Data Analytics and Machine Learning Group
Department of Informatics
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Machine Learning for Graphs and Sequential Data

Exam:	IN2323 / Endterm	**Date:**	Wednesday 5$^{\text{th}}$ August, 2020
Examiner:	Prof. Dr. Stephan Günnemann	**Time:**	11:30 – 12:45

Working instructions

- This exam consists of **14 pages** with a total of **10 problems**.
  Please make sure now that you received a complete copy of the exam.
- The total amount of achievable credits in this exam is 43 credits.
- Detaching pages from the exam is prohibited.
- Allowed resources:
  - all materials that you will use on your own (lecture slides, calculator etc.)
  - **not allowed are any forms of collaboration between examinees and plagiarism**
- You have to sign the code of conduct.
- Make sure that the **QR codes are visible** on every uploaded page. Otherwise, we cannot grade your exam.
- Only write on the provided sheets, **submitting your own additional sheets is not possible**.
- Last two pages can be used as scratch paper.
- All sheets (including scratch paper) have to be submitted to the upload queue. Missing pages will be considered empty.
- **Only use a black or blue color (no red or green)!**
- Write your answers only in the provided solution boxes or the scratch paper.
- **For problems that say "Justify your answer" you only get points if you provide a valid explanation.**
- **For problems that say "Prove" you only get points if you provide a valid mathematical proof.**
- If a problem does not say "Justify your answer" or "Prove" it's sufficient to only provide the correct answer.
- Exam duration - 75 minutes.

Left room from __________ to __________ / Early submission at __________

Problem 1 **Normalizing Flows (4 credits)**

We consider two transformations $f_1(\boldsymbol{z}) = \begin{bmatrix} z_1 \\ z_2^{1/3} \end{bmatrix}$ and $f_2(\boldsymbol{z}) = \begin{bmatrix} z_1(|z_2| + 1) \\ z_2 \end{bmatrix}$ from $\mathbb{R}^2$ to $\mathbb{R}^2$.

The respective inverse transformation are $f_1^{-1}(\boldsymbol{x}) = \begin{bmatrix} x_1 \\ x_2^3 \end{bmatrix}$ and $f_2^{-1}(\boldsymbol{x}) = \begin{bmatrix} \frac{x_1}{|x_2|+1} \\ x_2 \end{bmatrix}$.

The respective Jacobians are

$$J_{f_1} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{3}z_2^{-\frac{2}{3}} \end{bmatrix} \qquad J_{f_2} = \begin{bmatrix} |z_2| + 1 & \mathrm{sign}(z_2)z_1 \\ 0 & 1 \end{bmatrix}$$

$$J_{f_1^{-1}} = \begin{bmatrix} 1 & 0 \\ 0 & 3x_2^2 \end{bmatrix} \qquad J_{f_2^{-1}} = \begin{bmatrix} \frac{1}{|x_2|+1} & \frac{-\mathrm{sign}(x_2)x_1}{(|x_2|+1)^2} \\ 0 & 1 \end{bmatrix}$$

0
1
2
3
4

We assume a Gaussian base distribution $p_1(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$. We observed one point $\boldsymbol{x}_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

We propose to stack the transformations f_1, f_2 to transform the base distribution p_1 in the distribution p_2 with normalizing flows. Compute the likelihood for $\boldsymbol{x}$ under the transformed distribution p_2 if the order of transformations is f_1 followed by f_2.

Hint: You might use the density of the unit variate Gaussian $p = \mathcal{N}(0, 1)$ at the following points: $p(1/2) = 0.3521$, $p(1/3) = 0.3774$, $p(1/9) = 0.3965$, $p(5) = 1.4867e^{-06}$, $p(8) = 5.0523e^{-15}$, $p(10) = 7.6946e^{-23}$

Problem 2 Variational Inference (5 credits)

We are performing variational inference in some latent variable model $p_\theta(x, z)$ using the following family of variational distributions $\mathcal{Q}_1 = \{\mathcal{N}(z|\phi, 1) : \phi \in \mathbb{R}\}$.

a) Assume that the variational distribution $q \in \mathcal{Q}_1$ is fixed, and we are trying to maximize the ELBO w.r.t. θ using gradient ascent. Is it necessary to use the reparametrization trick in this case? If yes, explain how to do it for our family of distributions $\mathcal{Q}_1$; if not, provide a justification.

0
1
2
3

b) Consider another family of distributions $\mathcal{Q}_2 = \{\mathcal{N}(z|0, s^2) : s \in (0, \infty)\}$. Which of the following statements is true? Justify your answer.

0
1
2

1. $\max_{\theta, q \in \mathcal{Q}_1} \text{ELBO}(\theta, q) < \max_{\theta, q \in \mathcal{Q}_2} \text{ELBO}(\theta, q)$
2. $\max_{\theta, q \in \mathcal{Q}_1} \text{ELBO}(\theta, q) = \max_{\theta, q \in \mathcal{Q}_2} \text{ELBO}(\theta, q)$
3. $\max_{\theta, q \in \mathcal{Q}_1} \text{ELBO}(\theta, q) > \max_{\theta, q \in \mathcal{Q}_2} \text{ELBO}(\theta, q)$
4. It's impossible to tell without additional information.

Problem 3 Robustness of Machine Learning Models (6 credits)

Suppose we have trained a binary classifier $f : \mathbb{R}^d \to \{0, 1\}$ and want to certify its robustness via randomized smoothing. Therefore, the *smoothed classifier* $g_{\sigma^2}(\boldsymbol{x}) = \mathbb{E}\left[\mathbb{I}\left[f(\boldsymbol{x} + \varepsilon) = 1\right]\right]$, where $\varepsilon \sim \mathcal{N}(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$.

Fact: $\Phi^{-1}(g_{\sigma^2}(\boldsymbol{x}))$ is $1/\sigma$-**Lipschitz** w.r.t. $\boldsymbol{x}$ and the L_2 norm, where $\Phi(z)$ denotes the cumulative distribution function (CDF) of the standard normal distribution.

0 1 2 3 4

a) **Using the above fact about the Lipschitz-continuity** of $\Phi^{-1}(g_{\sigma^2}(\boldsymbol{x}))$, show that the largest certifiable L_2 radius r around a sample $\boldsymbol{x}$ is identical to the result shown in the lecture. More precisely, show that

$$r = \sigma \Phi^{-1}(g_{\sigma^2}(\boldsymbol{x})).$$

Hint: You may assume we can evaluate $g_{\sigma^2}(\boldsymbol{x})$ in closed form and you may use the following results: $\lim_{z \to 0} \Phi^{-1}(z) = -\infty, \quad \Phi^{-1}(0.5) = 0, \quad \lim_{z \to 1} \Phi^{-1}(z) = \infty$.

0 1 2

b) A fellow student has a promising idea: by letting $\sigma \to \infty$ we can make the Lipschitz constant of the smoothed classifier arbitrarily small, leading to arbitrarily large certifiable radii, i.e. a very robust model. Is this a good idea? Why or why not?

$$x^* = \phi\left(\phi^{-1} g_{\sigma^2}(x) - \frac{r}{\sigma}\right) > 0.5$$

$$\phi^{-1} g_{\sigma^2}(x) > \frac{r}{\sigma}$$

If robust $= 0.5$

$$r = \sigma \cdot \phi^{-1} g_{\sigma^2}(x)$$

$$\|(\boldsymbol{W}\mathbf{x}_1 + \boldsymbol{b}) - (\boldsymbol{W}\mathbf{x}_2 + \boldsymbol{b})\|_p \leq k\|\mathbf{x}_1 - \mathbf{x}_2\|_p$$

$$\|\phi^{-1} g_{2\sigma^2}(x) - \phi^{-1}(0.5)\|_2 \leq \frac{1}{\sigma}\|x - \tilde{x}\|_2$$

$$\|x - \tilde{x}\|_2 = r \geq \sigma \phi^{-1} g_{2\sigma_2}(x)$$

NO

$\sigma \to \infty$, $\Rightarrow$ large radius $\Rightarrow$ more noisy and other class data $\Rightarrow$ no certifying

loss accuracy

Problem 4 **Markov Property (3 credits)**

We consider the following sequences of random variables $U_0, U_1, \dots, U_t$.

a) $U_t = \begin{bmatrix} X_t \\ Z_t \end{bmatrix}$ where X_t are observed variables and Z_t are latent variables of an Hidden Markov Model. Does the sequence of variables U_t fulfill the Markov property i.e. $P(U_t|U_{t-1}) = P(U_t|U_{t-1}, ..., U_0)$? Justify your answer.

0
1

b) We consider an AR(p) process X_t. Under what condition on p and k does the sequence of variables $U_t = [X_{t-1}, ..., X_{t-k}]$ fulfill the Markov property i.e. $P(U_t|U_{t-1}) = P(U_t|U_{t-1}, ..., U_0)$? Justify your answer.

0
1

c) We consider a recurrent neural network which produces X_t. Does the sequence of variables $U_t = X_t$ fulfill the Markov property i.e. $P(U_t|U_{t-1}) = P(U_t|U_{t-1}, ..., U_0)$? Justify your answer.

0
1

Q4

a) ~~Nope~~

~~unobserved variables $\Rightarrow$ Markov property~~

~~$p(z_t | z_{t-1}, \dots, z_1) = p(z_t | z_{t-1})$~~

observe varing $\Rightarrow$ nonmarkov

$p(x_t | z_t) = p(x_t | z_t, z_{t-1}, \dots z_1, x_{t-1}, \dots 1)$

Yes x_t and z_t are c independ- of x_{t-2} z_{t-2} ..
give z_{t-1}

b) $p(V_t | V_{t-1}, \cdots, V_0)$

$= p(x_{t-1}, \cdots, x_{t-k} | x_{t-2}, \cdots, x_0)$

$= p(x_{t-1} | x_{t-2}, \cdots, x_0)$ $\Leftarrow$ AR(p)

$= p(x_{t-1} | x_{t-2}, \cdots, x_{t-p-1})$

$p(V_t | V_{t-1})$

$= p(x_{t-1}, \cdots x_{t-k} | x_{t-2}, \cdots, x_{t-k-1})$

$= p(x_{t-1} | x_{t-2}, \cdots, x_{t-k-1})$

$p \leq k$

c) hidden state

Problem 5 Markov Chain (3 credits)

0
1
2
3

We consider a Markov chain X_t in $\{1, C\}$ with parameters $\pi, \boldsymbol{A}$. We assume we observed the sequence $S_k = [\underbrace{v_0, \ldots, v_0}_{k \text{ times}}, \underbrace{v_1, \ldots, v_1}_{k \text{ times}}, \ldots, \underbrace{v_T, \ldots, v_T}_{k \text{ times}}]$ where each value is observed k times. The parameter k can be seen as a discretization parameter of the time space.

Compute the likelihood of the sequence under the parameters $\pi, \boldsymbol{A}$ i.e. $P_{\pi,\boldsymbol{A}}(S_k)$. What happens to this quantity if you increase the discretization parameter from k to $k' > k$ but keep the same model parameter $\pi, \boldsymbol{A}$?

$$P(X_{t+1}=j \mid X_t = i) = A_{ij} \quad P(X_1 = k) = \pi_k .$$

$$P(S_k) = \pi_{v_0} \times \underbrace{\prod_{0}^{T-1} A_{v_t, v_{t+1}}}_{v_t \to v_{t+1}} \times \underbrace{\prod_{0}^{T} A_{v_t, v_t}^{k-1}}_{v_t \to v_t}$$

$$A \leq 1 , \; k \uparrow , \; P \downarrow .$$

Problem 6 **Temporal Point Process (6 credits)**

Consider an inhomogeneous Poisson process (IPP) on the interval $[0, 4]$ with the intensity function

$$\lambda(t) = \begin{cases} a & \text{if } t \in [0, 3] \\ b & \text{if } t \in (3, 4] \end{cases}$$

where $a > 0$, $b > 0$ are some positive parameters.

a) Assume that you observed a sequence of events $\{0.2, 1.0, 1.5, 2.9, 3.1, 3.8\}$ generated by the above IPP. What is the maximum likelihood estimate of the parameters a and b?

0 1 2 3 4

b) Assume that $a = 1$ and $b = 5$. What is the expected number of events generated by the IPP in this case?

0 1 2

$$P(\{\cdots\}) = \lambda(t_1)\cdots\lambda(t_n)\cdot\exp\left(-\int_0^T \lambda(u)\,du\right)$$

$$\log P = \log\lambda(t_1) + \cdots \log\lambda t_n - \left[3a + b\right]$$

$$= 4\log a + 2\log b - 3a - b$$

$$\frac{\partial l}{\partial a} = \frac{4}{a} - 3 = 0 \qquad a = \frac{4}{3}$$

$$\frac{\partial l}{\partial b} = \frac{2}{b} - 1 = 0 \qquad b = 2$$

$$\# \int_0^T \lambda(u)\,du$$

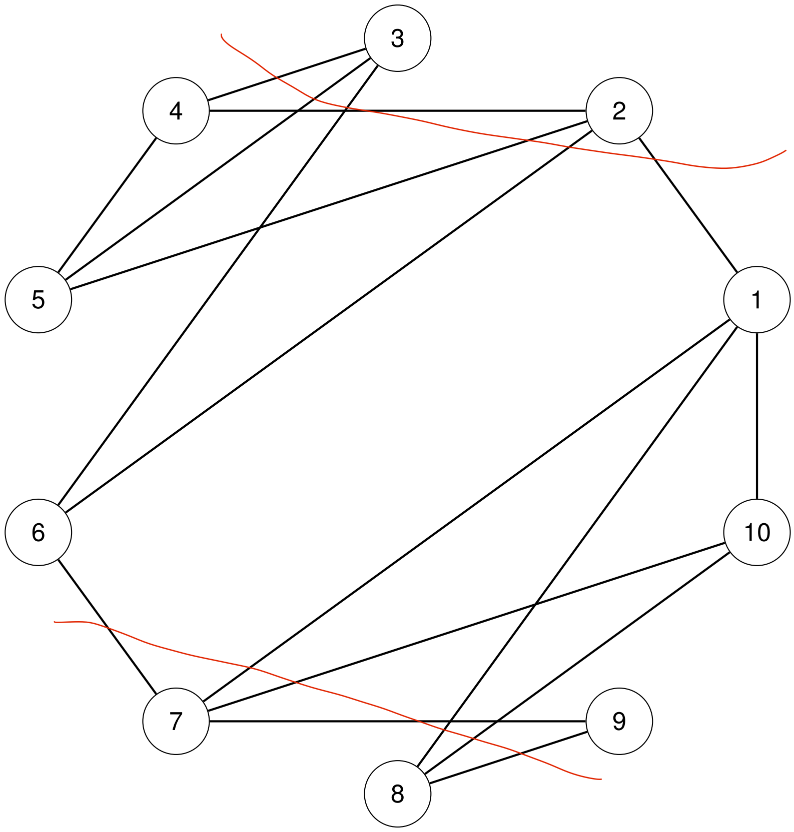
$$= au\Big|_0^3 + bu\Big|_3^4$$

$$= 3 + 5 = 8$$

Problem 7 Clustering with the Planted Partition Model (4 credits)

0
1
2
3
4

The following graph has been generated from a planted partition model with in-community edge probability p and between-community edge probability q.



Assuming $p < q$, find the maximum likelihood community assignments under a PPM.
Give your solution as two sets of node labels making up the two discovered communities. Justify your answer.

PPM → 2 cluster

$p < q$ more edge between community

$$\left(\frac{(1-p)q}{(1-q)p}\right)^{E_{cut}(z)}$$

$p < q \Rightarrow p > 1$

Find maximum cut

Problem 8 PageRank in a Wheel (6 credits)

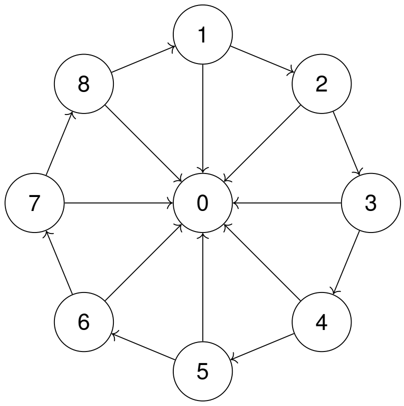


Figure 8.1: Example of a directed wheel graph with $n + 1 = 9$ nodes

Consider a directed graph of size $n + 1$ with a cycle of n nodes and an additional central node that every other node connects to (see figure). So we have a graph with node set $\mathcal{V} = \{0, 1, \dots, n\}$ and edge set

$$\mathcal{E} = \{(i, i+1) \mid i \in \{1, \dots, n-1\}\} \cup \{(n, 1)\} \cup \{(i, 0) \mid i \in \{1, \dots, n\}\}.$$

We want to compute the PageRank scores with a link-follow probability of β (a teleport probability of $1 - \beta$) and some arbitrary teleport vector $\boldsymbol{\pi}$, $\sum_{i=0}^{n} \pi_i = 1$. Note that we index $\boldsymbol{\pi}$ from 0 to n.
We define the predecessor function pa as the index of the predecessor of a node in the directed cycle, i.e.

$$\mathrm{pa}(1) = n \quad \text{and} \quad \mathrm{pa}(i) = i - 1 \;\; \forall i \in \{2, \dots, n\}.$$

You can write $\mathrm{pa}^k(i)$ for the k-th predecessor of node i, i.e. $\mathrm{pa}^3(i) = \mathrm{pa}(\mathrm{pa}(\mathrm{pa}(i)))$ and $\mathrm{pa}^0(i) = i$.

a) Set up the PageRank equations for all nodes in scalar form, i.e. each r_i separately instead of matrix form. 0 1 2

b) Why is this graph problematic for PageRank without random teleportation ($\beta = 1$)? 0 1

$$r_1 = \beta \frac{r_n}{2} + (1-\beta)\pi_1$$

$$r_n = \beta \frac{r_{n-1}}{2} + (1-\beta)\pi_n$$

$$r_{n-1} = \frac{\beta}{2} r_{n-2} + (1-\beta)\pi_{n-1}$$

$$r_1 = \frac{\beta}{2}\left(\frac{\beta}{2} r_{n-1}\right) + \frac{\beta}{2}(1-\beta)\pi_n + (1-\beta)\pi_1$$

$$r_1 = \frac{\beta}{2}\left(\frac{\beta}{2}\cdot\left(\frac{\beta}{2} r_{n-2}\right)\right) + \left(\frac{\beta}{2}\right)^2 \cdot (1-\beta)\pi_{n-1} + \cdots$$

$$r_1 = \left(\frac{\beta}{2}\right)^n r_1 + (1-\beta)\cdot\sum_{i+1}^{n}$$

$$r_i = \beta \frac{r_{pa(i)}}{2} + (1-\beta)\pi_i \qquad i \in \{1,\dots,n\}$$

$$r_0 = \beta \sum_{i}^{n} \frac{r_i}{2} + (1-\beta)\pi_0$$

node 0 is disconnected from other part

can't jump out dead end

0
1
2
3

c) Show that the PageRank for node $i \in \{1, \ldots, n\}$ in the outer cycle is given by

$$r_i = \frac{(1-\beta)}{1-\left(\frac{\beta}{2}\right)^n} \sum_{j=0}^{n-1} \left(\frac{\beta}{2}\right)^j \pi_{\mathrm{pa}^j(i)}.$$

c) Show that the PageRank for node $i \in \{1, \dots, n\}$ in the outer cycle is given by

$$r_i = \frac{(1-\beta)}{1-\left(\frac{\beta}{2}\right)^n} \sum_{j=0}^{n-1} \left(\frac{\beta}{2}\right)^j \pi_{\mathrm{pa}^j(i)}.$$

$r_i = \beta \frac{r_{pa(i)}}{2} + (1-\beta)\pi_i \qquad i \in \{1, \dots, n\}$

$r_1 = \beta \cdot \frac{r_n}{2} + (1-\beta)\pi_1 \quad = \frac{\beta}{2} \cdot \frac{\beta}{2} \cdot r_{n-1} + \frac{\beta}{2}(1-\beta)\pi_n + (1-\beta)\pi_1$

$\left(\frac{\beta}{2}\right)^{n-1}(1-\beta)\pi_2$ ...

$r_n = \beta \cdot \frac{r_{n-1}}{2} + (1-\beta)\pi_n \quad = \frac{\beta}{2} \cdot \frac{\beta}{2} \cdot \frac{\beta}{2} \cdot r_{n-2} + \left(\frac{\beta}{2}\right)^2 (1-\beta)\pi_{n-1}$

$+ \frac{\beta}{2}(1-\beta)\pi_n$

$+ (1-\beta)\pi_1$

$\Rightarrow pa^k(1)$

$r_{n-1} = \beta \cdot \frac{r_{n-2}}{2} + (1-\beta) \cdot \pi_{n-1}$

$\vdots$

$r_2 = \beta \cdot \frac{r_1}{2} + (1-\beta)\pi_2 \quad = \left(\frac{\beta}{2}\right)^n r_1 + (1-\beta) \sum_{k=0}^{n-1} \left(\frac{\beta}{2}\right)^k \pi_{pa^k(1)}$

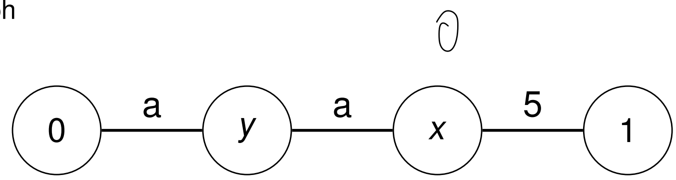
$r_i = \left(\frac{\beta}{2}\right)^n r_i + (1-\beta) \sum_{k=0}^{n-1} \left(\frac{\beta}{2}\right)^k \pi_{pa^k(i)}$

$r_i = \frac{1-\beta}{1-\left(\frac{\beta}{2}\right)^n} \sum_{k=0}^{n-1} \left(\frac{\beta}{2}\right)^k \pi_{pa^k(i)}$

Problem 9 **Label Propagation (4 credits)**

0
1
2
3
4

Consider the following graph



The nodes labeled 0 and 1 are observed and from class 0 and 1, respectively. One edge has a fixed weight, the other two have a variable edge weight of $a \geq 0$. The two center nodes are unobserved and we call their labels x and y.

We want to predict classes for the two center nodes that minimize the Label Propagation objective exactly,

$$\frac{1}{2} \sum_{ij} W_{ij} \left(y_i - y_j\right)^2$$

where W is the weighted adjacency matrix and y_i, y_j are the labels of the nodes.

Find the set of all possible edge weights a that guarantee that node x is assigned to class 0. Justify your answer.

$$a \cdot (0-y)^2 + a(x-y)^2 + 5(1-x)^2$$

$$ay^2 + ax^2 - 2axy + ay^2 + 5 - 10x + 5x^2$$

$x=0 \quad y=0 \quad \Rightarrow E=5$

$x=1 \quad y=0 \quad \Rightarrow E=a$

$x=0 \quad y=1 \quad \Rightarrow E=2a+5$

$x=1 \quad y=1 \quad \Rightarrow E=a$

$\underline{\underline{a>5}} \qquad a > 2a+5$

$-a>5$

$a<-5$

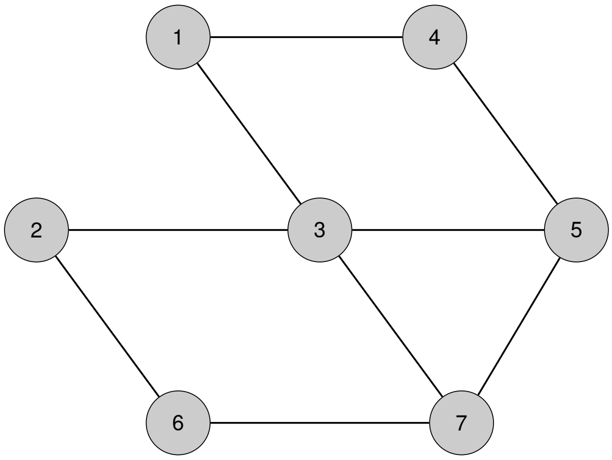
contr

Problem 10 Adversarial Attacks on Graph Neural Networks (2 credits)

Suppose you are given the following two-layer graph neural network.

$$f(\boldsymbol{A}, \boldsymbol{X}) = \boldsymbol{Z} = \text{Softmax}\left(\hat{\boldsymbol{A}}\text{ReLU}\left(\hat{\boldsymbol{A}}\boldsymbol{X}\boldsymbol{W}_1\right)\boldsymbol{W}_2\right)$$

$\boldsymbol{X} \in \mathbb{R}^{N\times D}$ are the node features, $\boldsymbol{Z}$ are the node predictions, $\boldsymbol{W}_x$ are weight matrices of appropriate dimensions and $\hat{\boldsymbol{A}} = \tilde{\boldsymbol{D}}^{-\frac{1}{2}}\tilde{\boldsymbol{A}}\tilde{\boldsymbol{D}}^{-\frac{1}{2}}$ is the propagation matrix as defined for GCNs. Here, $\tilde{\boldsymbol{A}} = \boldsymbol{A} + \boldsymbol{I}$, where $\boldsymbol{A}$ is the adjacency matrix and $\boldsymbol{I}$ is the identity matrix, and $\tilde{\boldsymbol{D}}$ is a diagonal matrix of node degrees $\tilde{\boldsymbol{D}}_{ii} = \sum_j \tilde{\boldsymbol{A}}_{ij}$.
The model was trained for the task of semi-supervised node classification, and we want to predict a class c for node 6 in the following graph $\boldsymbol{A}$:



0
1
a) An adversary with complete knowledge about the graph $\boldsymbol{A}$ and the trained model $f(\boldsymbol{A}, \boldsymbol{X})$ may delete one edge to perturb the prediction for node 6. Deleting which of the following edges would lead to a greater change to the prediction for node 6? Justify your answer.

1. The edge connecting node 5 and 7
2. The edge connecting node 3 and 5
3. There is not enough information to determine which deletion leads to a greater change.

0
1
b) Assume we instead have a Personalized Propagation of Neural Predictions (PPNP) model instead of the two-layer GCN. How does this affect your choice? Justify your answer.

① 5 - 7

Two layer Network.

3-5 decline after GCN

②

limit - infinite propagation

each node influence other node

not enough information

Additional space for solutions–clearly mark the (sub)problem your answers are related to and strike out invalid solutions.