PyTorch and Graph Neural Networks (GNNs)

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AI IN ASTRONOMY

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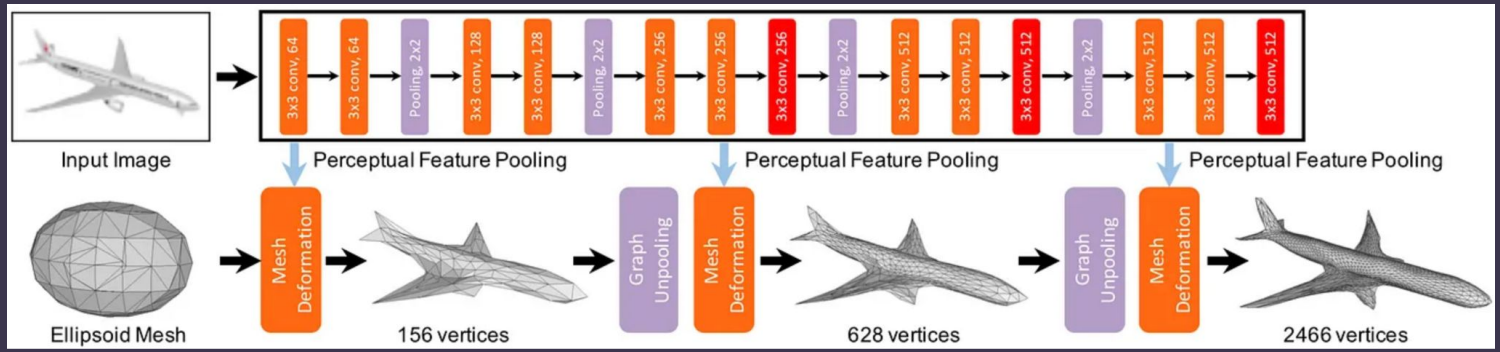
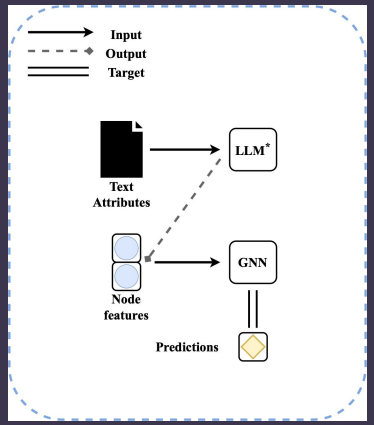
What are GNNs being used for?

Computer Vision



Pixel2Mesh: Generating 3D Mesh Models from Single RGB Images

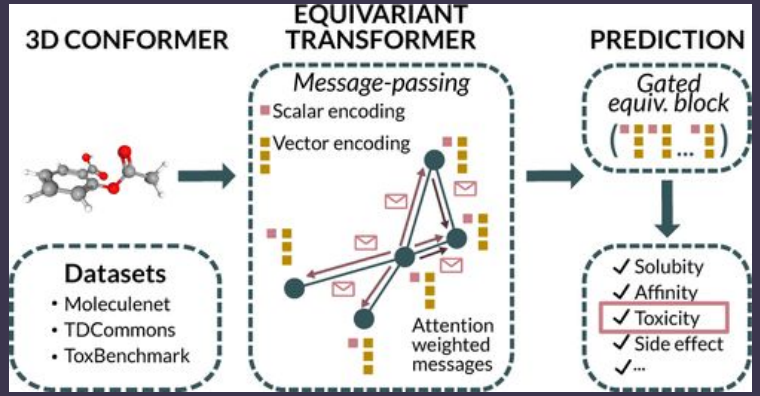
Large Language Models



Exploring the Potential of Large Language Models (LLMs) in Learning on Graphs

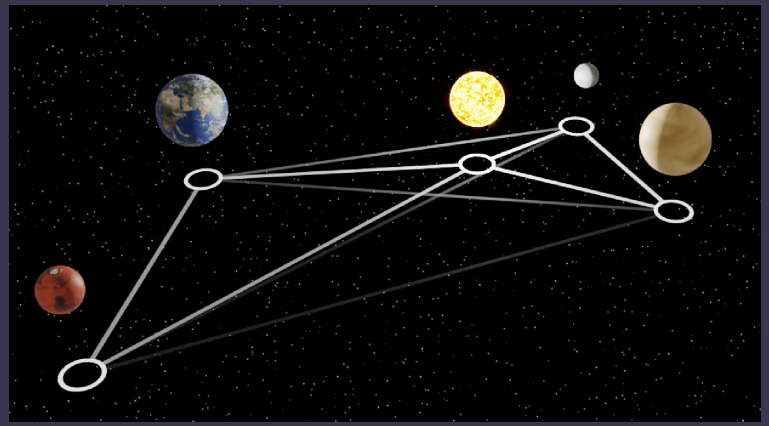
What are GNNs being used for?

Chemistry



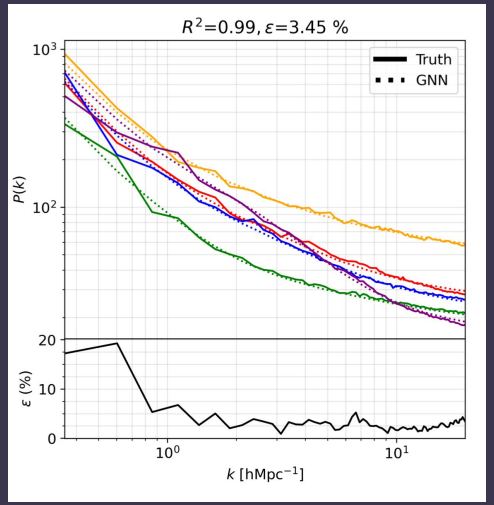
[Equivariant Graph Neural Networks for Toxicity Prediction]

Astrophysics

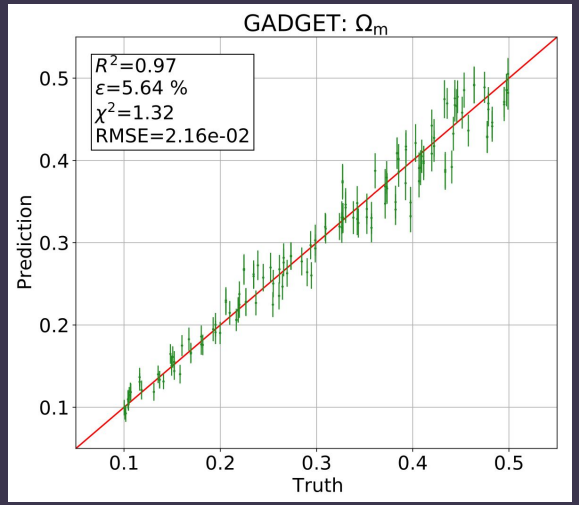


[Rediscovering orbital mechanics with machine learning]

Cosmology

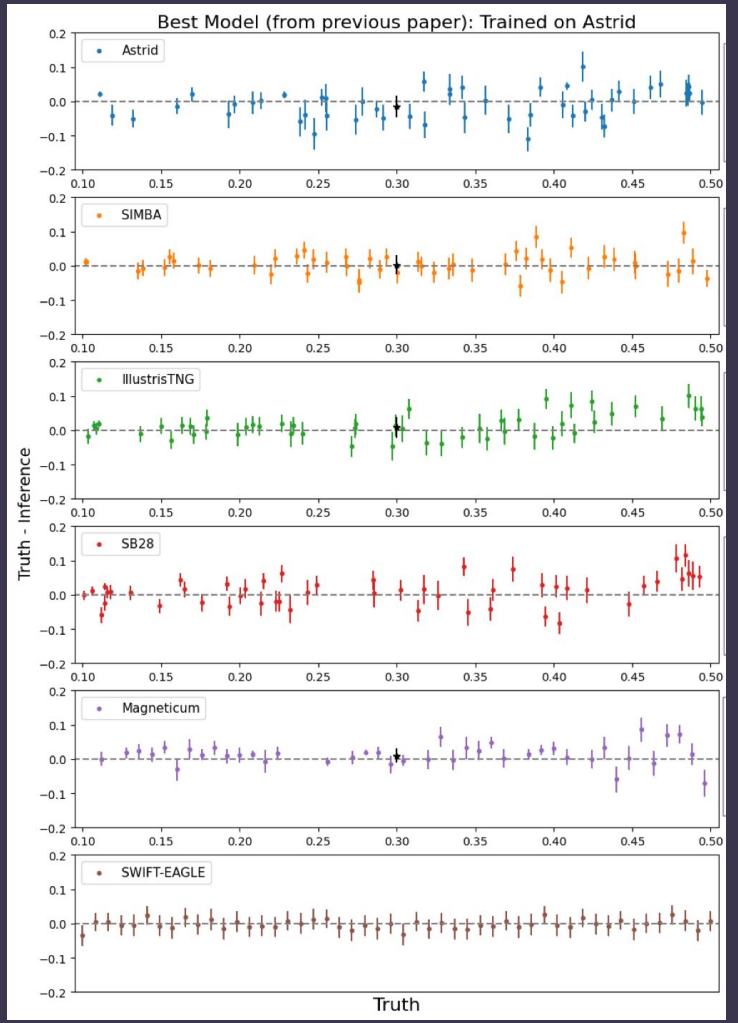


GNNs to to compute the power spectrum from galaxies

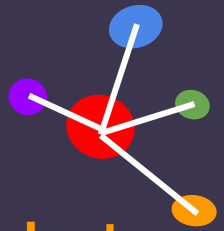


GNNs to predict the matter content of the universe using halos

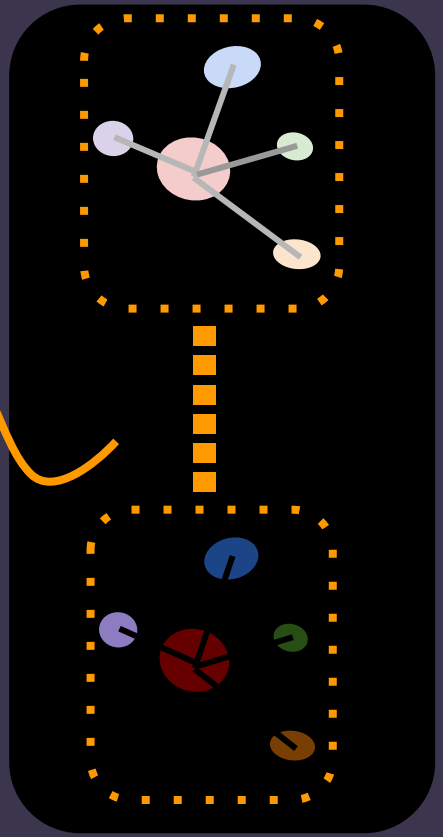
GNNs to predict the matter content of the universe using galaxies



How some of these GNNs work?



Input



Message passing scheme

Edge Model

$$\mathbf{e}_{ij}^{(\ell+1)} = \mathcal{E}^{(\ell+1)}\left(\left[\mathbf{n}_i^{(\ell)}, \mathbf{n}_j^{(\ell)}, \mathbf{e}_{ij}^{(\ell)}\right]\right)$$

Node Model

$$\mathbf{n}_i^{(\ell+1)} = \mathcal{N}^{(\ell+1)}\left(\left[\mathbf{n}_i^{(\ell)}, \bigoplus_{j\in\mathfrak{N}_i} \mathbf{e}_{ij}^{(\ell+1)}, \mathbf{g}\right]\right)$$

Multi Pooling Operation

$$\bigoplus_{j\in\mathfrak{N}_i} \mathbf{e}_{ij}^{(\ell+1)} = \left[\max_{j\in\mathfrak{N}_i} \mathbf{e}_{ij}^{(\ell+1)}, \sum_{j\in\mathfrak{N}_i} \mathbf{e}_{ij}^{(\ell+1)}, \frac{\sum_{j\in\mathfrak{N}_i} \mathbf{e}_{ij}^{(\ell+1)}}{\sum_{j\in\mathfrak{N}_i}}\right]$$

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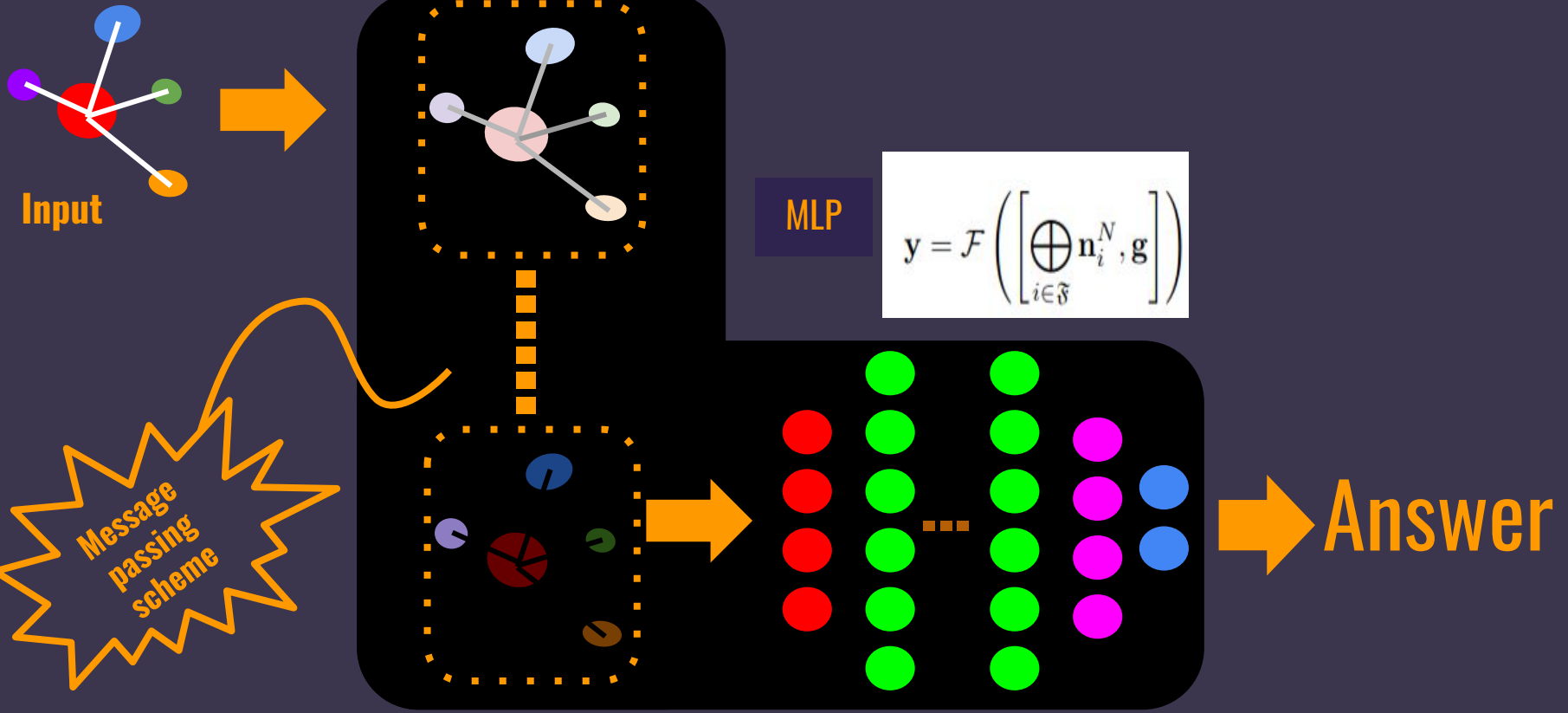

Hands-on activity

STEP 1: go to github and download the repo using:

$ git clone https://github.com/natalidesanti/pytorch_and_GNNs

STEP 2: open the **GNNs** notebook in your preferred machine (your own or in Google Colab)