



# §4.3 MLBD MRes practical Graph Neural Networks

Jarvist Moore Frost.



Twitter: @JarvistFrost

Imperial College London  
Email: [jarvist.frost@ic.ac.uk](mailto:jarvist.frost@ic.ac.uk)  
<https://jarvist.github.io>

# Intended Learning Outcomes §4.3

Demonstrate how and why graph neural networks are built, by solving a graph ML task within PyTorch.

- Be able to summarise the motivation and origin of Graph Neural Networks. (Classwork)
- Describe the main mathematical features of graph neural networks, concentrating on graph convolutional networks (GCN) (Google Research notebooks, classwork)
- Work through the PyTorch GCN example. (Jupyter)
- Run well defined machine-learning experiments to explore and document the parameter space of model construction and learning, communicating progress with your peers. (Jupyter)

# Two fantastic Google Research articles on Graph NNs

Google Research interactive review articles:-

- Daigavane, Ameya, Balaraman Ravindran, and Gaurav Aggarwal. '*Understanding Convolutions on Graphs*'. Distill 6, no. 8 (17 August 2021): 10.23915/distill.00032.  
<https://doi.org/10.23915/distill.00032>.
- Sanchez-Lengeling, Benjamin, Emily Reif, Adam Pearce, and Alex Wiltschko. '*A Gentle Introduction to Graph Neural Networks*'. Distill 6, no. 8 (17 August 2021): 10.23915/distill.00033.  
<https://doi.org/10.23915/distill.00033>.

Implementations of graph neural networks in PyTorch:-

- University of Amsterdam Deep Learning 'Tutorial 7' by Phillip Lippe  
[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)
- Kung-Hsiang, Huang (Steeve) '*Hands-on Graph Neural Networks with PyTorch & PyTorch Geometric*.' May 30, 2019  
<https://towardsdatascience.com/hands-on-graph-neural-networks-with-pytorch-pytorch-geometric-359487e221a8>

# Installing PyTorch Geometric

You should be able to add PyTorch Geometric to your conda environment with:

By hand:

```
conda activate MLBD-MRes
```

```
conda install pyg -c pyg -c conda-forge
```

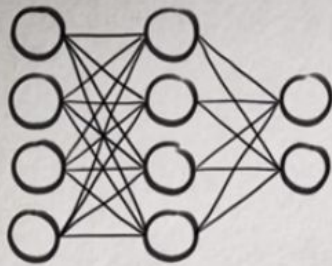
```
conda install -c conda-forge pytorch-lightning
```

Re-sync the environment file:

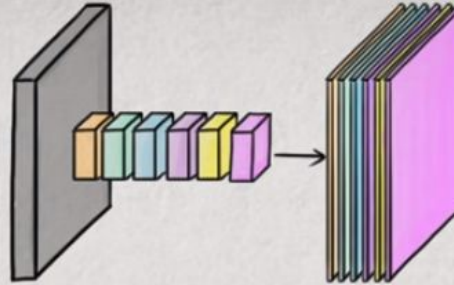
```
git pull
```

```
conda env update --file environment.yml
```

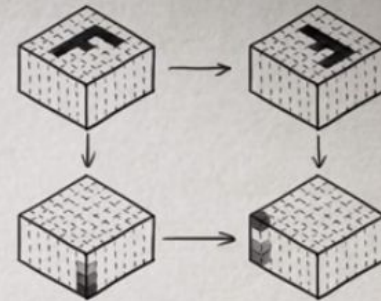
# Self-study



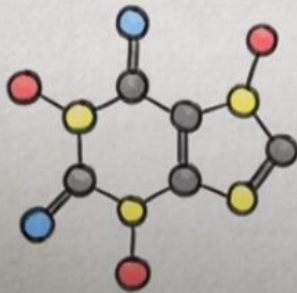
**Perceptrons**  
Function regularity



**CNNs**  
Translation



**Group-CNNs**  
Translation + Rotation



**GNNs**  
Permutation



**DeepSets / Transformers**  
Permutation



**Intrinsic CNNs**  
Isometry / Gauge choice