Data Analytics and Machine Learning
Department of Informatics
Technical University of Munich

Eexam
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- During the attendance check a sticker containing a unique code will be put on this exam.
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# Machine Learning for Graphs and Sequential Data

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| **Exam:** | IN2323 / Endterm | **Date:** | Friday 19th August, 2022 |
| **Examiner:** | Prof. Dr. Stephan Günnemann | **Time:** | 08:15 – 09:30 |

| | P 1 | P 2 | P 3 | P 4 | P 5 | P 6 | P 7 | P 8 | P 9 |
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## Working instructions

- This exam consists of **16 pages** with a total of **9 problems**.
  Please make sure now that you received a complete copy of the exam.
- The total amount of achievable credits in this exam is 72 credits.
- Detaching pages from the exam is prohibited.
- Allowed resources:
  - one A4 sheet of handwritten notes (two sides, not digitally written and printed).
- **No other material (e.g. books, cell phones, calculators) is allowed!**
- Physically turn off all electronic devices, put them into your bag and close the bag.
- There is scratch paper at the end of the exam (after problem 9).
- Write your answers only in the provided solution boxes or the scratch paper.
- If you solve a task on the scratch paper, clearly reference it in the main solution box.
- All sheets (including scratch paper) have to be returned at the end.
- **Only use a black or a blue pen (no pencils, red or greens pens!)**
- **For problems that say "Justify your answer" you only get points if you provide a valid explanation.**
- **For problems that say "Derive" you only get points if you provide a valid mathematical derivation.**
- **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", "Derive" or "Prove", it is sufficient to only provide the correct answer.

Left room from ________ to ________ / Early submission at ________

## Problem 1 Generative models (6 credits)

Recall the variational autoencoder (VAE), which can be summarized by the following pseudocode

$$\begin{aligned} \mu, \sigma &= f_\theta(\mathbf{x}) \\ \epsilon &\sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \\ \mathbf{z} &= \epsilon * \sigma + \mu \\ \tilde{\mathbf{x}} &= g_\phi(\mathbf{z}), \end{aligned}$$

and is trained to model a distribution $p(\mathbf{x})$ via maximization of the evidence lower bound.
We now want to develop a VAE that can model a distribution of images conditioned on a label, i.e. $p(\mathbf{x} \mid y)$ where $\mathbf{x} \in \mathbb{R}^d$ is the image and $y$ is the label, for example, “dog” or “cat”.

0 1 2

a) Modify the above pseudocode for the VAE to condition the model on the label $y$. You can change the dimensions of functions’ domains and codomains if necessary.

0 1 2 3 4

b) After training is completed we want to sample new images from our variational autoencoder. Write the pseudocode to generate an image given a label $y$. You should use the solution to the previous problem as a starting point.

# Problem 2 Robustness (10 credits)

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We are interested in robustness certification for a model with discrete input data $\mathbf{x} \in \{0, 1, \dots, C\}^N$ and an adversary that changes exactly $\delta \in \mathbb{N}$ elements of $\mathbf{x}$.
The perturbation set can be expressed as

$$\mathcal{P}(\mathbf{x}) = \left\{ \tilde{\mathbf{x}} \in \{0, 1, \dots, C\}^N \middle| ||\mathbf{x} - \tilde{\mathbf{x}}||_0 = \delta \right\} \tag{2.1}$$

with $||\mathbf{x}||_0 = \sum_{n=1}^{N} \mathbb{I}[x_n \neq 0]$.
Specify a set of **linear constraints** on $\tilde{\mathbf{x}}$ to model the perturbation set in Eq. (2.1). You may introduce at most $\mathcal{O}(N)$ constraints and $\mathcal{O}(N)$ variables. You are allowed to use integer-valued variables.
*Note:* A linear constraint is an equality or inequality between two expressions that are **linear functions** of the variables.

## Problem 3 **Autoregressive models (8 credits)**

You are given an AR(3) model according to the formula

$$X_t = 17 + 4X_{t-1} + \frac{1}{4}X_{t-2} - X_{t-3} + \varepsilon_t \ ,$$

with independently distributed noise variables $\varepsilon_t \sim \mathcal{N}(0, \sigma)$.

0 1 2 3

a) Write down the characteristic polynomial $\Phi(z)$ and show that it can be factorised according to $(2 + z)\left(z^2 - \frac{9}{4}z + \frac{1}{2}\right)$.

0 1 2 3 4 5

b) Decide if the process $X_t$ is stationary. Justify your answer.

## Problem 4 Hidden Markov Models (10 credits)

Consider a hidden Markov model with 2 states $\{1, 2\}$ and 6 possible observations $\{\mathrm{p}, \mathrm{a}, \mathrm{n}, \mathrm{e}, \mathrm{r}, \mathrm{t}\}$. The initial distribution $\pi$, transition probabilities **A** and emission probabilities **B** are

$$\pi = \begin{array}{c} 1 \\ 2 \end{array} \begin{pmatrix} 1/5 \\ 4/5 \end{pmatrix} \qquad \mathbf{A} = \begin{array}{c} \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{pmatrix} 1/5 & 4/5 \\ 3/5 & 2/5 \end{pmatrix} \end{array} \qquad \mathbf{B} = \begin{array}{c} \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cccccc} \mathrm{p} & \mathrm{a} & \mathrm{n} & \mathrm{e} & \mathrm{r} & \mathrm{t} \end{array} \\ \begin{pmatrix} 0 & 1/5 & 0 & 2/5 & 0 & 2/5 \\ 1/5 & 1/5 & 1/5 & 1/5 & 1/5 & 0 \end{pmatrix} \end{array},$$

where $\mathbf{A}_{ij}$ specifies the probability of transitioning from state $i$ to state $j$.

a) You have observed the sequence $X = [\mathrm{pattern}]$. Specify all probability distributions $\mathbb{P}()$ that correspond to smoothing / offline inference on $X$.
*Note:* You do not need to perform any calculations or insert parameter values. 0 1 2

b) Write down the MAP objective given the observed sequence $X = [\mathrm{pattern}]$. 0 1

c) In another instance, you observe the sequence $X = [\mathrm{tea}]$. Given $X$, what is $\mathbb{P}(Z_3|X)$? [An unnormalised vector suffices]. Justify your answer. What is this type of inference called? 0 1 2 3 4 5 6 7

# Problem 5 Graph learning & Variational inference (10 credits)

Consider the following probabilistic model for generating a **directed, weighted** graph with $N$ nodes, continuous adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ and two communities, represented by vector $\mathbf{z} \in \{0, 1\}^N$:

$$p_\lambda(\mathbf{A} \mid \mathbf{z}) = \prod_{n=1}^{N} \prod_{m=1}^{N} p_\lambda(A_{n,m} \mid z_n, z_m) \tag{5.1}$$

$$p_\theta(\mathbf{z}) = \prod_{n=1}^{N} \text{Bern}(z_n \mid \theta) = \prod_{n=1}^{N} \theta^{z_n} \cdot (1 - \theta)^{1 - z_n} \tag{5.2}$$

with $\theta \in [0, 1]$. The conditional density $p_\lambda(A_{n,m} \mid z_n, z_m)$ will be specified later.
In the following, assume that we have observed a single graph $\mathbf{A} \in \mathbb{R}^{N \times N}$. We want to perform **mean-field variational inference** with variational family

$$q_\phi(\mathbf{z}) = \prod_{n=1}^{N} \text{Bern}(z_n \mid \phi_n) = \prod_{n=1}^{N} \phi_n^{z_n} \cdot (1 - \phi_n)^{1 - z_n}. \tag{5.3}$$

Note that $\phi \in [0, 1]^N$, i.e. we have one parameter per node.

0 1 2

a) Why is evaluating the ELBO $\mathcal{L}((\lambda, \theta), \phi) = \mathbf{E}_{\mathbf{z} \sim q_\phi}\left[\log p_{\lambda,\theta}(\mathbf{A}, \mathbf{z}) - \log q_\phi(\mathbf{z})\right]$ not tractable for large graphs (e.g. $N > 1000$)?

0 1 2 3 4

b) Assume that we approximate the ELBO with a single Monte Carlo sample $\mathbf{z} \in \{0, 1\}^N$, i.e.

$$\mathcal{L}((\lambda, \theta), \phi) \approx \log p_{\lambda,\theta}(\mathbf{A}, \mathbf{z}) - \log q_\phi(\mathbf{z}). \tag{5.4}$$

Let

$$p_\lambda(A_{n,m} \mid z_n, z_m) = \begin{cases} \lambda_1 \exp(-\lambda_1 A_{n,m}) & \text{if } A_{n,m} \geq 0 \land z_n = z_m, \\ \lambda_2 \exp(-\lambda_2 A_{n,m}) & \text{if } A_{n,m} \geq 0 \land z_n \neq z_m, \\ 0 & \text{else.} \end{cases}$$

with $\lambda_1, \lambda_2 > 0$. Assume that $\lambda_2$, $\theta$ and $\phi$ are fixed.
Prove that the optimal value of $\lambda_1$, i.e. the value that maximizes $\log p_{\lambda,\theta}(\mathbf{A}, \mathbf{z}) - \log q_\phi(\mathbf{z})$ is

$$\lambda_1^* = \frac{|\{n, m \mid z_n = z_m\}|}{\sum_{n,m \mid z_n = z_m} A_{n,m}}.$$

*Note:* You may also write on the next page.

c) To allow optimization w.r.t. $\phi$, we want to apply the reparameterization trick. Specify a base distribution $b(\epsilon)$ and a transformation $T(\epsilon, \phi)$ such that

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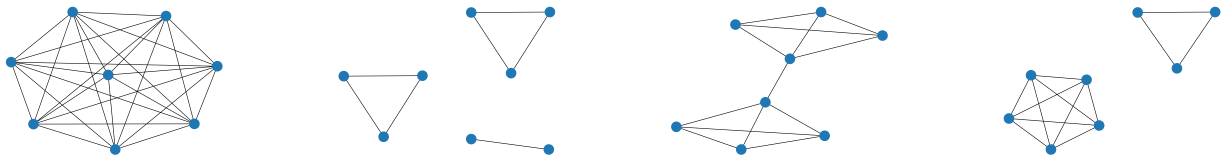
$$\mathbf{E}_{\mathbf{z}\sim q_\phi}\left[\log p_{\lambda,\theta}(\mathbf{A}, \mathbf{z}) - \log q_\phi(\mathbf{z})\right] = \mathbf{E}_{\epsilon\sim b}\left[\log p_{\lambda,\theta}(\mathbf{A}, T(\epsilon, \phi)) - \log q_\phi(T(\epsilon, \phi))\right]. \tag{5.5}$$

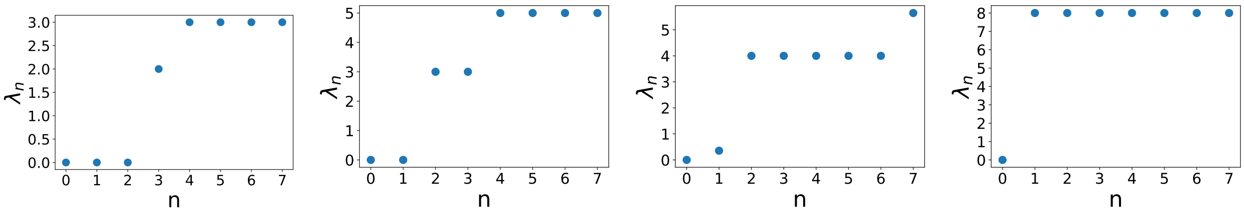
# Problem 6 Graphs – Laws & patterns (8 credits)

0 1 2 3 4 5 6 7 8

You are given four graphs (a-d), each consisting of eight nodes. You are further given four eigenspectra (1-4), i.e. eigenvalues of the graph Laplacian ordered in ascending order. Assign each of the graphs (a-d) to an eigenspectrum (1-4). Justify your answer.



(a) (b) (c) (d)




(1) (2) (3) (4)

# Problem 7 Page Rank (8 credits)

The PageRank scores (without teleports) of the graphs a-d have been computed with power iteration. Match the graphs a-d with the results 1-4. Justify your answer.

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1. Does not converge.
2. Does not converge.
3. Converges to $r_A = 0.167$, $r_B = 0.167$, $r_C = 0.167$, $r_D = 0.5$.
4. Converges to $r_A = 0.125$, $r_B = 0.375$, $r_C = 0.25$, $r_D = 0.25$.

## Problem 8 **Graph Neural Networks (6 credits)**

Below, you can find three different types of Graph Neural Network modules. The node embedding $h_u^{(t+1)}$ of node $u$ at layer $t+1$ is calculated with:

- Network Propagation (NP): $h_u^{(t+1)} = \sum_{v \in N(u) \cup \{u\}} h_v^{(t)}$
- Graph Convolution (GCN): $h_u^{(t+1)} = \phi_{gcn}(h_u^{(t)}, \oplus_{v \in N(u)} \psi_{gcn}(h_v^{(t)}))$
- Message Passing (MP): $h_u^{(t+1)} = \phi_{mp}(h_u^{(t)}, \oplus_{v \in N(u)} \psi_{mp}(h_v^{(t)}, h_u^{(t)}))$

where $\oplus$ is some permutation invariant function without learnable parameters, the functions $\psi_{gcn}, \psi_{mp}$ transform hidden features, functions $\phi_{gcn}, \phi_{mp}$ are update functions and $N(u)$ is the neighbourhood of node $u$.

0 1 2 3

a) Prove that network propagation is a special case of graph convolution.
*Hint:* You can do this by providing specific realizations of $\oplus$, $\psi_{gcn}$ and $\phi_{gcn}$.

0 1 2 3

b) Prove that graph convolution is a special case of message passing.
*Hint:* You can do this by providing specific realizations of $\psi_{mp}$ and $\phi_{mp}$.

## Problem 9 Limitations of Graph Neural Networks (6 credits)

a) Briefly explain two challenges when attacking GNNs using adversarial attacks.

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b) We model the absence or presence of an edge in a graph with $N$ nodes using a binary vector $\mathbf{x} \in \{0,1\}^{N^2}$. Now, we want to use randomized smoothing to certify that a smoothed classifer using GNNs as base-classifers is robust against attacks on the graph structure.

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Recall that a smoothed classifier $g(\mathbf{x})_c$ returns the probability that the base classifier $f$ classifies a smoothed sample $\tilde{\mathbf{x}} \sim \phi(\mathbf{x})$ as class $c$, i.e. $g(\mathbf{x})_c := \mathbb{P}(f(\phi(\mathbf{x})) = c)$ with a randomization scheme $\phi(\mathbf{x})$.

What is the problem when we want to use Gaussian noise as our randomization scheme? How could that problem be solved?

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