CTU
CZECH TECHNICAL UNIVERSITY IN PRAGUE

THESIS REVIEWER'S REPORT

I. IDENTIFICATION DATA

Thesis title:	**Out-of-Distribution Detection in GAS Chromatography Mass Spectrometry Data**
Author's name:	Pavel Linder
Type of thesis :	master
Faculty/Institute:	Faculty of Electrical Engineering (FEE)
Department:	Cybernetics
Thesis reviewer:	Ing. Vojtěch Franc, Ph.D.
Reviewer's department:	Cybernetics

II. EVALUATION OF INDIVIDUAL CRITERIA

Assignment — challenging

How demanding was the assigned project?

The diploma thesis was challenging due to the need to grasp an extensive literature in a rapidly evolving domain (out-of-distribution detection) and apply that knowledge to address a largely unexplored problem (chromatography data classification).

Fulfilment of assignment — fulfilled

How well does the thesis fulfil the assigned task? Have the primary goals been achieved? Which assigned tasks have been incompletely covered, and which parts of the thesis are overextended? Justify your answer.

The tasks set out in the thesis assignment were successfully accomplished by a considerable margin, with special praise deserving the comprehensive literature review section and the number of implemented OOD detection methods.

Methodology — correct

Comment on the correctness of the approach and/or the solution methods.

The approach used in the thesis seems reasonable for solving the problem at hand. I have one comment on the evaluation methodology used. Specifically, the performance of the compound classifier is evaluated on all in-distribution data, which would be fine if the OOD detector was perfect, which is obviously not the case. A more reasonable approach is to measure the ID classifier performance on ID sample accepted by the evaluated OOD detector, which reflects the performance in a real deployment. That is, the ID classifier performance should be evaluated for each OOD detector separately. This is not a serious error as the field of OOD detection is still evolving and suitable evaluation metrics have not been established in the community.

Technical level — B - very good.

Is the thesis technically sound? How well did the student employ expertise in the field of his/her field of study? Does the student explain clearly what he/she has done?

The thesis is technically sound up to a few inaccuracies, not fully unclear explanations and typos, which however do not overshadow the overall very good level of the work.

Formal and language level, scope of thesis — A - excellent.

Are formalisms and notations used properly? Is the thesis organized in a logical way? Is the thesis sufficiently extensive? Is the thesis well-presented? Is the language clear and understandable? Is the English satisfactory?

The thesis is well organized, has a logical structure, well-written text, and reads smoothly.

Knowledge of English is at a good level.

Selection of sources, citation correctness	A - excellent.
Does the thesis make adequate reference to earlier work on the topic? Was the selection of sources adequate? Is the student's original work clearly distinguished from earlier work in the field? Do the bibliographic citations meet the standards?	
The citations and references to previous works are at very good level.	

Additional commentary and evaluation (optional)

Comment on the overall quality of the thesis, its novelty and its impact on the field, its strengths and weaknesses, the utility of the solution that is presented, the theoretical/formal level, the student's skillfulness, etc.

Please insert your comments here.

III. OVERALL EVALUATION, QUESTIONS FOR THE PRESENTATION AND DEFENSE OF THE THESIS, SUGGESTED GRADE

Summarize your opinion on the thesis and explain your final grading. Pose questions that should be answered during the presentation and defense of the student's work.

Assessing the complexity of the assignment, the extent of work accomplished, and the technical proficiency demonstrated, the thesis surpasses the average by a considerable margin.

The grade that I award for the thesis is A - excellent.

Questions for the defense:

- It is claimed (page 48), that the "AUPR is more informative than AUROC" in case of imbalanced data. I would say the opposite because the AUPR depends on the prior distribution while AUROC does not. Please explain you statement.

- I've expressed concerns about the evaluation methodology for the ID classifier performance (see above). Do you share these concerns? If not, please provide a justification for the chosen approach.

Date: 01/18/24 Signature: