
Domain Adaptive Graph Neural Networks for Constraining Cosmological Parameters Across Multiple Data Sets

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Abstract

Deep learning models have been shown to outperform methods that rely on summary statistics, like the power spectrum, in extracting information from complex cosmological data sets. However, due to differences in the subgrid physics implementation and numerical approximations across different simulation suites, models trained on data from one cosmological simulation show a drop in performance when tested on another. Similarly, models trained on any of the simulations would also likely experience a drop in performance when applied to observational data. Training on data from two different suites of the CAMELS hydrodynamic cosmological simulations, we examine the generalization capabilities of Domain Adaptive Graph Neural Networks (DA-GNNs). By utilizing GNNs, we capitalize on their capacity to capture structured scale-free cosmological information from galaxy distributions. Moreover, by including unsupervised domain adaptation via Maximum

Mean Discrepancy (MMD), we enable our models to extract domain-invariant features. We demonstrate that DA-GNN achieves higher accuracy and robustness on cross-dataset tasks (up to 28% better relative error and up to almost an order of magnitude better χ^2). Using data visualizations, we show the effects of domain adaptation on proper latent space data alignment. This shows that DA-GNNs are a promising method for extracting domain-independent cosmological information, a vital step toward robust deep learning for real cosmic survey data.

1 Introduction

Accurate determination of cosmological parameters using big data from astronomical surveys is a task of paramount importance in modern science. Historically, the extraction of valuable cosmological information has relied on computing summary statistics [31, 16, 15]. More recently, deep learning methods, such as 2D and 3D Convolutional Neural Networks (CNNs), showed great promise in extracting rich non-linear information that summary statistics struggle to capture [32, 39, 29]. However, CNNs lack scale-invariance, as their analysis is firmly anchored to the grid size of the convolutional kernels, while any information on scales below that is lost. Choosing a superfine grid to avoid information loss, though, would simply yield almost entirely zeros in case of sparse and irregular data, such as galaxy clusterings. Thus, CNNs result in an inadequate method for structured sparse data. In contrast, Graph Neural Networks (GNNs) [23, 4, 49, 46] can handle structured cosmic web data in a scale-free manner [41, 14]. As with any other model, the typical procedure is to train GNNs on labeled data (like simulations) and then infer cosmological parameters from unlabeled data (like observations). However, there is a significant risk of these models not generalizing in the presence of the domain shift between simulations and observations. Systematic biases have been demonstrated even in experiments that train and test on simulations with different subgrid physics [41]. Domain adaptation (DA) techniques [11, 43, 18, 27] can be used to increase model robustness to this type of domain shift. Here we propose the use of Domain Adaptive Graph Neural Networks (DA-GNNs) and investigate the utility of distance-based DA losses i.e., Maximum Mean Discrepancy (MMD) [6]. MMD is an unsupervised DA technique because it does not require labeled data, which is paramount for future applications on observations. We show that our domain-adaptive models achieve stronger generalization across datasets than regular GNN models. Our work is a significant step towards building future models trained on simulations, yet robust enough to work on observational data.

Related Work GNNs have shown great potential for extracting information from large sparse datasets, such as the distribution of galaxies, galaxy clusters, and cosmic large-scale structure [25, 28, 41, 33, 42, 14]. Unfortunately, due to the complexity of most deep learning models, they often learn dataset-specific features, which renders them useless when testing on a different dataset (different simulations or astronomical observations). In astronomy, it has been shown that DA techniques applied to different types of CNNs can substantially improve model performance in cross-dataset applications [8, 10, 9, 37, 21, 2]. Recently, it has been shown that DA can be used on other types of deep learning algorithms such as GNNs [12, 24, 45, 47, 7, 44, 17]. However, DA on GNNs has not been used for any astrophysics or cosmology applications.

2 Data and Methods

Data We use galaxy catalogs from the CAMELS [38] magneto-hydrodynamic simulations, which follow the evolution of dark matter particles and fluid elements (baryons) from redshift $z = 127$ to $z = 0$. We use snapshots at $z=0$ from two different simulation suites: 1) IllustrisTNG [30] was generated with Arepo2¹ and employs the IllustrisTNG subgrid physics model; 2) SIMBA [13] was generated with Gizmo3² and employs the SIMBA subgrid physics model. Using two independent models and codebases to simulate galaxies, cosmic gas, and large-scale structure is critical to assess the generalization potential of the machine learning models. In particular, we use the LH set of both suites, which contains 1000 simulations evolved with different random seeds and different values of two cosmological parameters (total matter density Ω_m and the amplitude of density fluctuations σ_8)

¹<https://arepo-code.org/>

²<http://www.tapir.caltech.edu/~phopkins/Site/GIZMO.html>

and four astrophysical parameters (A_{SN1} , A_{SN2} , A_{AGN1} , A_{AGN2} related to supernovae efficiency and active galactic nuclei (AGN) feedback, respectively)³. We use the following features from the galaxy catalogs as input to our models: 3D positions, stellar mass, stellar radius, stellar metallicity, and maximum circular velocity.

Methods

Following [41], we generate graphs from 3D galaxy catalogs; these graphs are rotation and translation invariant with respect to the catalogs themselves. We later feed them as inputs to the DA-GNN, an architecture based on CosmoGraphNet with the addition of DA techniques. The model is composed of two parts. The first part is a graph encoder that transforms the graphs into a vector in the latent space through graph blocks [4]. The second part is a simple feedforward network that performs regression, predicting the posterior mean μ and standard deviation σ of the Ω_m cosmological parameter. This can be achieved by minimizing the following loss [26,40]:

$$\mathcal{L}_{\mu,\sigma} = \log\left(\sum_{i \in \text{batch}} (\Omega_{m,i} - \mu_i)^2\right) + \log\left(\sum_{i \in \text{batch}} ((\Omega_{m,i} - \mu_i)^2 - \sigma_i^2)^2\right), \quad (1)$$

where $\Omega_{m,i}$ is the ground-truth value for the i -th sample in the training set batch, and μ_i and σ_i are the mean and standard deviation, respectively, predicted for sample i .

2.1 Domain Adaptation

Our objective is to create models that generalize across domains i.e., cosmology simulations with different subgrid physics implementations. To assess this, we train on IllustrisTNG and test on SIMBA – and vice versa. We experiment with the use of MMD, a distance-based DA technique. MMD measures the distance of two probability distributions, based on the notion of embedding probabilities in a reproducing kernel Hilbert space. We include an MMD-based component in the network loss function, following [8, 48]. For two distributions Z^1 and Z^2 (with N samples each), this is calculated as:

$$\mathcal{L}_{MMD} = \log\left(\frac{1}{N-1} \sum_{i \neq j}^N [k(z_i^1, z_j^1) + k(z_i^2, z_j^2) - k(z_i^1, z_j^2) - k(z_i^2, z_j^1)]\right), \quad (2)$$

where k is the Gaussian Radial Basis Function kernel and z_q^p is the sample q of distribution p (Z^1 or Z^2) [6, 34, 22, 48, 8]. The loss is calculated on the latent space distributions produced by the graph encoder when processing samples from SIMBA and IllustrisTNG sets. Our final objective function is $\mathcal{L} = \mathcal{L}_{\mu,\sigma} + \lambda \mathcal{L}_{MMD}$, where $\lambda \geq 0$ controls the relative contribution of the MMD loss and is a hyperparameter of the model. We find that $\lambda \approx 0.1$ for the best-performing models in this work. The MMD component of the total loss causes the graph encoder to generate similar latent distributions for both simulations, which will improve the performance of the regressor on cross-dataset tasks.

Optimization and Computing Resources. We performed experiments on NVIDIA A100 40GB GPU. For each of the models, implemented using PyTorch Geometric [19], we perform a hyperparameter search using the Optuna library [1], with 50 trials per model. More details on code performance, model implementations, and selected hyperparameters can be found in the publicly available code⁴.

2.2 Evaluation

We split both IllustrisTNG and SIMBA data into training/validation/testing sets with a proportion of 70%/15%/15%. During training, we save the final models at the epoch with the best validation score. For performance metrics, we use the mean relative error ϵ (reported in percentages), the coefficient of determination R^2 , and the χ^2 ($N = 150$ test points), measured as:

$$\epsilon = \frac{1}{N} \sum_{i=1}^N \frac{|\Omega_{m,i} - \mu_i|}{\Omega_{m,i}}, \quad R^2 = 1 - \frac{\sum_{i=1}^N (\Omega_{m,i} - \mu_i)^2}{\sum_{i=1}^N (\Omega_{m,i} - \bar{\Omega}_m)^2}, \quad \chi^2 = \frac{1}{N} \sum_{i=1}^N \frac{(\Omega_{m,i} - \mu_i)^2}{\sigma_i^2}, \quad (3)$$

³CAMELS dataset documentation: <https://camels.readthedocs.io/en/latest/index.html>

⁴GitHub repository will be added after the anonymous review stage.

Table 1: Comparison of results: No Domain Adaptation (top) and MMD (bottom).

	I -> I			I -> S			S -> S			S -> I		
	R^2	ϵ	χ^2	R^2	ϵ	χ^2	R^2	ϵ	χ^2	R^2	ϵ	χ^2
NoDA	0.97	5.0	1.39	-1.04	43.8	59.43	0.97	5.2	1.79	0.22	25.0	185.54
MMD	0.97	4.7	1.12	0.69	15.7	17.99	0.97	5.9	1.54	0.68	16.7	19.96

where $\bar{\Omega}_m$ is the mean of Ω_m value in the test set. A value of χ^2 close to 1 suggests that the standard deviations are correctly predicted and can be seen as minimizing the second term of Equation 1. A higher (lower) value can be seen as an underestimation (overestimation) of the uncertainties [3].

3 Results

DA-GNN achieves significantly better results (up to 28% better relative error ϵ and up to almost an order of magnitude better χ^2) on cross-domain generalization with respect to CosmoGraphNet, whilst achieving comparable results on the same domain test set⁵, as shown in Table 1 and Figure 1. In [39], the authors were able to infer the value of Ω_m with higher cross-domain accuracy. However, that analysis utilizes the full matter surface density maps i.e., 2D images, instead of the full 3D galaxy distributions. In [14], the authors propose a GNN-based model that performs well cross-domain when trained on the Astrid simulation [5] alone. However, this apparent robustness is achieved by choosing Astrid as the training set and by using input features that are less subject to simulation code variability – galaxy positions and 1D velocities. When authors try training on other simulations or using more simulation-dependant parameters (e.g., stellar mass), cross-dataset performance drops significantly. Therefore, domain-shift robustness across different cosmological datasets requires DA.

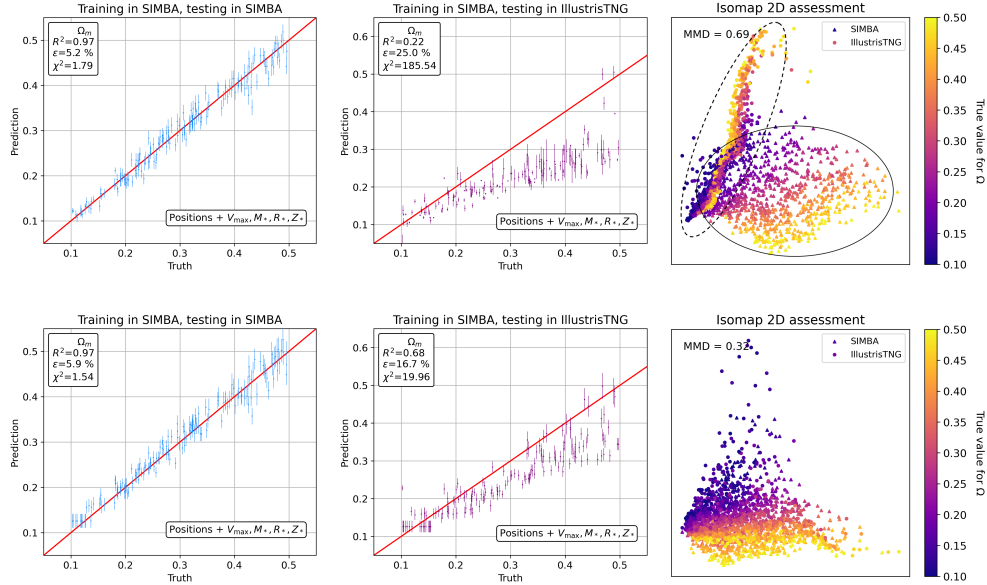


Figure 1: Comparison of models without (top row) and with DA (bottom row), trained on the SIMBA suite. From left to right, we report: scatter plot for the value of Ω_m on 1) same domain, 2) cross-domain and 3) the isomap showing how the GNN is encoding the two datasets in the latent space (SIMBA - triangles, IllustrisTNG - circles)⁶. In the non-domain adapted isomap, ellipses highlight regions where distributions lie, showing the difference between simulation encodings that leads to substantial drop in performance on the cross-domain task.

⁵In [41], authors get slightly better results for the same domain, and slightly worse for the cross-domain tests. We impute these differences to choices such as batch sizes and optimization techniques we took due to computational and time constraints.

⁶In Appendix A, the IllustrisTNG counterpart of this plot is presented.

Latent space organization Isomaps are two-dimensional projections of the multi-dimensional latent space [35]. Figure 1 shows the difference in the latent space structure without (top row) and with (bottom row) DA. Ellipses in the top right isomap highlight how the two distributions are encoded in different regions of the latent space. Without the MMD loss, the model encodes samples with very different values of Ω_m close to each other, if they originate from different simulations (circles and triangles of different colors are overlapping). This scenario leads to the fragility of the regressor, which cannot learn to output different values for the same latent space encodings. On the contrary, the DA-GNN (bottom right plot) correctly encodes the samples in a domain-invariant way. Visually, circle and triangle distributions are overlapping, which indicates domain mixing. Furthermore, the direction in the color gradient shows that the DA-GNN encodes information such that the regressor can now more correctly predict cosmological parameters based on the encodings of both simulations.

4 Conclusions

We propose and demonstrate a method for unsupervised DA for cosmological inference with GNNs. We use an MMD-based loss to enable the domain-invariant encoding of features by the GNN. This approach enhances cross-domain robustness: compared to previous methods, DA-GNNs reduce prediction error and improve uncertainty estimates.

Limitations The cross-domain accuracy remains worse when compared to single-domain performance. Although reaching the same accuracy might not be possible, more flexible approaches such as adversarial-based DA techniques [20, 36], instead of distance-based ones such as MMD, might yield better results. Moreover, due to computational and time constraints, our models have been trained and tested only on two of the four available CAMELS simulation suites. Using more suites would yield better cross-domain efficacy and reliability at assessment time. These limitations will be addressed in future work.

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Author Contributions:

A. Roncoli: *Methodology, Software, Validation, Formal analysis, Investigation, Writing - Original Draft, Visualization;*

A. Ćiprijanović: *Conceptualization, Methodology, Project administration, Resources, Software, Supervision, Writing - Original Draft, Funding Acquisition;*

M. Voetberg: *Software, Writing (review and editing);*

F. Villaescusa-Navarro: *Software, Writing (review and editing);*

B. Nord: *Supervision, Resources, Writing (review and editing).*

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A Additional Plots

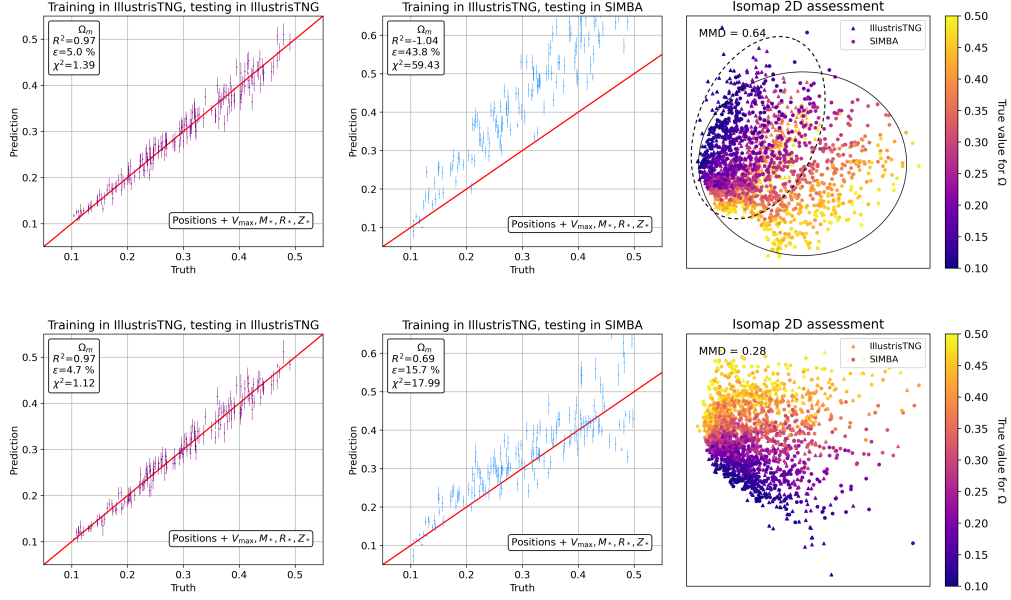


Figure 2: Comparison of models without (top row) and with DA (bottom row), trained on the IllustrisTNG suite. From left to right, we report: scatter plot for the value of Ω_m on 1) same domain, 2) cross-domain and 3) the isomap showing how the GNN is encoding the two datasets in the latent space (IllustrisTNG - triangles, SIMBA - circles). In the non-domain adapted isomap, ellipses highlight regions where distributions lie, showing the difference between simulation encodings that leads to substantial drop in performance on the cross-domain task.