

# Assignment 15

## Graph neural networks (GNNs)

### EECE-6822 Machine Learning

Cris Ababei  
Electrical and Computer Engr., Marquette University

### 1. Objective

The objective of this activity is to run several code examples that study and illustrate various concepts related to Graph neural networks (GNNs).

### 2. Prerequisite Readings

Raschka

- Ch.18: Graph Neural Networks for Capturing Dependencies in Graph Structured Data

### 3. Code Examples

#### Example 2: Graph Neural Networks ←

This code example is from **Ch.18** from Sebastian Rashka's book:

[\*B3-Raschka] Sebastian Raschka, Yuxi Liu, and Vahid Mirjalili, *Learning with PyTorch and Scikit-Learn: Develop machine learning and deep learning models with Python*, Packt Publishing, 2022.

The source code (Jupyter Notebook) is located at the GitHub repository. You should read first the chapter itself from the book, before going through the code.

<https://github.com/rasbt/machine-learning-book/tree/main/ch18>

This chapter explores the following topics:

- An introduction to graph data and how it can be represented for use in deep neural networks
- An explanation of graph convolutions, a major building block of common GNNs
- A tutorial showing how to implement GNNs for molecular property prediction using PyTorch
- Geometric
- An overview of methods at the cutting edge of the GNN field

#### Example 3: Other tutorials

---A Gentle Introduction to Graph Neural Networks in Python

<https://machinelearningmastery.com/a-gentle-introduction-to-graph-neural-networks-in-python/>

---Tutorial 7: Graph Neural Networks

[https://uvadlc-notebooks.readthedocs.io/en/latest/tutorial\\_notebooks/tutorial7/GNN\\_overview.html](https://uvadlc-notebooks.readthedocs.io/en/latest/tutorial_notebooks/tutorial7/GNN_overview.html)

### 4. Assignment

In the examples we looked at, GNNs were developed in Python and Pytorch. Your task in this assignment is to search and find examples of GNN implementations in Keras and Tensorflow. Investigate them; apply them to a problem that was investigated with GNNs in Pytorch and then compare the two approaches.

## 5. Deliverables

You must write (typed) a report and upload it as a PDF file on D2L. The report should be named "**hw15\_report\_LastName.pdf**". You should also create a .zip archive with all your code and implementations of all parts of the assignment. Upload also this archive .zip file with the name "**hw15\_implementation\_code\_LastName.zip**" to D2L. Hence, your D2L should contain two items: the report and the .zip file. **Do not include the report inside the .zip and upload only the .zip. They should be two separate items!**

The report should include the following sections and subsections. Make sure section titles are in bold font and pages are numbered.

- 1) **Title + course info + your name**
- 2) **Summary.** Describe in one paragraph what the objective of the assignment is.
- 3) **Description of Experiments and Discussion.** Describe the experiments you did. All tables and figures should be numbered and should have captions. All plots in all figures should have axes labels and titles. Present a meaningful discussion with the interpretation of the results you obtained. Explain if you expected the results or not; discuss the intuition behind it.
- 4) **Conclusion.** Present your conclusions; highlight what are your main takeaways that you learned from this assignment. Describe what issues you encountered and how you solved them.
- 5) **References.** Include all references that you used, as a numbered list. Cite them in the report itself; do not just list them! If your report has References that are not numbered and cited in the report, points will be deducted!