Supplementary material:
Learning Adaptive Neighborhoods for Graph Neural Networks

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A. Node classification Experiments

A.1. Datasets

Transductive datasets. We evaluate on the three citation benchmark datasets Cora, Citeseer and Pubmed [26] introduced by [41]. Each citation graph contains nodes corresponding to documents and edges indicating citations. Node features are bag-of-words features and node labels are categorized by topic. We follow the semi-supervised setting in [41] and [16] along with their train/test splits. **Inductive datasets.** In an inductive setting, we evaluate our approach on three datasets: 1. Flickr [42] — categorizing images based on their descriptions; 2. Reddit [42] — predicting the communities of online posts from user comments. 3. PPI [11] — classifying protein-protein interactions.

A.2. Dataset details

In Table 1 we provide dataset statistics on the node classification datasets used in this paper.

Table 1. Dataset statistics. ‘s’ stands for single class classification and ‘m’ for multi-class.

Dataset	Nodes	Edges	Features	Classes	Train / Val / Test
Cora	2,708	5,429	1,433	7 (s)	140 / 500 / 1,000
Citeseer	3,327	4,732	3,703	6 (s)	120 / 500 / 1,000
PubMed	19,717	44,338	500	3 (s)	100 / 500 / 1,000
PPI	56,944	81,8716	50	121 (m)	44,906 / 6,514 / 5,524
Flickr	89,250	899,756	500	7 (s)	44,760 / 22,312 / 22,312
Reddit	232,965	11,606,919	602	41 (s)	153,756 / 23,295 / 55,911

A.3. Implementation details

We integrate our DGG into the official publicly available code of all baselines, without architectural modification. Models are trained and evaluated as their original implementation.

In our DGG, all MLPs use a single fully-connected layer of dimension 64. In our DGG, all MLPs use a single fully-connected layer of dimension 64. We use a Gumbel-Softmax temperature of 2.5. When adding Gumbel noise to the edge log-probabilities, we do not add any to the self-loops (i.e. the diagonal of the edge probability matrix). During training, we keep the Gaussian and Gumbel noise on, but turn it off during inference. While in practice it can be left on, we found it does not significantly impact the results.

A.4. Training details

We train the entire network end-to-end using the classification loss from the downstream model and an annealed MSE loss on the adjacency matrix generated by the DGG:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{class}} + \frac{\alpha}{M} \sum_{i=1}^{M} (y_i - \hat{y_i})^2, \tag{1}$$

where the first term is the classification loss from the downstream GCN, the second term is the MSE loss applied to every element $\hat{y_i}$ of the adjacency matrix $\mathbf{A} \in \hat{\mathbb{R}}^{N \times N}$ for which we have a node label, and α is loss weight. The model can be trained by annealing α smoothly or in a stepwise manner. In practice we keep α constant for the first 100 epochs and then set it to zero for the rest of the training schedule (where the total number of epochs is determined by the schedule of the downstream GCN).

A.5. Comparison with bespoke architectures experiment settings

In Table 4 of the main paper we compare against bespoke SOTA architectures which learn the graph structure. Here we explain the choice of our backbone and the experiment setting to compare against each architecture:

1. Setting 1: IDGL [3] uses an attention mechanism so we choose the Graph Attention Network (GAT) [35] as our backbone. The experiment setting is the same as that in [16].

2. Setting 2: Both LDS [9] and SLAPS [8] use regular graph convolutions so we choose the GCN [16] as our backbone. In this setting there is no input graph, and the training split includes half of the validation graph.

3. Setting 3: NodeFormer [37] is based on a Transformer [34] so we choose GAT [35] as our backbone. The data splits now include 50 %, 25 % and 25 % of the full graph for training, validation and testing respectively.
4. Setting 4: VGCN [7] uses a variational framework, and as there is no directly applicable backbone, we compare it against our best performing backbone GAT [35]. The training split includes half of the validation set.

A.6. Robustness to noise

We test the effect of the DGG when the input graph has random edges added across it. We do this by adding edges between previously unconnected nodes. Broadly, the results in Fig. 1 demonstrate the detrimental effects of noisy edges on classification accuracy, but the inclusion of the DGG can mitigate this. Interestingly, the state-of-the-art GCNII [2] demonstrates the largest drops in accuracy as the noise increases, which may be attributed to the depth of their graph convolution layers. In such deeper message-passing models, the edge structure is even more significant, highlighting the importance of learning a structure that prevents the propagation of irrelevant information.

B. Trajectory Prediction Experiments

B.1. Dataset details

ETH and UCY. ETH [27] and UCY [18] are two common benchmarks for pedestrian trajectory prediction. These datasets consist of 5 subsets of widely used real-world pedestrian trajectories [**?**, **?**, 22, **?**]. The primary challenge in these datasets are the frequent interactions of agents in very crowded scenes. Furthermore, the number of pedestrians varies considerably. Some frames contain only 2 pedestrians, while many have over 50.

SportVU. The STATS SportVu [32] is a tracking dataset composed of multiple NBA seasons. Each scene consists of two teams of 5 players, with each team categorized as either making an offensive or defensive play in a particular game. Each play contains 50 timesteps sampled at 5Hz, with the player trajectories expressed in (x, y, z) coordinates.

Stanford Drone. The Stanford Drone Dataset (SDD) [28] is a large dataset with 20 different top-down scenes across multiple areas at Stanford University. Each scene consists of agents of different types, from pedestrians and skaters to cars and buses. Trajectories are recorded at 2.5Hz and expressed in (x, y) world coordinates. Despite the heterogeneity of agents, the maximum number of agents in any one scene is 21.

Baselines. We integrate our DGG module into two state-of-the-art trajectory prediction pipelines: **Social-STGCNN** [22] built upon a spatio-temporal convolutional network using graphs to represent pedestrian trajectories and **DAGNet** [23] built upon a VAE backbone [14] with a graph attention network modelling agent interactions across a fully-connected graph. Our DGG is placed within both networks to generate the adjacency matrix on the fly and forms part of its forward and backward pass. To integrate the DGG with DAGNet's attention mechanism, the adjacency generated is multiplied by the attention weights.

Implementation details. We integrate DGG into the publicly available code of each method, without any architectural modification. We use the same DGG hyperparameters as for node classification except the intermediate loss is disabled and the training signal is entirely from the downstream task.

B.2. Qualitative results

In Fig. 2 we plot the node-degree distribution learned by our DGG across multiple datasets. While on average, a pedestrian may only look at their 2 nearest neighbors in crowded scenes such as Zara1 and Univ, this can increase to almost 5 nearest neighbors in some cases. This suggests that both a fully-connected graph, or one with a fixed node-degree like DGM [13] are both suboptimal.

Figure 3 compares our predicted trajectories to DGM [13], on the SportVU dataset. As shown, our trajectories are closer to the ground truth. We illustrate this further in Fig. 4, which shows the graph generated by our DGG for 3 different basketball players in a game. The figure demonstrates how our DGG lets each player look at a different number of neighbors, while DAGNet [23] forces each player to look at all others in the game.

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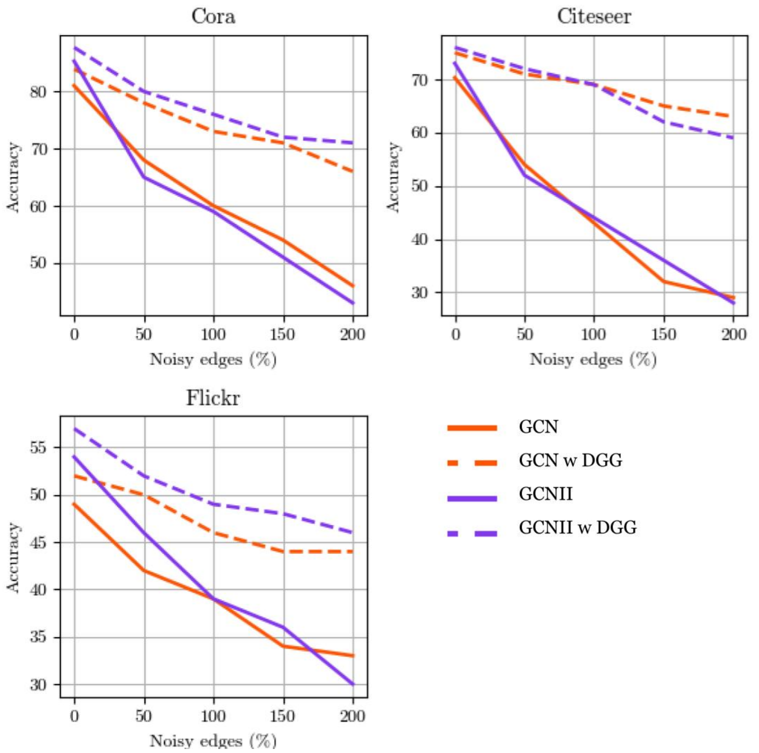

Figure 1. Node classification accuracy with noisy edges added to the input graph of different datasets.

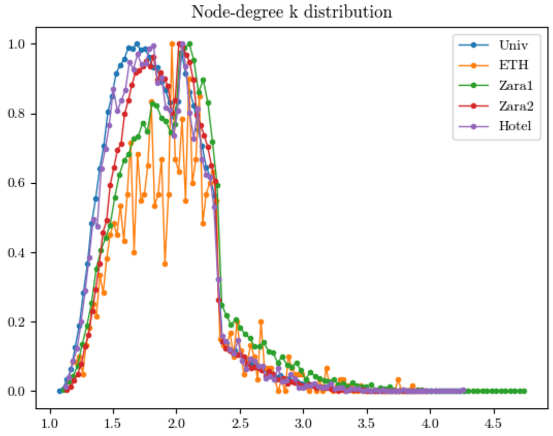

Figure 2. Distribution of the learned node degree k over the test split for different trajectory prediction datasets.

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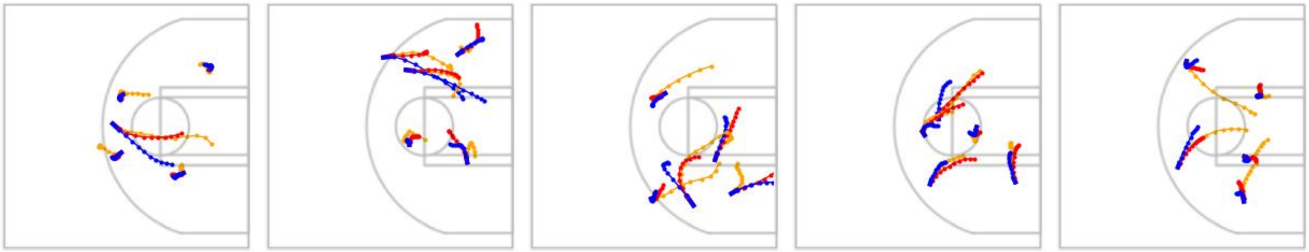
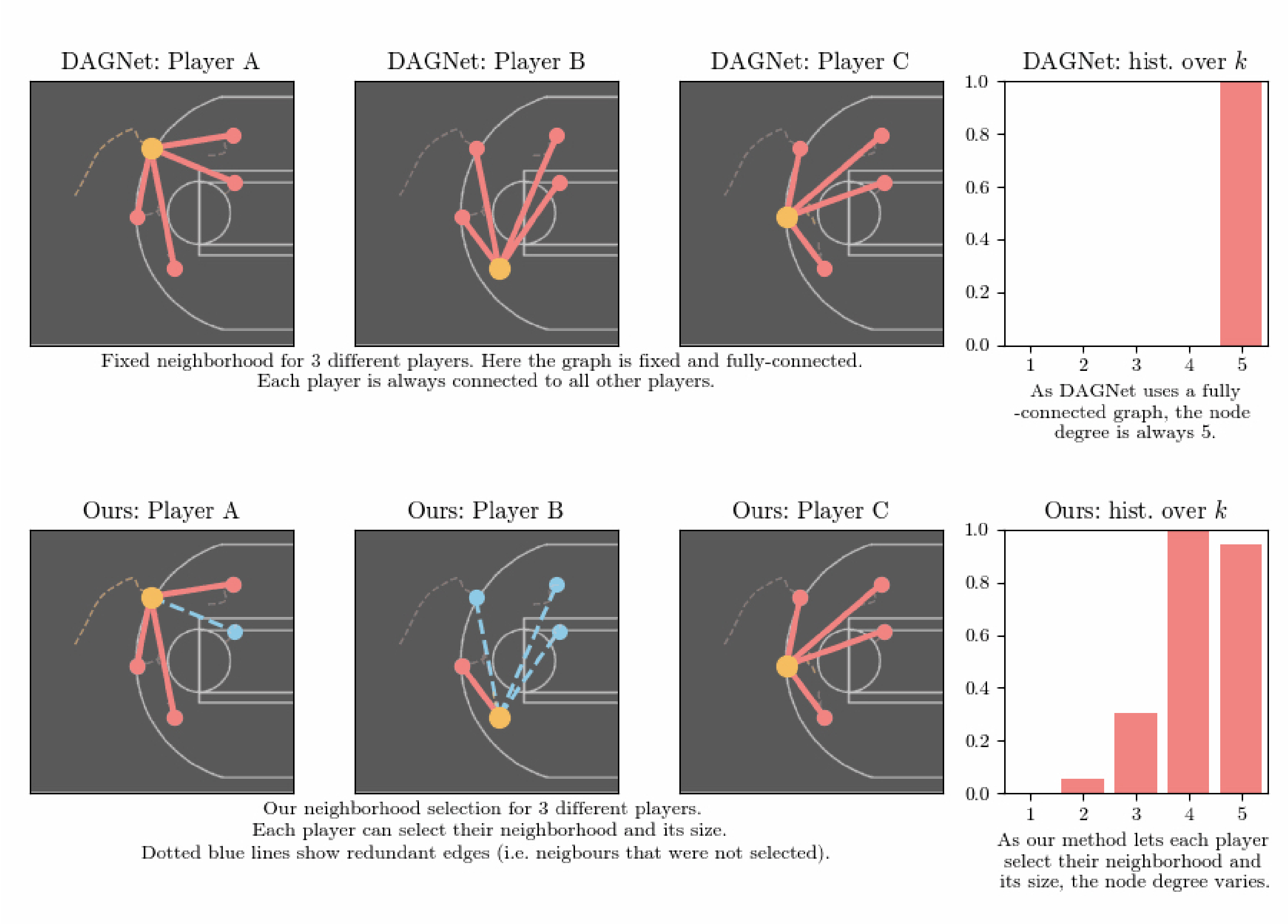


Figure 3. Qualitative results for trajectory prediction on the SportVU dataset. Orange: ground truth; Blue: DGM prediction; Red: our prediction.



Fixed neighborhood for 3 different players. Here the graph is fixed and fully-connected.
Each player is always connected to all other players.

As DAGNet uses a fully -connected graph, the node degree is always 5.

Our neighborhood selection for 3 different players.
Each player can select their neighborhood and its size.
Dotted blue lines show redundant edges (i.e. neigbours that were not selected).

As our method lets each player select their neighborhood and its size, the node degree varies.

Figure 4. Graph topology visualization in basketball players on the SportVU dataset: ours vs. DAGNet [23]. We display the selected neighborhood for 3 different players and a histogram of the node-degree k accumulated over the dataset/scene. First row: DAGNet's fully-connected graph, second row: our DGG.

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