Subgraph Pattern Matching with Deep Representations

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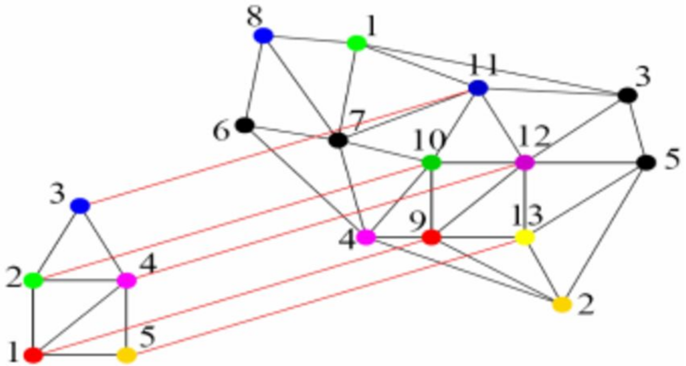
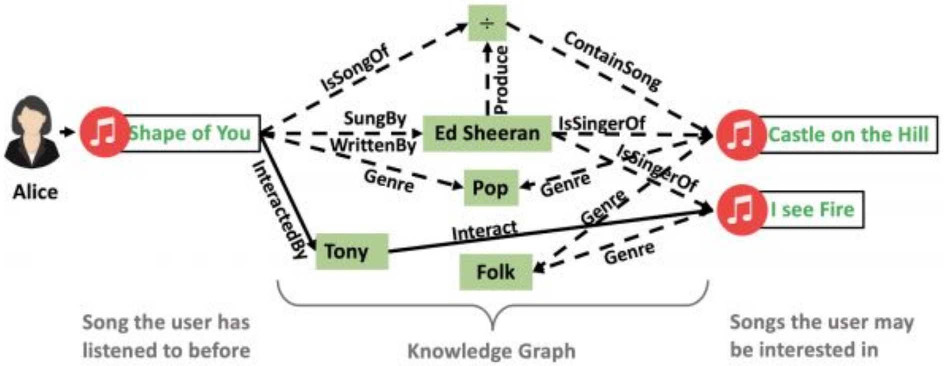
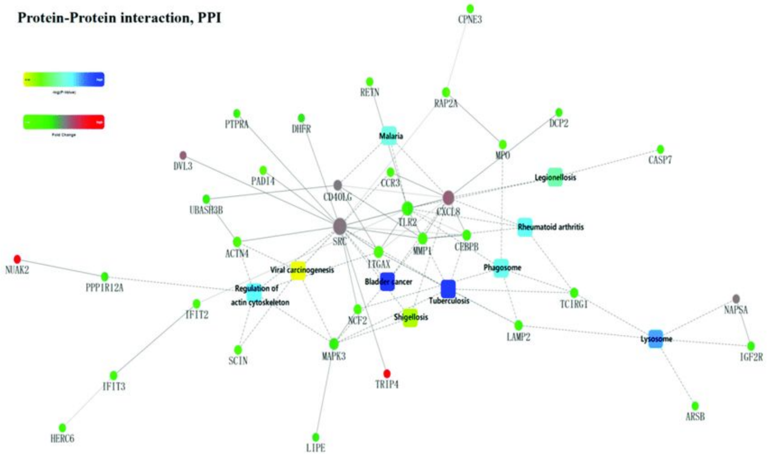
Mentor: Rex Ying, Jiaxuan You, Jure Leskovec

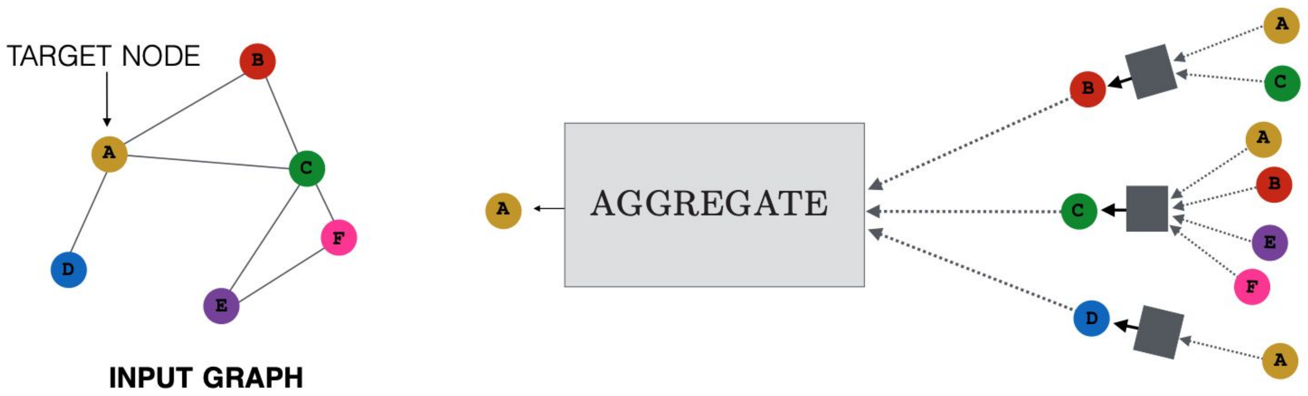
Subgraph Matching



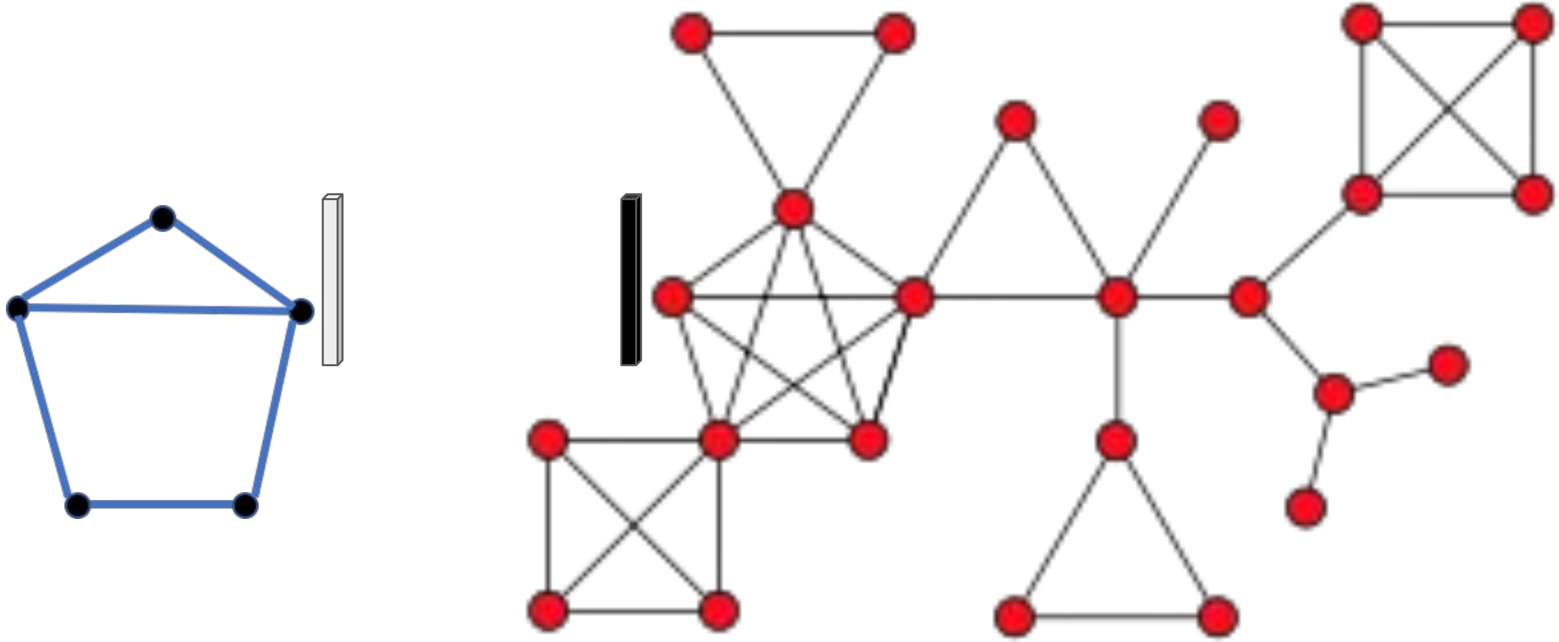




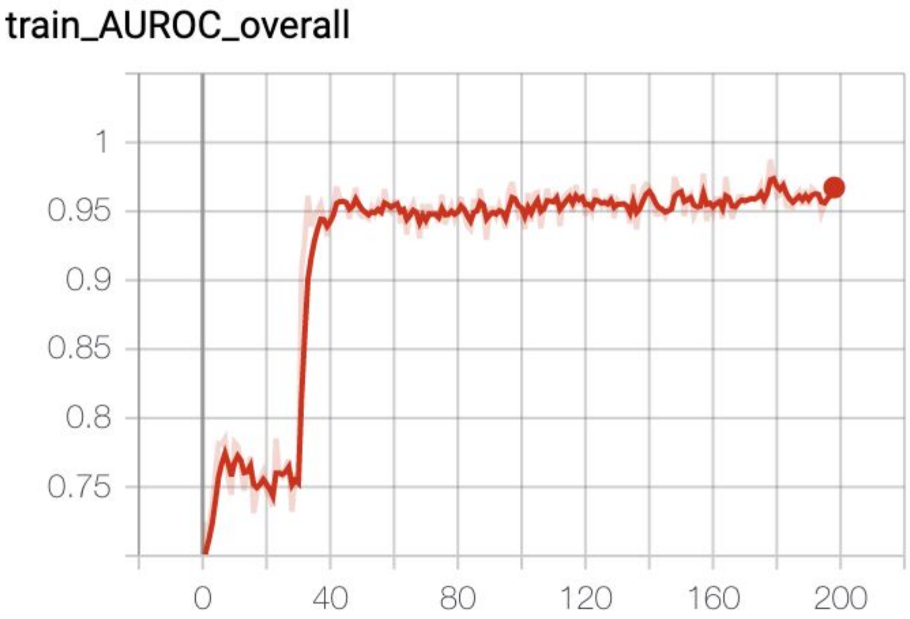
Method: Graph Convolutional Networks (GCNs)

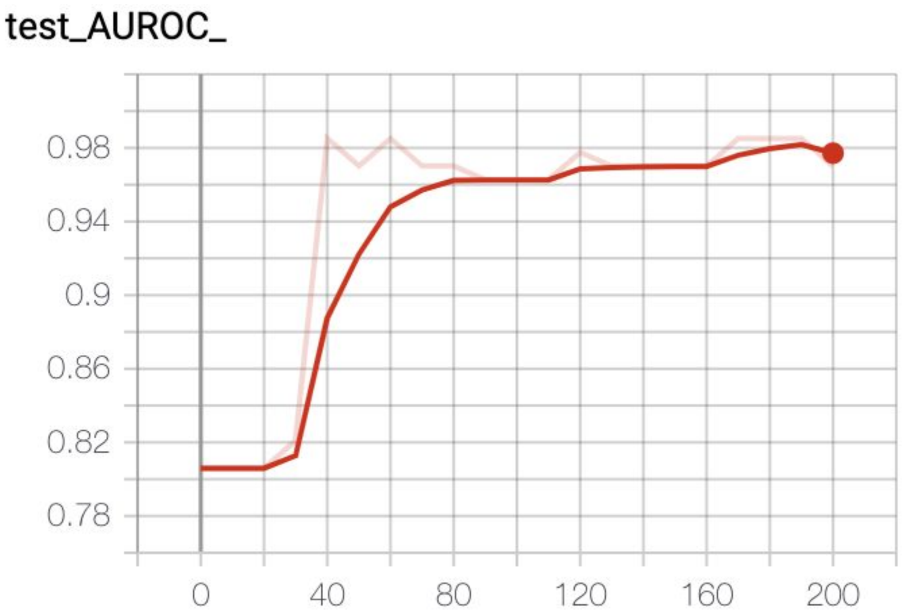


Single Query Matching

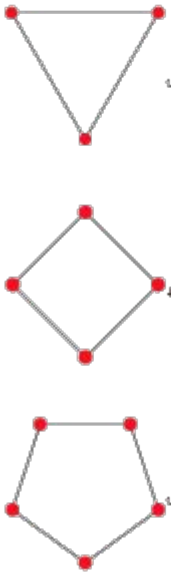


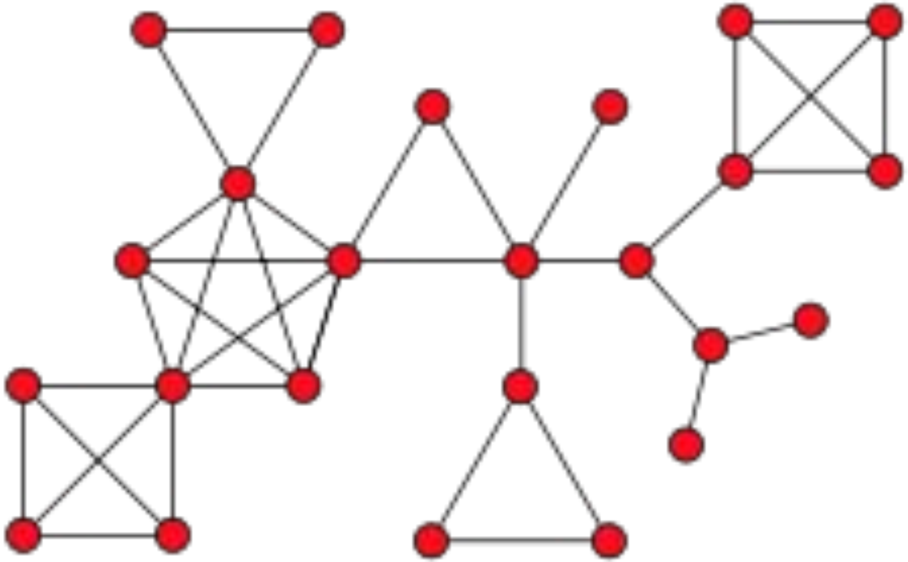
Single Query Matching



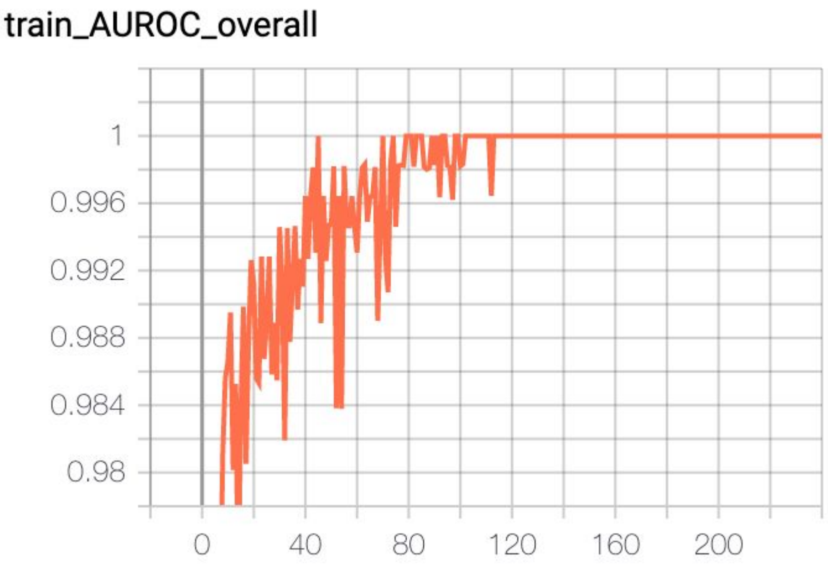


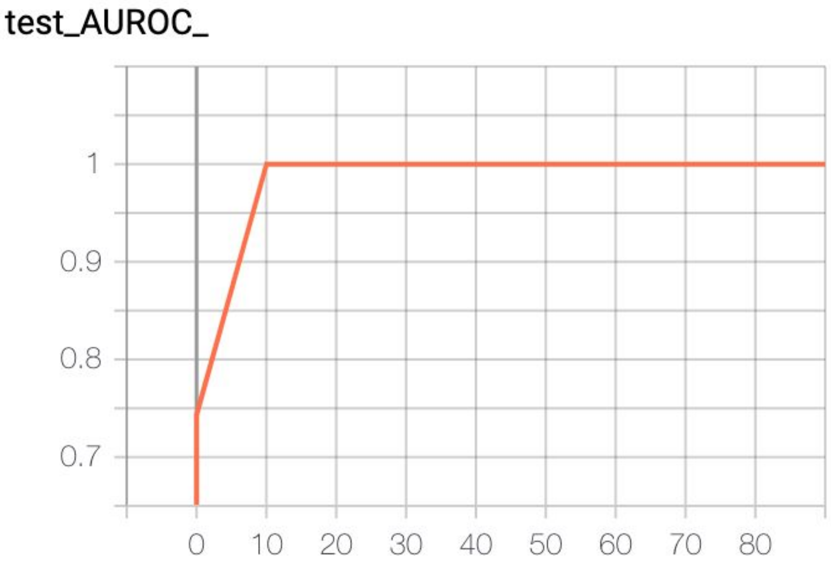
Family Classification



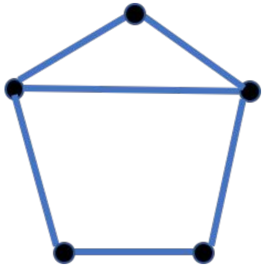


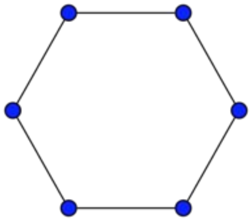
Family Classification

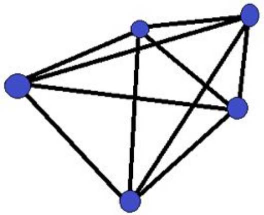


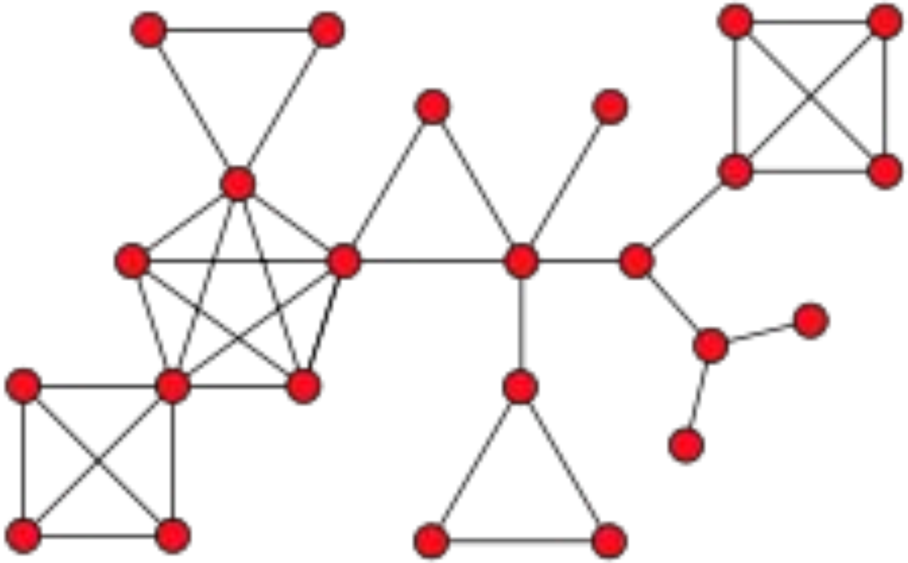


Generalizing

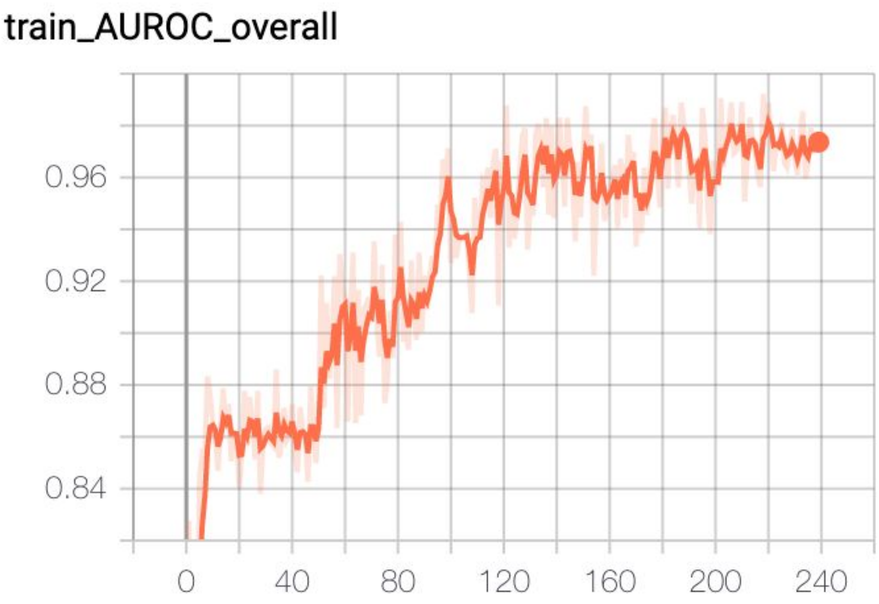


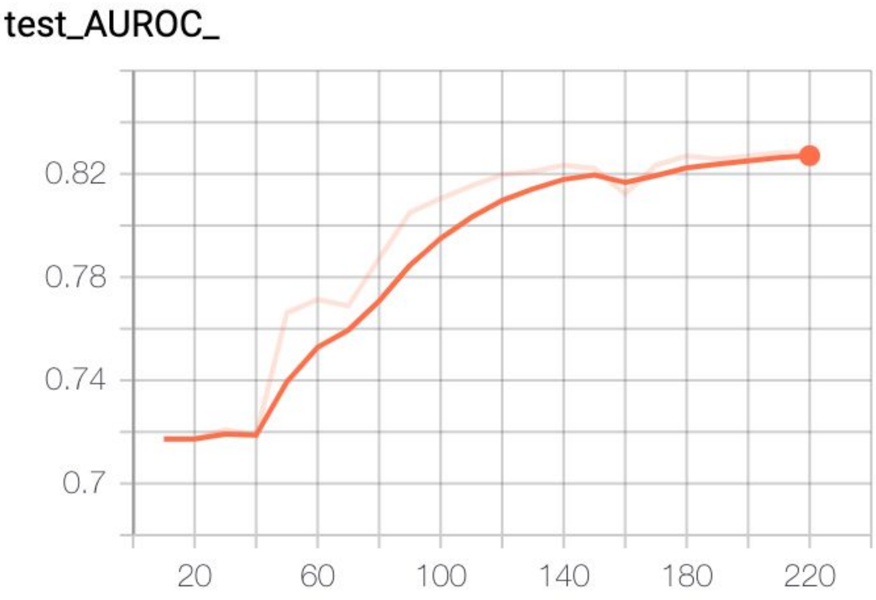




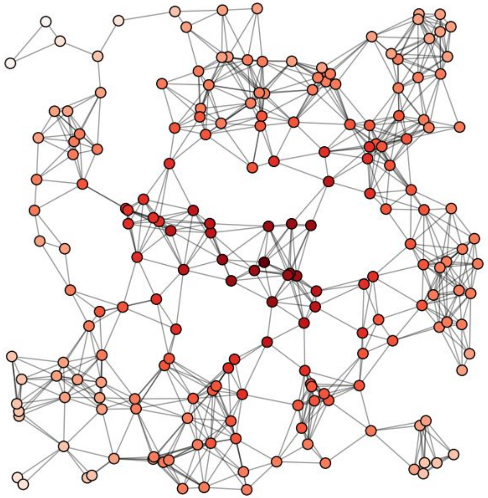


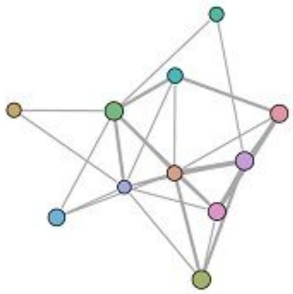
Generalizing

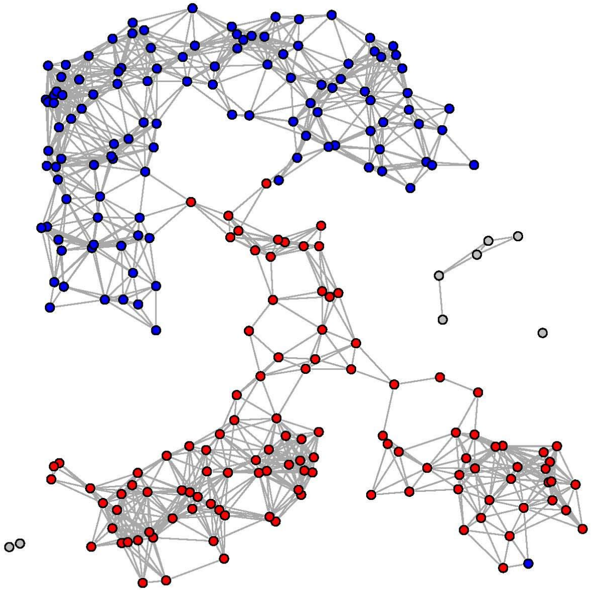




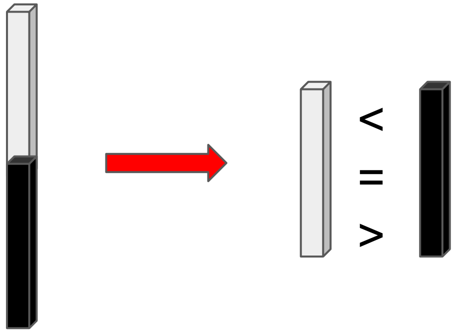
Random Training (In Progress)







Order embedding



- Query graph node embedding (Y),
  Test graph node embedding (X)

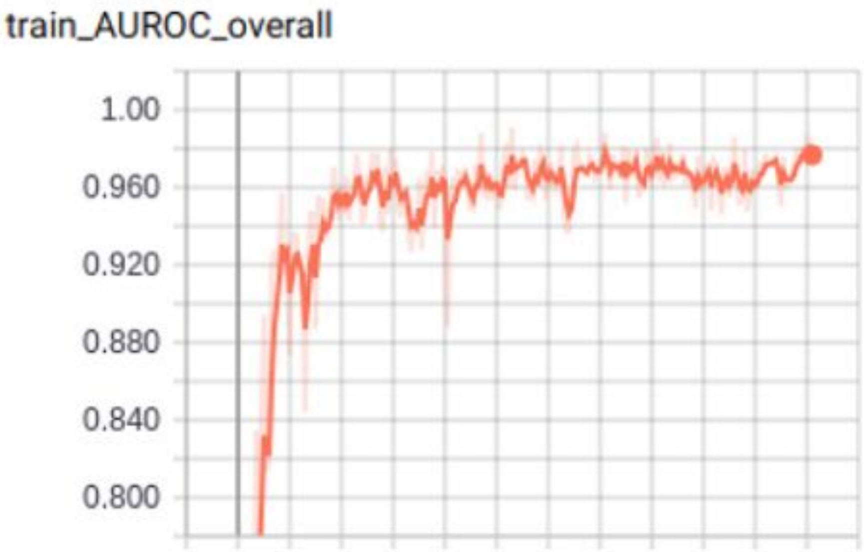
- Comparing embeddings directly reduces computational cost.

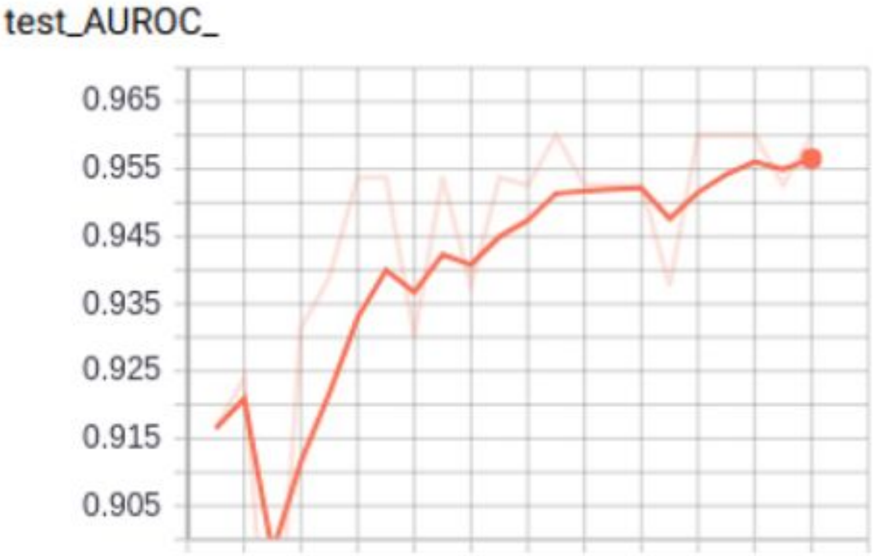
- Penalizing Order Violations: $E(x, y) = ||\max(0, y - x)||^2$
- Max-margin loss

$$\sum_{(u,v)\in P} E(f(u), f(v)) + \sum_{(u',v')\in N} \max\{0, \alpha - E(f(u'), f(v'))\}$$

- Hyperparameters introduced: Margin *a*, dimension threshold *b*

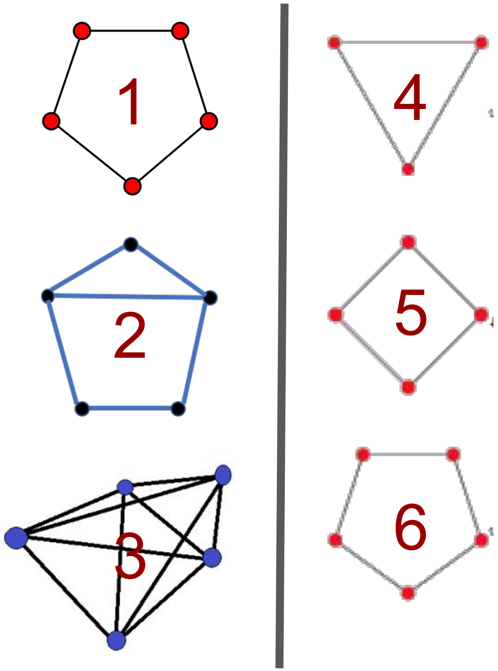
Order embedding on multi-query experiment





Order embedding Results

- Compare the node embeddings for common subgraph

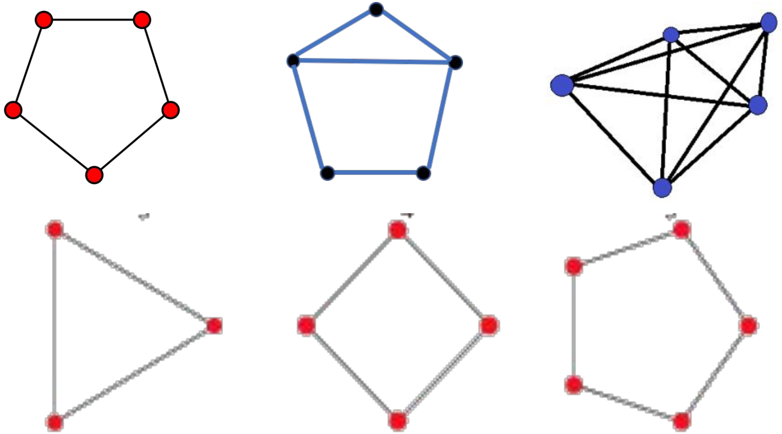


- ❑ 1 is subgraph of 2 and 2 is subgraph of 3.
- ❑ Node embeddings have dimension 60.
- ❑ Out of 60 elements,
  0 elements in embedding 1 > 2 (expect < 12)
  9 elements in embedding 2 > 3 (expect < 12)
  27 elements in embedding 4 > 5 (expect > 12)
  36 elements in embedding 5 > 6 (expect > 12)

Order embedding Results

1

2



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Conclusions & Future Work

- Delivered a Graph Convolutional Neural Network model for subgraph matching.
- Order embedding method was used to train node embeddings that can be compared directly to reduce computational cost.