0.1 i

First iteration:

- 1: 0.750
- 2: 0.750
- 4: 0.417
- 6: 0.625
- 7: 0.209
- 9: 0.406

Second iteration:

- 1: 0.875
- 2: 0.764
- 4: 0.324
- 6: 0.602
- 7: 0.162
- 9: 0.401

0.2 ii

Nodes belonging to class "+": 1, 2, 6

Nodes belonging to class "-": 4, 7, 9

i)

$b_1(x_1) = \frac{1}{Z}\phi_1(x_1)\Pi_{j \in N_1} m_{j1}(x_1)$

$= \frac{1}{Z}\phi_1(x_1)m_{21}(x_1)$

$= \frac{1}{Z}\phi_1(x_1)\Sigma_{x_2}\phi_2(x_2)\psi_{21}(x_2, x_1) \times m_{32}(x_2) \times m_{42}(x_2)$

$= \frac{1}{Z}\phi_1(x_1)\Sigma_{x_2}\phi_2(x_2)\psi_{21}(x_2, x_1)\Sigma_{x_3}\phi_3(x_3)\psi_{32}(x_3, x_2)\Sigma_{x_4}\phi_4(x_4)\psi_{42}(x_4, x_2)$

$= \Sigma_{x_2}\Sigma_{x_3}\Sigma_{x_4}\frac{1}{Z}\psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)\psi_{42}(x_2, x_4)\phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\phi_4(x_4)$

ii)

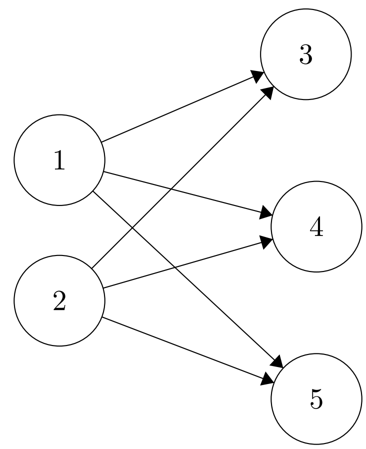
$p(x_1|y_1, y_2, y_3, y_4)$

$= \Sigma_{x_2}\Sigma_{x_3}\Sigma_{x_4}p(x_1, x_2, x_3, x_4|y_1, y_2, y_3, y_4)$

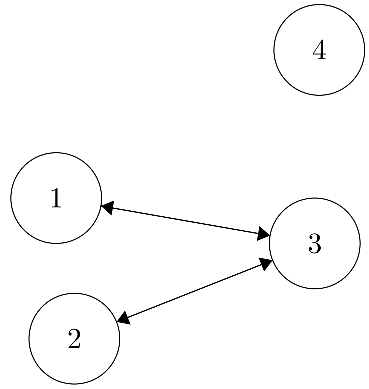
$= \Sigma_{x_2}\Sigma_{x_3}\Sigma_{x_4}\frac{1}{Z}\psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)\psi_{42}(x_2, x_4)\phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\phi_4(x_4)$

$= b_1(x_1)$

Suppose we have a graph as follows:



Suppose that we want to make node 1, 2 in the same class and 3, 4,5 in another class. One way to optimize this simpler loss function is just to make the embedding of every node similar to each other. In that way, the loss function can reach 0, but it is useless because it cannot distinguish test data.



In this example, suppose that 1-3 is a positive pair while 2-3 is a negative pair. If we optimize the no margin version of the loss function, one possible way of embedding is to make the distance between negative pair and positive pair the same. This is useless because with a new pair 3-4 which have the same distance as 1-3 or 2-3, it is impossible to tell if the new pair is positive or negative.

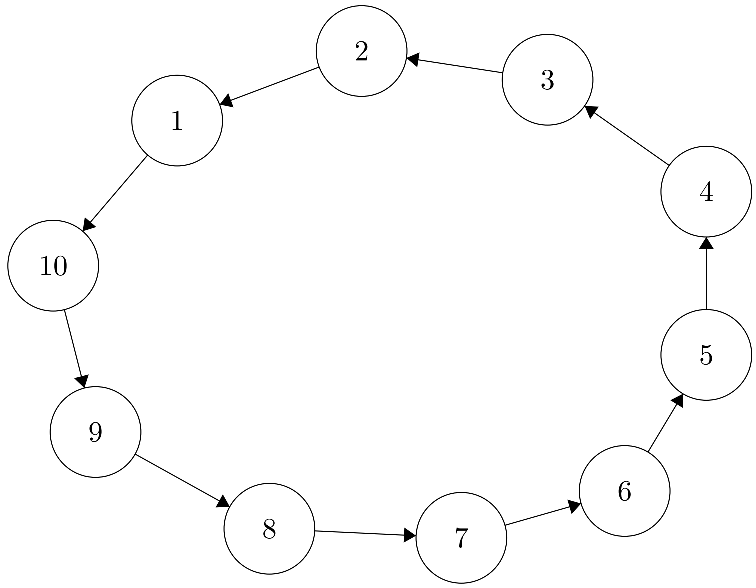
If the embedding is not normalized, length of the embedding is going to be taken into account in the training procedure. Because, of this, one way of minimizing the loss function is making the norm of the embedding vectors of one class large while the other one is small. However, in the training procedure, the positive pairs can come from both class. Therefore, it is hard to make data type from one class

In this graph, if the relationship l is symmetric, it cannot be expressed because $l(2) = 1$, but it cannot be said that $l(1) = 2$.

i)

There must be at least 3 layers of message passing to make these nodes distinguishable.

ii)



All nodes from 1 to 10 are classified as True. In order to perform this task, the GNN must have at least 5 layers because this is the minimum number of path you must take along all neighbors path of a node to make sure that a path is not part of a length 10 cycle.

i)

The transition matrix is $M_{ij} = A_{ij}/D_{ii}, \forall i, j$.

ii)

The transition matrix is $M_{ij} = \frac{1}{2} A_{ij}/D_{ii} + \frac{1}{N}$ with N being the number of nodes.

It is proved that GCN is a special form of Laplacian smoothing, and as you appy the symmetrically normalized Laplacian matrix many times, the value converge at $\frac{\sqrt{deg_i}}{\Sigma_i \sqrt{deg_i}}$.

i)

```
reachability = previous_reachability

for j in neighbor[i]:
    reachability |= reachable(previous_node)

return reachability

return False
```

ii)

$h_v^k = I_{\Sigma_{u \in N_i} h_u^{k-1} > 1 | h_v^{k-1} > 1}$ with I being an indicator function.

The number of nodes in CORA is 2168.

The number of graphs in ENZYMES is 480.

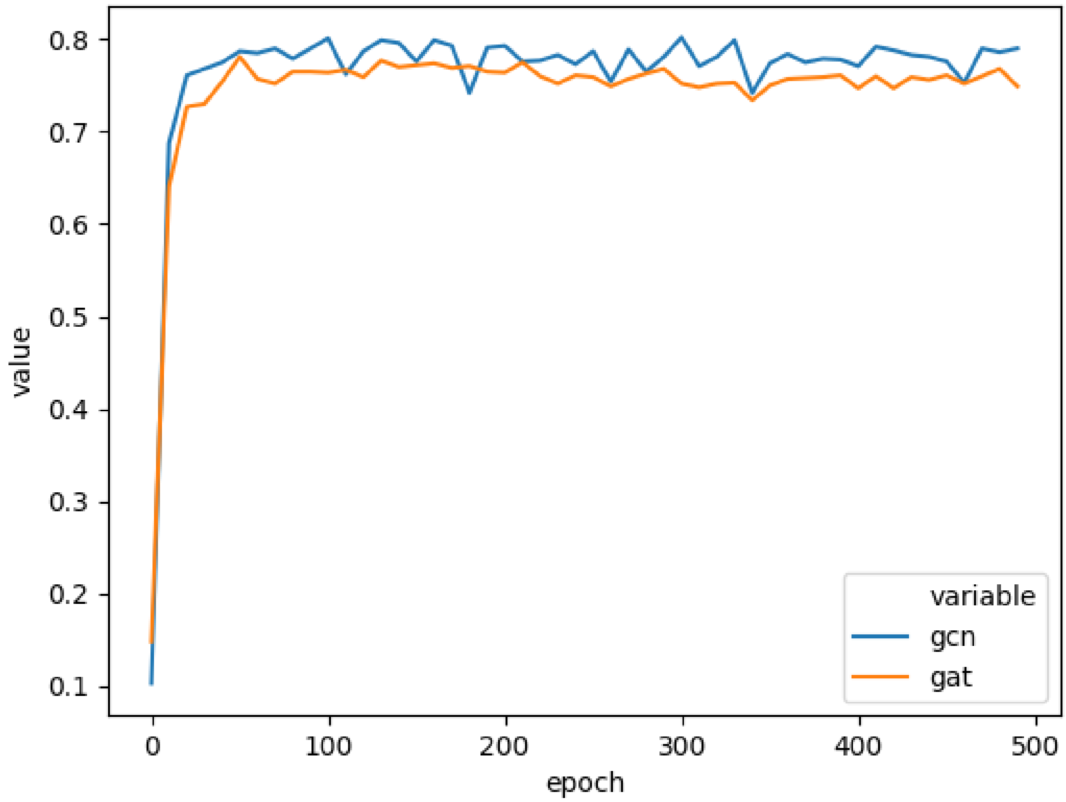


Figure 1: Node classification

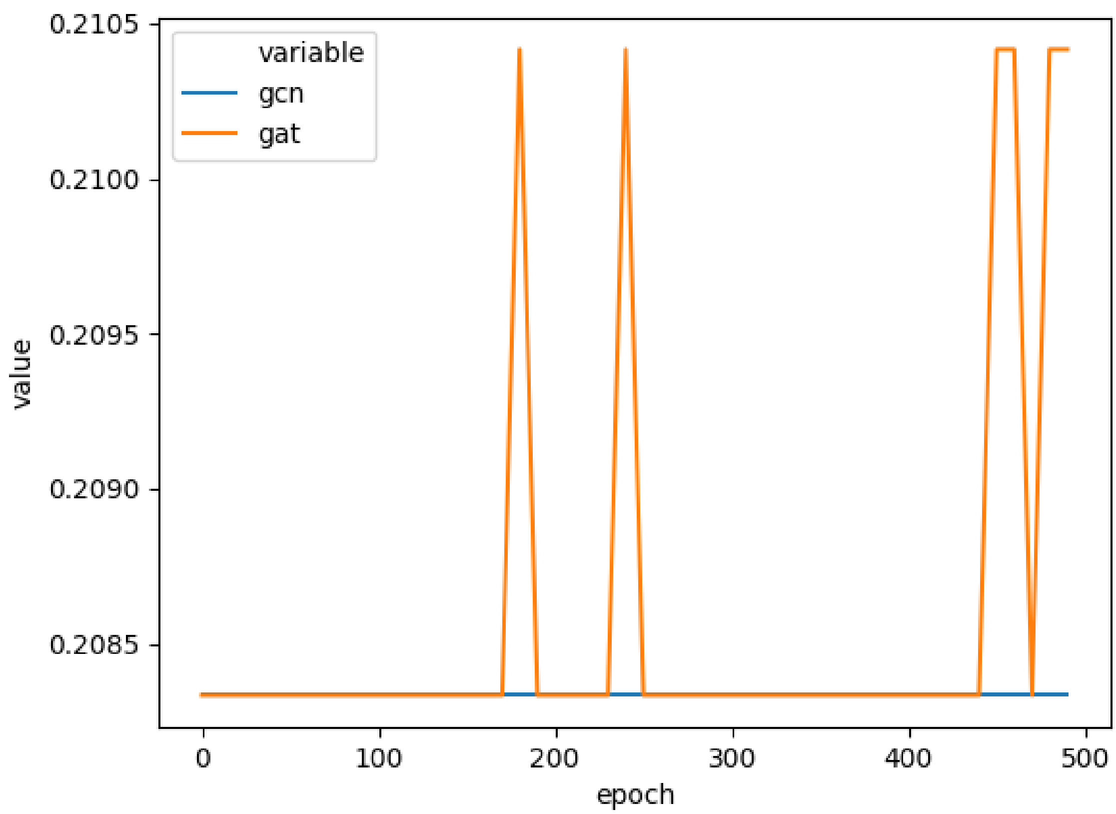


Figure 2: Graph Classification

Information sheet
CS224W: Machine Learning with Graphs

Assignment Submission Fill in and include this information sheet with each of your assignments. This page should be the last page of your submission. Assignments are due at 11:59pm and are always due on a Thursday. All students (SCPD and non-SCPD) must submit their homework via GradeScope (http://www.gradescope.com). Students can typeset or scan their homework. Make sure that you answer each (sub-)question on a separate page. That is, one answer per page regardless of the answer length. Students also need to upload their code on Gradescope. Put all the code for a single question into a single file and upload it.

Late Homework Policy Each student will have a total of *two* late periods. *Homework are due on Thursdays at 11:59pm PT and one late period expires on the following Monday at 11:59pm PT*. Only one late period may be used for an assignment. Any homework received after 11:59pm PT on the Monday following the homework due date will receive no credit. Once these late periods are exhausted, any assignments turned in late will receive no credit.

Honor Code We strongly encourage students to form study groups. Students may discuss and work on homework problems in groups. However, each student must write down their solutions independently, i.e., each student must understand the solution well enough in order to reconstruct it by him/herself. Students should clearly mention the names of all the other students who were part of their discussion group. Using code or solutions obtained from the web (GitHub/Google/previous year's solutions etc.) is considered an honor code violation. We check all the submissions for plagiarism. We take the honor code very seriously and expect students to do the same.

Your name: ______________________________

Email: ______________________ **SUID:** ______________________

Discussion Group: ______________________________

I acknowledge and accept the Honor Code.

(Signed) ______________________________