0.99	78.00 ± 1.49	69.70 ± 3.56	64.49 ± 5.47	66.40 ± 1.44	62.94 ± 1.98	62.88 ± 3.57
SEAL (Avg)	77.91 ± 0.91	75.98 ± 0.99	75.71 ± 0.66	77.50 ± 2.35	72.68 ± 3.21	66.95 ± 6.79	66.05 ± 0.78	65.14 ± 0.89	66.99 ± 1.32
SEAM, no embedding	86.24 ± 0.99	85.57 ± 0.94	88.61 ± 0.71	91.20 ± 1.03	96.16 ± 0.55	98.40 ± 0.22	83.39 ± 0.94	86.12 ± 0.66	87.86 ± 1.06
SEAM	90.78 ± 1.30	90.00 ± 1.84	91.53 ± 1.53	93.06 ± 0.61	97.26 ± 0.23	98.90 ± 0.18	83.81 ± 0.53	87.56 ± 0.79	88.59 ± 1.51

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

Evaluation

	3-star	5-star	7-star	3-clique	5-clique	7-clique	3-db-star	5-db-star	7-db-star
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SEAM: learning from Subgraphs, Embeddings and Attributes for Motif prediction

„db" – with deal-breaker edges

Evaluation

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)

[2] M. Zhang and Y. Chen. 2018. Link prediction based on graph neural networks. NeurIPS'18

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

„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)

[2] M. Zhang and Y. Chen. 2018. Link prediction based on graph neural networks. NeurIPS'18

	3-star	5-star	7-star	3-clique	5-clique	7-clique	3-db-star	5-db-star	7-db-star
CN (Mul)	49.99 ± 0.45	49.78 ± 0.39	50.19 ± 0.47	50.13 ± 0.65	50.37 ± 0.79	51.55 ± 0.32	52.93 ± 0.61	55.42 ± 0.58	54.81 ± 0.58
CN (Min)	49.98 ± 0.33	49.72 ± 0.49	50.26 ± 0.59	50.35 ± 0.27	50.48 ± 0.32	51.77 ± 0.40	52.99 ± 0.75	54.75 ± 0.48	54.60 ± 0.85
CN (Avg)	49.76 ± 0.32	49.50 ± 0.64	50.18 ± 0.64	50.28 ± 0.51	50.91 ± 0.35	51.70 ± 0.59	53.32 ± 0.35	54.93 ± 0.77	54.20 ± 0.68
AA (Mul)	63.05 ± 0.71	62.09 ± 0.57	60.67 ± 0.95	54.95 ± 0.92	51.25 ± 0.63	51.40 ± 0.68	53.92 ± 0.52	55.15 ± 0.77	54.93 ± 0.61
AA (Min)	63.34 ± 0.68	62.81 ± 0.80	61.59 ± 0.94	54.81 ± 0.77	51.26 ± 0.38	51.60 ± 0.68	54.15 ± 0.89	54.59 ± 0.65	54.94 ± 0.27
AA (Avg)	63.96 ± 0.68	63.66 ± 0.48	62.71 ± 0.52	55.78 ± 0.74	51.28 ± 0.55	51.79 ± 0.62	54.52 ± 0.57	55.20 ± 0.53	54.55 ± 0.39
Jaccard (Mul)	67.17 ± 0.92	62.01 ± 0.72	59.71 ± 0.93	69.62 ± 1.09	57.60 ± 0.73	52.75 ± 0.97	51.75 ± 1.10	51.68 ± 0.85	50.93 ± 0.64
Jaccard (Min)	69.20 ± 0.80	67.11 ± 0.46	65.24 ± 0.80	73.88 ± 0.88	63.36 ± 1.17	56.50 ± 0.94	52.30 ± 0.54	51.86 ± 0.77	50.87 ± 0.53
Jaccard (Avg)	70.12 ± 0.78	68.59 ± 0.71	68.69 ± 0.77	75.35 ± 0.60	67.93 ± 0.87	61.22 ± 1.11	51.76 ± 0.91	49.74 ± 0.75	47.66 ± 0.58
SEAL (Mul)	76.68 ± 0.61	74.00 ± 0.50	71.80 ± 0.95	76.25 ± 1.90	63.66 ± 4.01	59.48 ± 4.87	68.53 ± 0.88	67.49 ± 1.27	67.88 ± 1.43
SEAL (Min)	77.15 ± 0.43	74.62 ± 0.55	73.11 ± 0.99	78.00 ± 1.49	69.70 ± 3.56	64.49 ± 5.47	66.40 ± 1.44	62.94 ± 1.98	62.88 ± 3.57
SEAL (Avg)	77.91 ± 0.91	75.98 ± 0.99	75.71 ± 0.66	77.50 ± 2.35	72.68 ± 3.21	66.95 ± 6.79	66.05 ± 0.78	65.14 ± 0.89	66.99 ± 1.32
SEAM, no embedding	86.24 ± 0.99	85.57 ± 0.94	88.61 ± 0.71	91.20 ± 1.03	96.16 ± 0.55	98.40 ± 0.22	83.39 ± 0.94	86.12 ± 0.66	87.86 ± 1.06
SEAM	90.78 ± 1.30	90.00 ± 1.84	91.53 ± 1.53	93.06 ± 0.61	97.26 ± 0.23	98.90 ± 0.18	83.81 ± 0.53	87.56 ± 0.79	88.59 ± 1.51

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

„db" – with deal-breaker edges

Evaluation

With correlation

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AA (Min)	63.34 ± 0.68	62.81 ± 0	[illegible]	[illegible]	[illegible]	[illegible]	4.15 ± 0.89	54.59 ± 0.65	54.94 ± 0.27
AA (Avg)	63.96 ± 0.68	63.66 ± 0	[illegible]	[illegible]	[illegible]	[illegible]	4.52 ± 0.57	55.20 ± 0.53	54.55 ± 0.39
Jaccard (Mul)	67.17 ± 0.92	62.01 ± 0	[illegible]	[illegible]	[illegible]	[illegible]	1.75 ± 1.10	51.68 ± 0.85	50.93 ± 0.64
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Jaccard (Avg)	70.12 ± 0.78	68.59 ± 0	[illegible]	[illegible]	[illegible]	[illegible]	1.76 ± 0.91	49.74 ± 0.75	47.66 ± 0.58
SEAL (Mul)	76.68 ± 0.61	74.00 ± 0	[illegible]	[illegible]	[illegible]	[illegible]	8.53 ± 0.88	67.49 ± 1.27	67.88 ± 1.43
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Much more results and sensitivity analyses in the paper ☺

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Motif Prediction with Graph Neural Networks

Thank you for your attention

SPCL