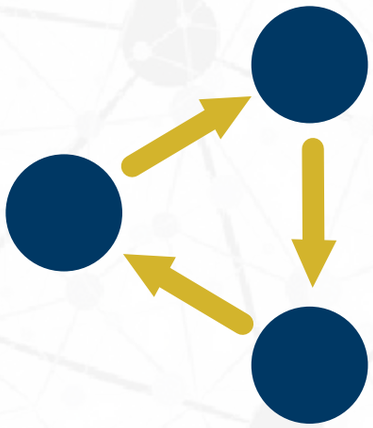
東京工業大学
Tokyo Institute of Technology

MURATA LAB



Mid-term Presentation

Motif-aware method for graph analysis

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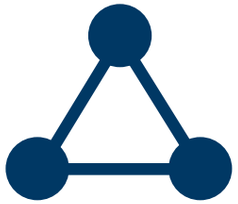
2017/02/03

Roadmap

Result of motif methods | Proposal of future models



Deep architecture
Skip-gram methods
Spectral methods

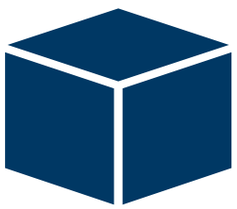
EMBEDDINGS

Diversity models
Generative models
Motif Spectral

IN PROGRESS

NETWORK MOTIF

Definition
Applications
Motif Conductance



OBSERVATION

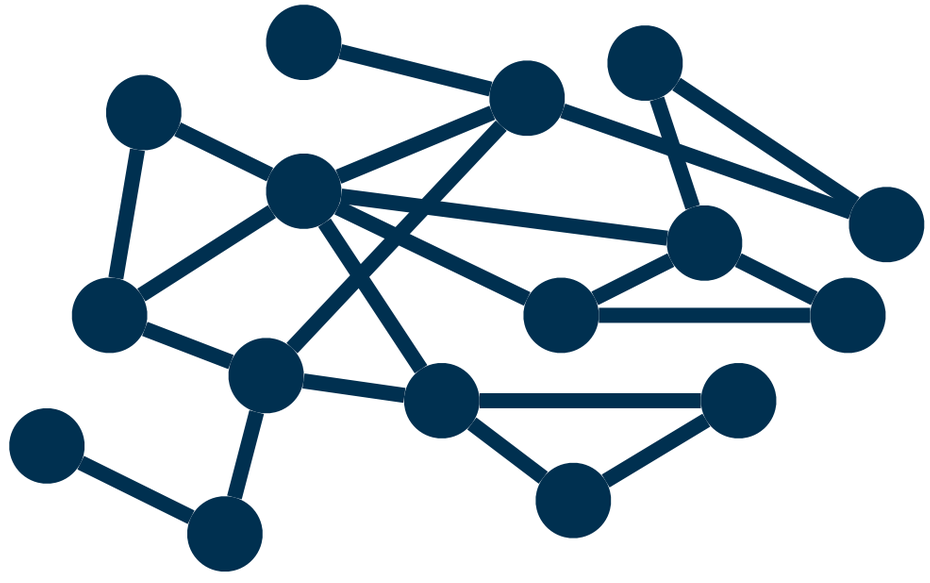
Experiments
Proposed models
Results

Definition and applications

Complex networks and significant subgraphs

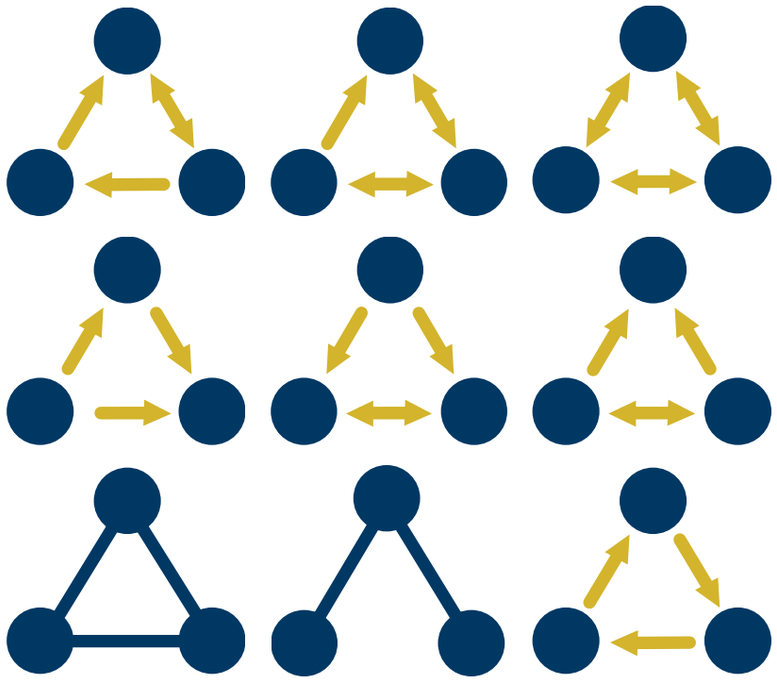
Scales of network analysis:

- Macroscopic (global view)
- Microscopic (interactions)
- Mesoscopic (sub-structures)



Network motifs are [1]

> patterns of statistically significant interconnections occurring in complex networks.



Applications

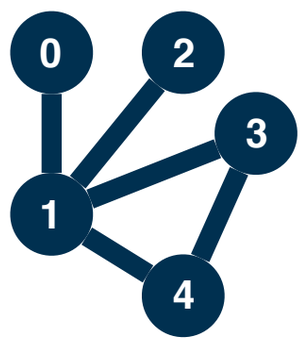
- Social networks [2]
- Biological systems [1,3,4]

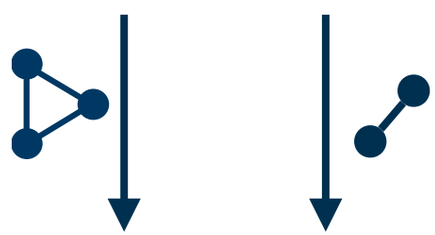
[4](*Franceschet, 2012*) [3](*Honey, 2007*) [2](*Holland, 1970*) [1](*Milo, 2002*)

Motif conductance
Network motifs in network analysis

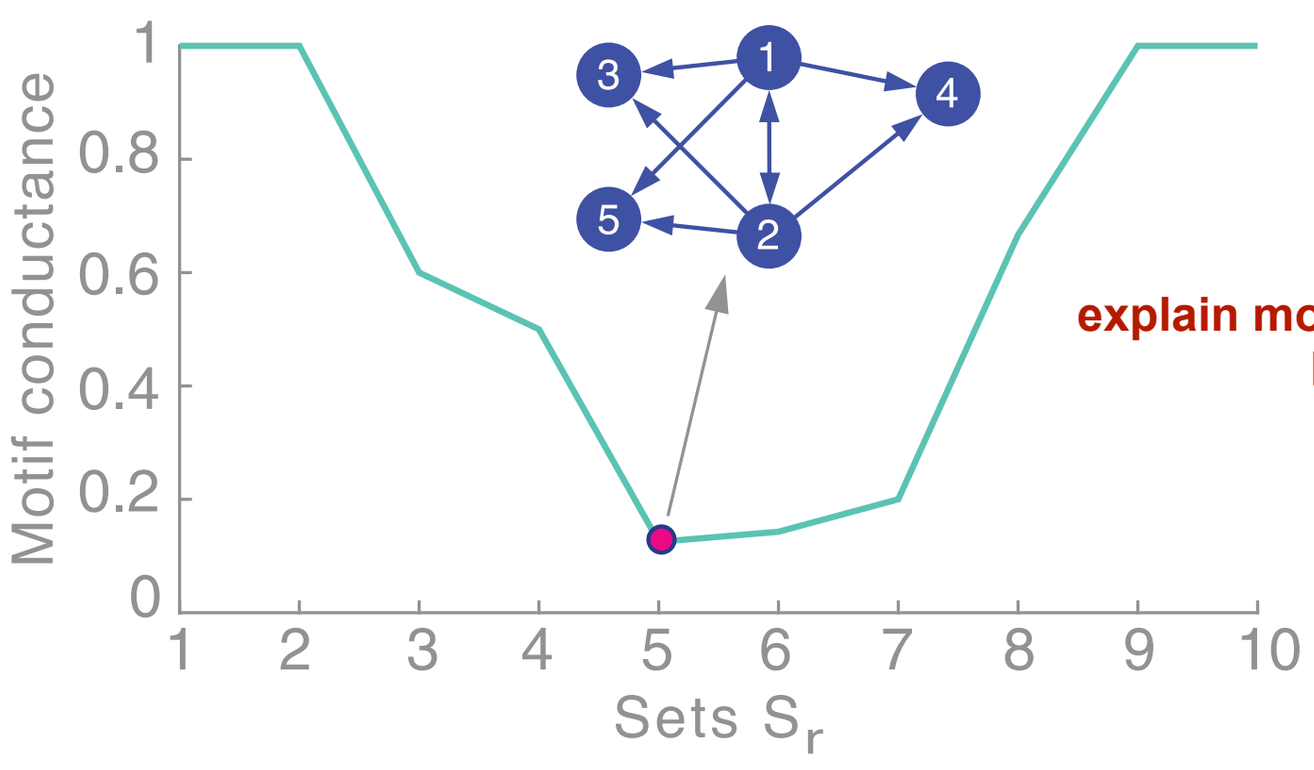
Motif conductance *(Benson, 2016)*

- Generalization of graph conductance.
- Motif-cooccurrence matrix.
- Good results for graph partitioning.





$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 2 & 2 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 2 \\ 0 & 2 & 0 & 2 & 0 \end{bmatrix}$$

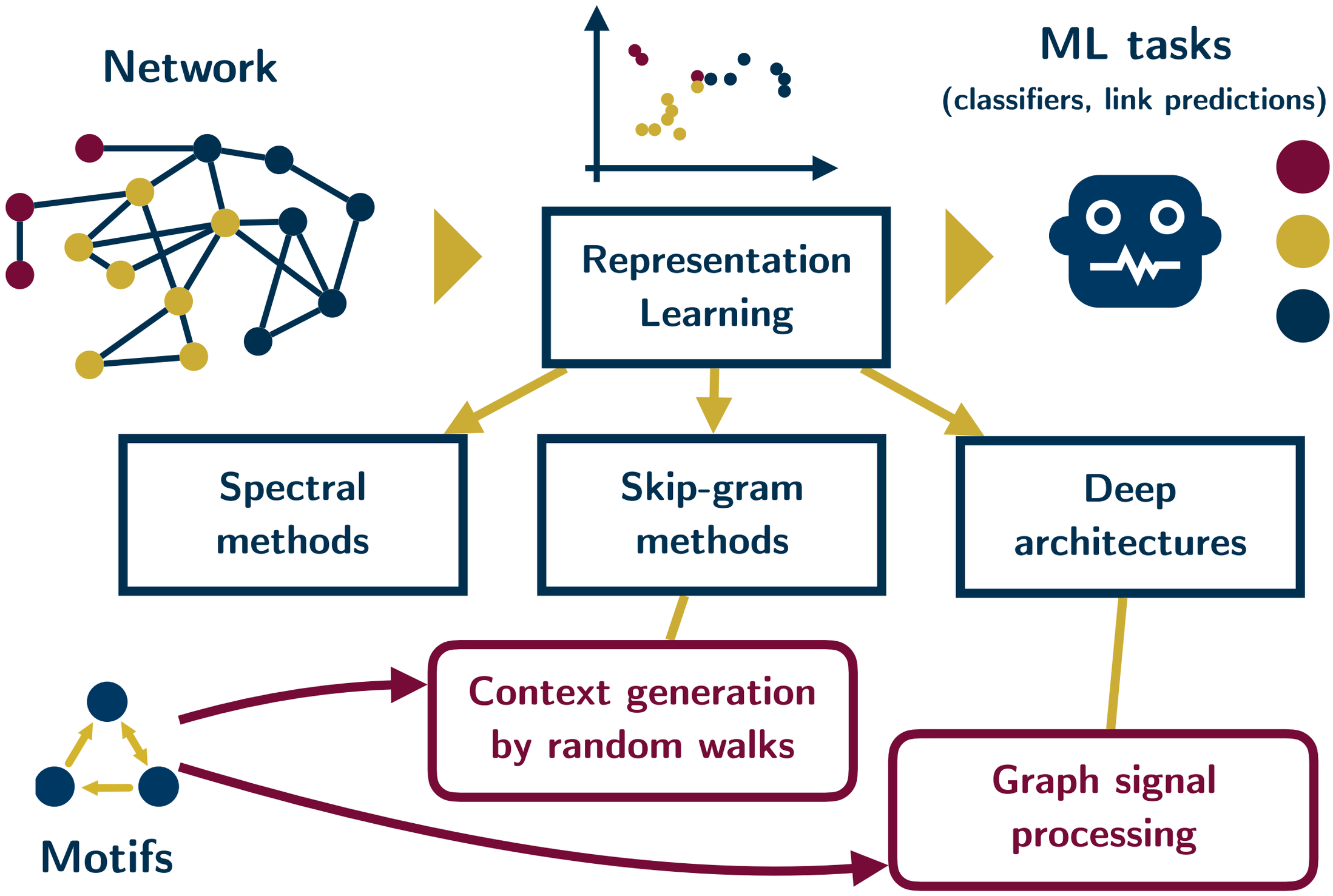


explain motif-conductance better

$$\phi_m(S) = \frac{\mathrm{cut}_M(S, \bar{S})}{\min[\mathrm{vol}_M(S), \mathrm{vol}_M(\bar{S})]}$$

Experiments

Graph embedding for classifying network node



Experiments
Motif analysis

Datasets:

- Blogcatalog3
- Cora, Citeseer, Pubmed
- Facebook (EgoNet)
- Transcription networks

Networks	*#nodes*	*#edge*
Blogcatalog3	10312	333983
Cora*	2708	5429
Citeseer*	3327	4732

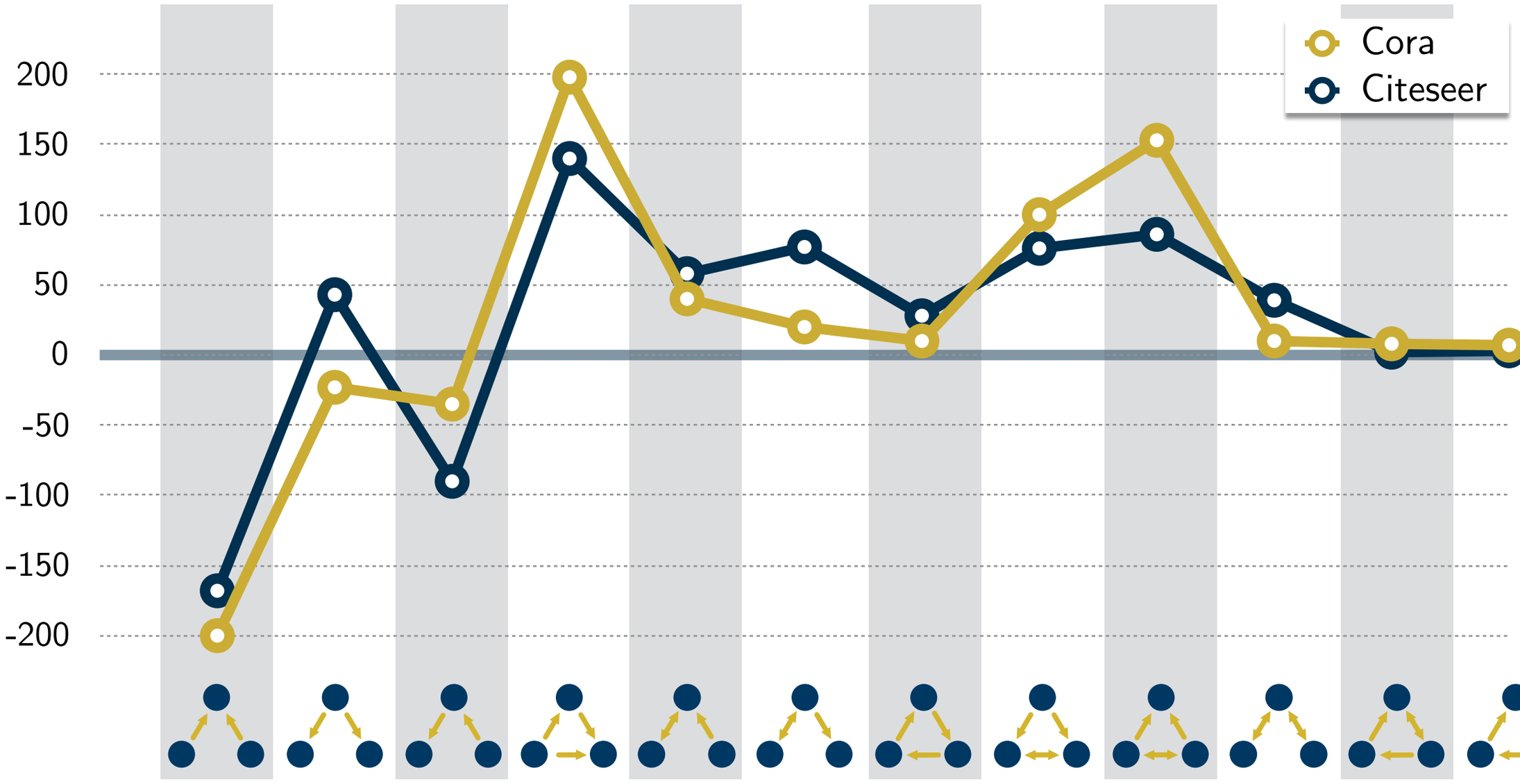
* Each node has a feature vector (tf-idf)

Deciding motif:

- Motif frequency
- Z-score
- Motif conductance

$$z_m = \frac{N_m(emp) - N_m(rnd)}{\sigma_m}$$

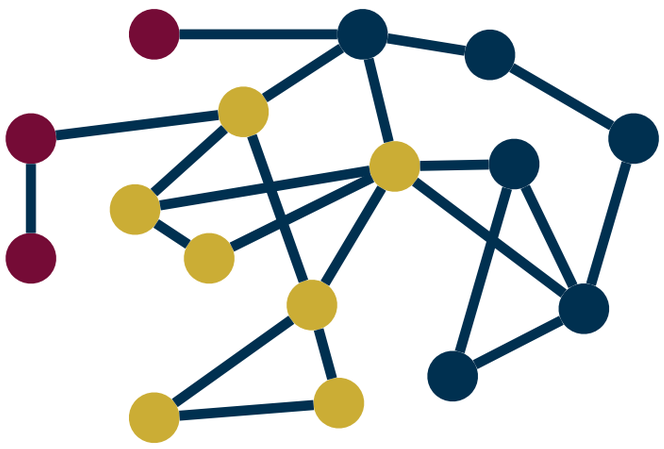
Significant graph - Directed size 3 motifs

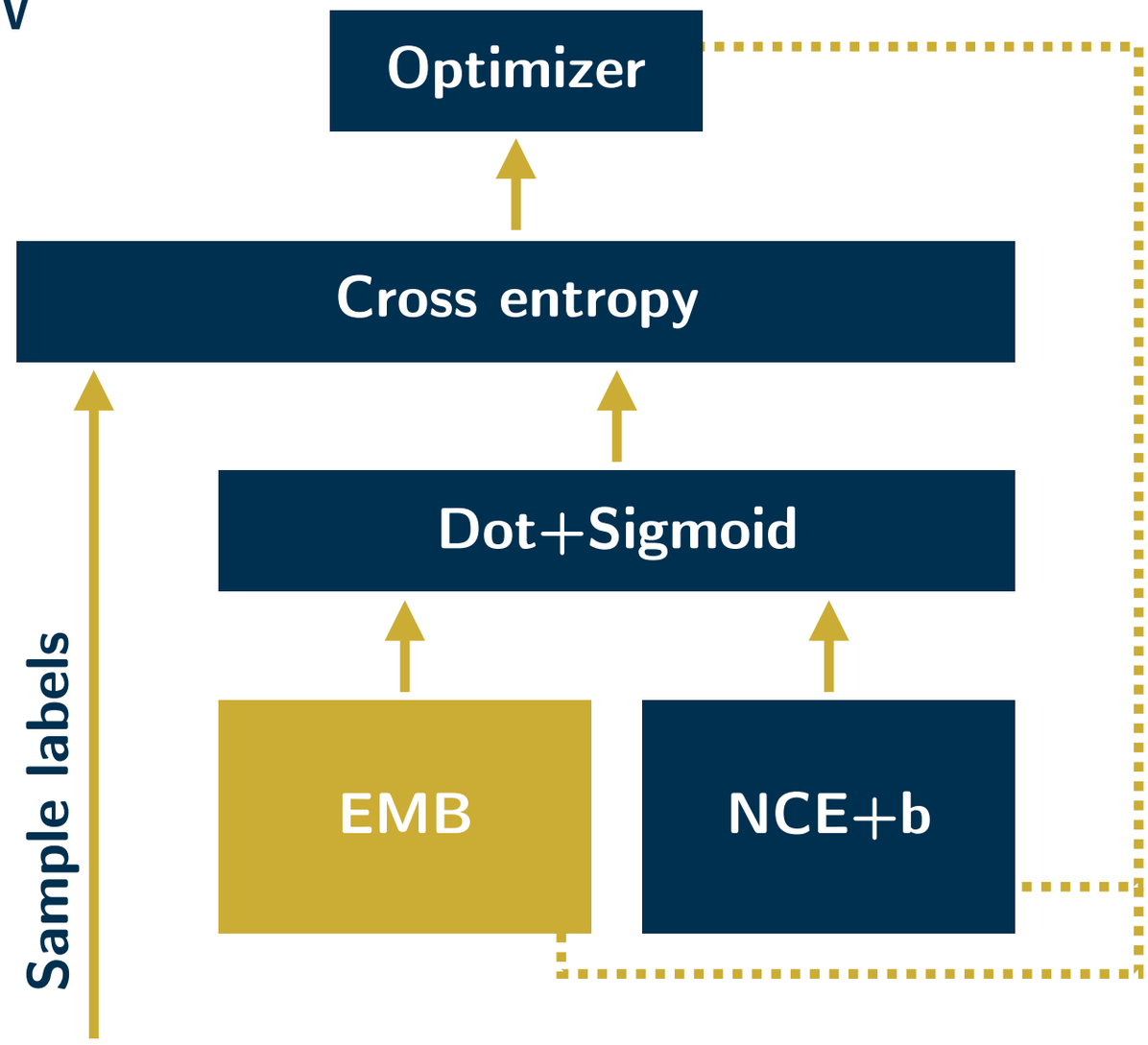


Experiments
Approach #1: motifwalk

Using motif as a guiding pattern

- DeepWalk := Skip-gram+RW
- LINE := DeepWalk+bi-fan
- node2vec := Skip-gram +bias-ed walk
- motifwalk := Skip-gram +motif walk





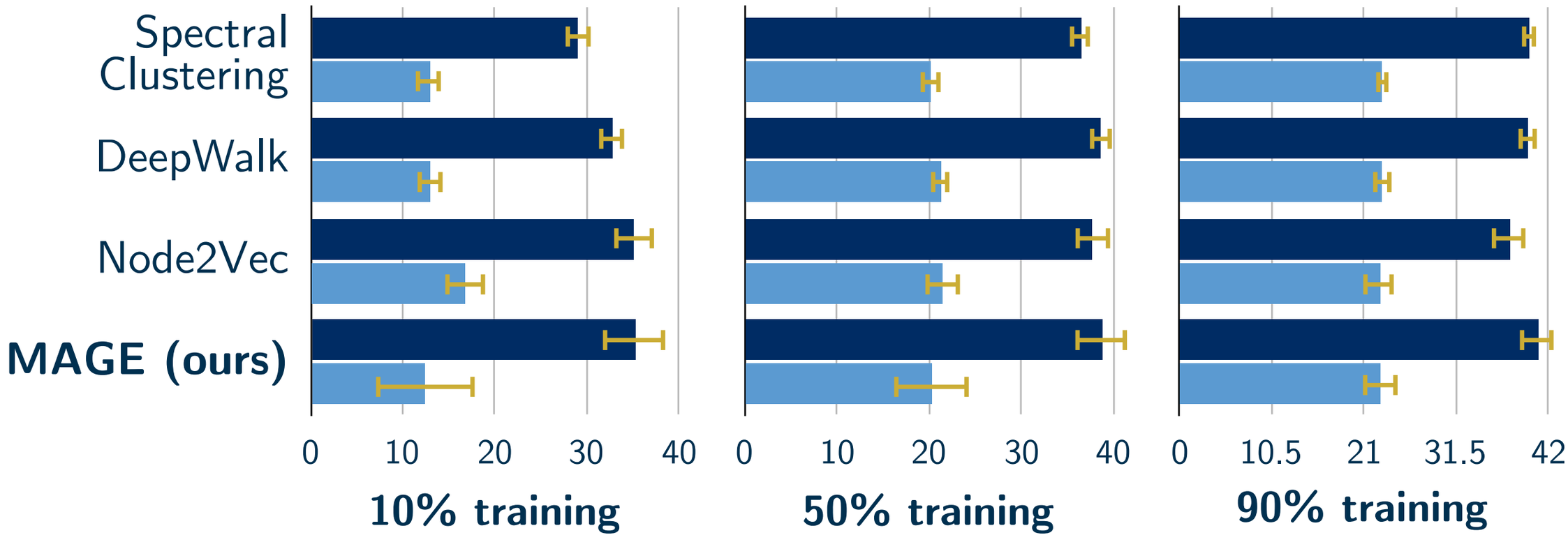
Add animation to explain the motif walk vs random walk

Generated context:

Experiments
Approach #1: motifwalk

Node multi-label classification

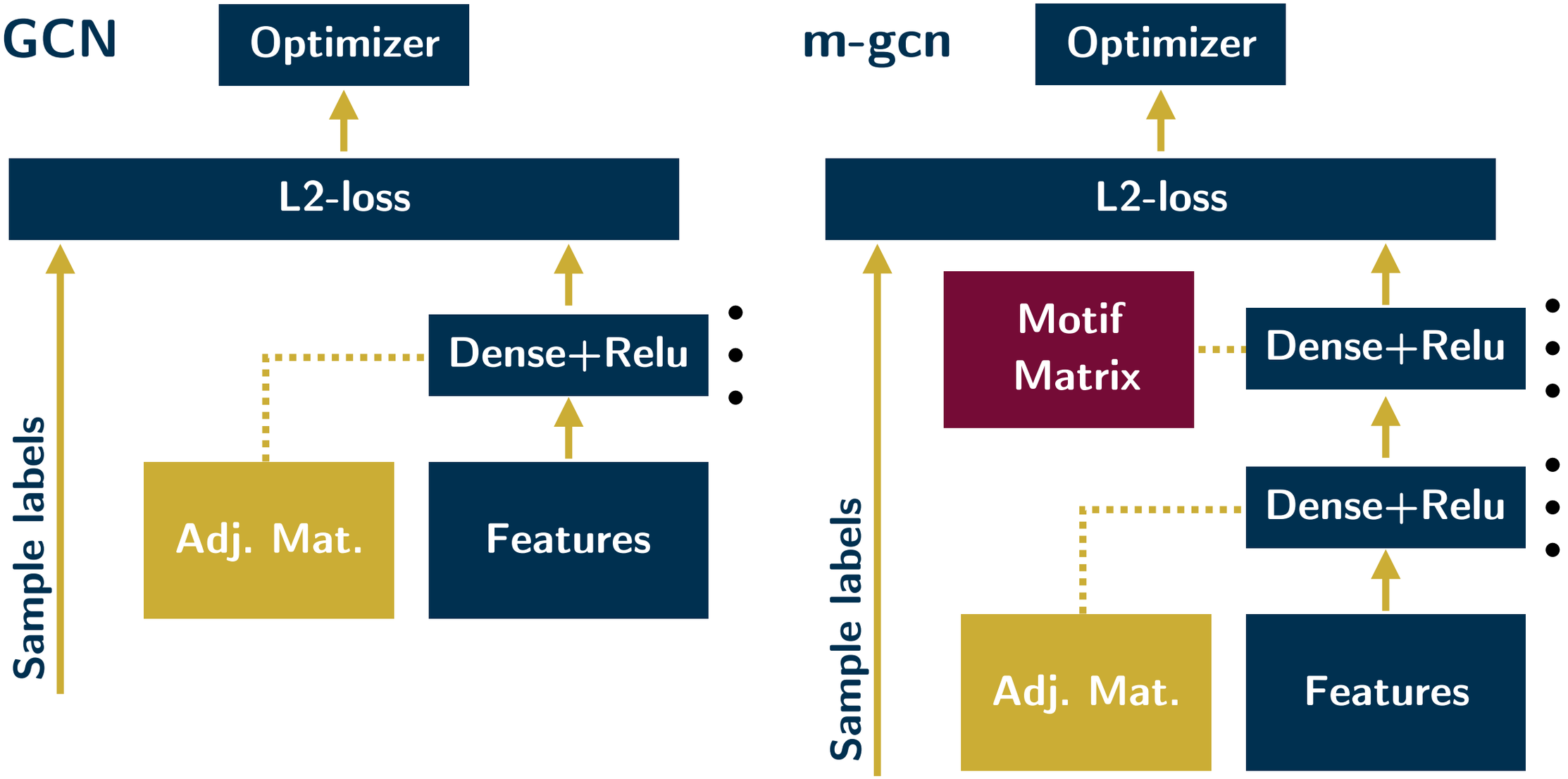
- Blogcatalog3 - f1 score
- 39 classes (imbalanced), nodes can have multiple labels



- Bottleneck at context generation.

Experiments
Approach #2: m-gcn

Motif laplacian for graph convolutional networks



Experiments

Approach #2: m-gcn

Node label classification

- Citation networks: Cora, citeseer, pubmed. - f1 and acc.
- 3 to 6 classes, each node has exactly one label.

Methods	Cora		Citeseer		Pubmed	
	accuracy	macro	accuracy	macro	accuracy	macro
Spectral Clus.	59.5	-	42.7	-	65.3	-
DeepWalk	67.2	-	43.2	-	65.3	-
GCN	81.5	-	70.3	-	79.0	-
m-gcn (ours)	**83.3**	-	**71.4**	-	**80.4**	-

- Explaining why does it work.
- Minor contribution.

In progress

Generative models | Diversity models

My interests:

- Network sampling (diversity oriented).
- Turn m-gcn into a generative model.

Agenda:

- Investigate graph spectral theory.
- Determinantal processes on graphs.
- Graph motif sampling model definition.
- (opt.) Generative Adversarial Networks and Auto-Encoders.

References

(Diestel, 2000) Graph Theory.

(Mikolov, 2013) Distributed Representations of Words and Phrases and their Compositionality.

(Bengio, 2013) Deep Learning of Representations: Looking Forward.

(Ng, 2001) On Spectral Clustering: Analysis and an algorithm.

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(Tang, 2015) LINE: Large-scale Information Network Embedding.

(Cao, 2015) GraRep: Learning Graph Representations with Global Structural Information.

(Grover, 2016) node2vec: Scalable Feature Learning for Networks

(Yang, 2016) Semi-Supervised Classification with Graph Convolutional Networks

(Alon, 2007) Network motifs: theory and experimental approaches.

(Benson, 2016) Higher-order organization of complex networks.

Motif generalizes link

Motif here!

Skip-gram model

Applying NLP techniques to network science

Algorithm 1: Motif context sampling $P_m(\omega)$.

Data: Undirected Graph $G = (V, E)$;
Input: start vertex, walk length, motif $M = (V', E')$, bias β;
Result: Vertices in the local motif structure;
vertexList ⟵ [start vertex]
current ⟵ start vertex
initialize dequeue buffer Q of size $|V'|$
while *vertexList.length* $<$ *walk length* **do**
    candidate ⟵ random(neighboor(current))
    Q.append(candidate)
    if *Isomorphic(Q, M)* **then**
        if random $< \beta$ **then**
            vertexList.append(candidate)
        else
            continue
    else
        if random $> \beta$ **then**
            vertexList.append(candidate)
        else
            continue
return vertexList

NPL Skipgram

Graph convolutional networks

Spectral methods meets neural networks

Laplacian, normalized, convolution operations