Chapter 1
New applications of Graph Neural Networks in Cosmology

Farida Farsian, Federico Marulli, Lauro Moscardini, Carlo Giocoli

Abstract Upcoming cosmological surveys will provide unprecedented amount of data, which will require innovative statistical methods to maximize the scientific exploitation. Standard cosmological analyses based on abundances, two-point and higher-order statistics of cosmic tracers have been widely used to investigate the properties of the cosmic web and Large Scale Structure. However, these statistics can only exploit a subset of the entire information content available. Our goal is thus to implement new data analysis techniques based on machine learning to extract cosmological information through forward modelling, by directly exploiting
the spatial coordinates and other observed properties of galaxies and galaxy clusters. Specifically, we investigated a new representation of large-scale structure data in the form of graphs. This data format can be directly fed to Graph Neural Networks, a recently proposed class of supervised Deep Learning algorithms. We tested the method on dark matter halo catalogues in different cosmologies, finding promising results. In particular, the method can discriminate among different dark energy models with high accuracy, through both binary classification (99% accuracy) and multi-class classification (97% accuracy). Moreover, it provides constraints on the value of $w_0$, through regression, with high precision.

1.1 Introduction

Accurate and fast statistical data analysis techniques are essential to extract the full cosmological information content in the data provided by current and next-generation cosmological experiments (e.g. Euclid and LSST). A possible response to these needs could be pulling the information out of raw data available in galaxy or galaxy cluster catalogues. To do so, we propose to consider the large-scale structure data in the form of graphs and let a so-called Graph Neural Network (GNN) to obtain all the specifications of the tracer distribution field. GNNs are a class of Deep Learning methods designed to perform inferences on irregular and sparse data described by graphs. Indeed, they can capture the graph structure of data which is often very rich, and are particularly suitable for learning global permutation invariant quantities, which makes them ideal to be used with large-scale galaxy catalogues.

1.2 Graph Neural Networks

To build a GNN for cosmological inference analyses, we have used the Spektral package which is based on Tensorflow and Keras. Our GNN architecture consists of two blocks of EdgeGNN and two blocks of GeneralConv, followed by the pooling layers – TopKpool layers and the Global average pooling layer.

We test our GNN model on a large set of dark matter halo catalogues extracted from the Quijote N-body simulations, which provide enough statistics to train Neural Networks on cosmologies with different dark energy equation of state parameters. The box size of this simulation is $1 \ Gpc/h$ with more than 8.5 trillions of particles at a single redshift. In particular, we consider 500 mock catalogues extracted from the Quijote simulations at redshift $z = 0$, and for three $w_0$ values: $[-0.95, -1.0, -1.05]$. Massive halos are the most relevant probes for the analysis.

\[\text{https://graphneural.network}\]
performed in this work, and we have applied a mass halo cut of \(7 \times 10^{14} \, M_\odot\) which means we have around one thousand halos per realization.

The first step of the implemented method consists in building the graph assigned to each dark matter halo catalogue, to give it as input to the GNN. Each halo is considered as a node of the graph, while the halo mass and coordinates are held as node features. Then we assign an edge between nodes. Two nodes, \(i\) and \(j\), have an edge \((e_{i\rightarrow j})\) if they are closer than a certain distance \(r\). We keep \(r\) as one of the hyper-parameters of the method, and implemented a grid search algorithm to optimise its value. The results presented here are obtained with \(r = 100 \, Mpc/h\).

1.3 Results

To assess the performance of the implemented GNN on the built cosmic graphs, we check its ability in distinguishing and classifying halo graphs with different values of \(w_0\). Then we move to the regression problem, which is more desirable for the purpose of this project. For all the cases, we performed a graph-level analysis on 360 realizations as the training, 40 as the validation and 100 as the test set.

Firstly, we perform a binary classification on \(w_0 = [-0.95, -1.05]\). The implemented GNN is able to distinguish among these values with 100% of accuracy in both the training and validation phases, and 99% accuracy for the test set. The next stage of our analysis is dedicated to a multi-class classification, with the three values of \(w_0\) as classes. In this case, the GNN reaches 99% of accuracy in the training and validation phases, and 97% accuracy on the test set.

As a final step, we exploit the GNN to provide a prediction on the value of \(w_0\) for the constructed halo graphs. As it is shown in Fig. 1.1 the GNN predicts the value of \(w_0\) very accurately, with 2% of statistical error for all the three sets of halo catalogues considered. The error bars show the standard deviation of the GNN predictions for the 100 test set realizations.
References

1. A. Blanchard et al. [Euclid], Astron. Astrophys. 642 (2020), A191 doi:10.1051/0004-6361/202038071 [arXiv:1910.09273 [astro-ph.CO]].
2. Wu Z., Pan S., Chen F., Long G., Zhang C., Yu P. S., 2019, arXiv, arXiv:1901.00596.
3. Zhou J., Cui G., Hu S., Zhang Z., Yang C., Liu Z., Wang L., et al., 2018, “Graph neural networks: A review of methods and applications”, arXiv, arXiv:1812.08434
4. Wang Y., Sun Y., Liu Z., Sarma S. E., Bronstein M. M., Solomon J. M., 2018, “Dynamic Graph CNN for Learning on Point Clouds”, arXiv, arXiv:1801.07829
5. You J., Ying R., Leskovec J., 2020, “Design Space for Graph Neural Networks”, arXiv, arXiv:2011.08843
6. Gao H., Ji S., 2019, “Graph U-Nets”, arXiv, arXiv:1905.05178
7. F. Villaescusa-Navarro, C. Hahn, E. Massara, A. Banerjee, A. M. Delgado, D. K. Ramanah, T. Charnock, E. Giusarma, Y. Li and E. Allys, et al. “The Quijote simulations,” Astrophys. J. Suppl. 250 (2020) no.1, 2 doi:10.3847/1538-4365/ab9d82 [arXiv:1909.05273 [astro-ph.CO]].