
Graph Networks with Spectral Message Passing

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Abstract

Graph Neural Networks (GNNs) are the subject of intense focus by the machine learning community for problems involving relational reasoning. GNNs can be divided into spatial and spectral approaches, which represent different ways to generalize the convolutional inductive bias to graph structured data. Here we introduce Spectral Graph Networks, which apply message passing in both the spatial and spectral domains. Briefly, our model projects vertex features of the spatial graph to and from the Laplacian eigenvectors, which are each represented as vertices in a fully connected “spectral graph.” We apply this model to various benchmark tasks including graph-based MNIST classification, molecular classification (MoleculeNet), and molecular property prediction (QM9). The Spectral GN promotes efficient training, reaching high performance with fewer training iterations despite having more parameters. The model also provides robustness to edge dropout and outperforms baselines for the classification tasks.

1 Introduction

Many machine learning problems involve data that can be represented as a graph, whose *vertices* and *edges* correspond to sets of entities and their relations, respectively. These problems have driven the development of graph neural networks (GNNs) [Scarselli et al., 2008], which adapt the notion of convolution on Euclidean signals to the graph domain [Bronstein et al., 2017]. Here we introduce a new GNN architecture which bridges two dominant approaches within the field—the spatial and spectral approach—to favorably trade-off their comparative strengths and weaknesses.

Spatial approaches involve a form of learned message-passing [Gilmer et al., 2017] that propagates information over the graph by a local diffusion process. Spectral approaches [Bruna et al., 2013] generalize the Fourier transform of Euclidean signals to graphs, providing access to information over short and long spatiotemporal scales simultaneously. Spatial approaches have tended to be more popular recently; however, a limitation is that propagating information over long ranges can require many rounds of message-passing, resulting in fine-grained information being corrupted or lost.

To overcome this limitation, our Spectral Graph Network (GN) architecture performs message-passing over the input graph’s structure—the “spatial graph”—as well as message-passing in a high-level “spectral graph”. This allows long-range information to be pooled, processed, and transmitted between any vertices in the spatial graph, which confers an inductive bias toward explicitly incorporating the global topology of the graph into its processing. We test our Spectral GN on a graph MNIST classification task and on two distinct molecular property prediction tasks. Our model achieves

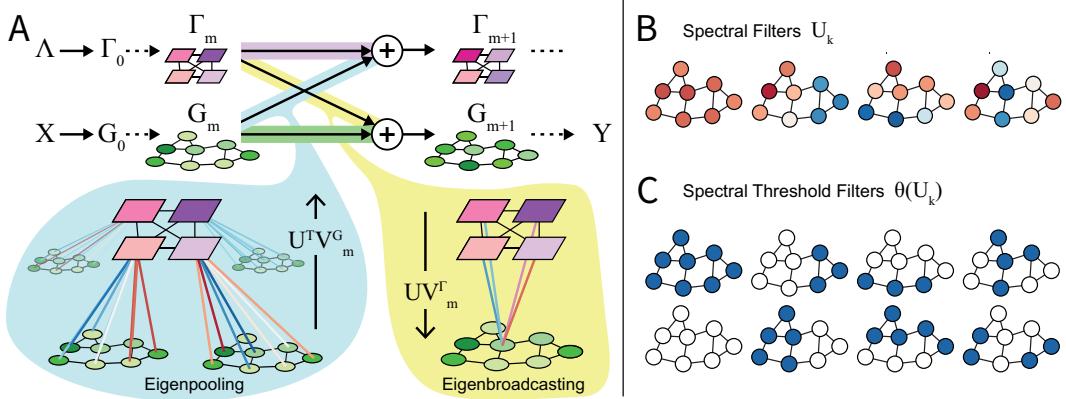


Figure 1: (A) Spectral GraphNet Schematic. The spatial graph, G_m , is processed by the GNN G network (green graphs and arrow). The spectral graph, Γ_m , is processed in parallel by the GNN $^\Gamma$ network (purple graphs and arrow). The eigenpooling operation (cyan bubble) communicates G_m 's vertex information to Γ_{m+1} , weighted by the eigenvector values (blue/red lines). The eigenbroadcasting operation (yellow bubble) communicates Γ_m 's vertex information to G_{m+1} , weighted by the eigenvector values. (B) Spectral Filters $U_{K=4}$ (first 4 non-thresholded eigenvectors). (C) Thresholded Spectral Filters $\theta(U_{K=4})$, first 4 eigenvectors $U_{K=4}$ (top row), and their negatives, $-U_{K=4}$ (bottom row), thresholded at 0. Vertex coloring indicates weights on each spatial latent applied before pooling.

high performances, more efficient training, and is more robust to dropped input vertices and edge sparsification in the model. These results demonstrate how spatial GNN approaches can benefit from low frequency information provided by spectral approaches.

2 Model

2.1 Graph Theory Background

Let $G = (V, E)$ be a graph containing vertices V and directed edges E . Let $v_i \in V$ be the vertex features for vertex i , $(e_k, r_k, s_k) \in E$ contain the edge features, sender indices, and receiver indices, respectively, and g be graph-level “global” features. The adjacency matrix, A , is defined such that $A_{ij} = 1$ if $(\cdot, i, j) \in E$ and 0 otherwise. The degree matrix D is diagonal with $D_{ii} = \sum_j A_{ij}$.

The graph Laplacian matrix is $L = D - A$ [Chung, 1994]. The eigendecomposition of L , $L = U \cdot \text{diag}(\Lambda) \cdot U^\top$, where U is the matrix of $|V|$ eigenvectors and Λ vector of eigenvalues. The operation $U^\top \phi$ projects a signal ϕ over graph nodes into the spectral domain. These K eigenvectors with the smallest eigenvalues distinguish vertices that will be slowest to share information under diffusion (or, similarly, message passing) [Shi and Malik, 2000]. Other applications include spectral clustering [Ng et al., 2002] and graph coarsening [Ortega et al., 2018].

2.2 Our Spectral GN model

Spatial and Spectral GraphNets. The input “spectral graph” is a complete graph with K vertices corresponding to the K smallest eigenvalues of input spatial graph X 's graph Laplacian. The vertex features are initialized to the eigenvalues, $\Lambda_{:K}$. The spatial and spectral input graphs are processed by vertex and edge-wise MLP encoders to yield G_0 and Γ_0 , respectively.

On the m -th message passing step, spatial and spectral GNNs, GNN G and GNN $^\Gamma$, are applied to G_m and Γ_m , respectively (horizontal lines between m and $m + 1$ steps in Figure 1A). After M rounds of message passing, an MLP decoder processes G_M and returns graph output Y . For graph-level classification, the loss is applied to the global feature of Y .

For the GNNs, we implemented the GN, Graph Convolution Network (GCN), and (for spectral processing only) the Graph Fourier Transform (GFT). The GCN is a popular, lightweight spatial

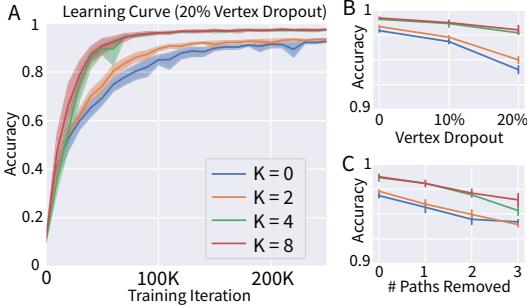


Figure 2: Graph MNIST results. **(A)** Learning curves showing classification test accuracy (y -axis) across training iterations (x -axis). **(B)** Accuracy (y -axis) of U -GN with increasing vertex dropout proportion (x -axis). **(C)** Accuracy (y -axis) of U -GN with increasing number of shortest paths removed (x -axis).

approach that has fewer parameters and no global term. The GFT, inspired by [Bruna et al., 2013], applies an MLP to the spectral latents ordered by eigenvalue.

Eigenpooling/broadcasting. Vertex features of G_m are projected onto the k -th vertex in the spectral domain via multiplication with the k -th eigenvector $U_{\cdot,k}$, or, in matrix form, $\bar{V}_{m+1}^{\Gamma} = U^{\top} V_m^G$ (Figure 1A, blue). For notational simplicity, we let U be the truncated K eigenvector matrix. These eigenpooled vertices, \bar{V}_{m+1}^{Γ} , are concatenated onto the spectral vertices, \hat{V}_{m+1}^{Γ} , to form V_{m+1}^{Γ} . Similarly, vertex features of Γ_m are projected to the i -th vertex in the spectral domain via multiplication with $U_{i,\cdot}$, or, in matrix form, $\bar{V}_{m+1}^G = U V_m^{\Gamma}$ (Figure 1A, yellow). These eigenbroadcasted spectral vertices, \bar{V}_{m+1}^G , are concatenated onto the spatial vertices, \hat{V}_{m+1}^G , to form V_{m+1}^G .

We also explored a modified version termed ‘‘Spectral Threshold GN’’ ($\theta(U)$ -GN), which thresholds U at 0, and uses $\text{concat}[\theta(U), \theta(-U)]$ as the projection matrix (Figure 1B,C). It thus has $2K$ the number of spectral graph vertices, whose input for initialization are the duplicated eigenvalues. The U -GN refers to a Spectral GN with no thresholding.

Further considerations. By treating the eigenvectors as an unordered set *labelled* by eigenvalue, our approach helps circumvent instabilities and degeneracies that challenge previous approaches which treat them as a sequence *ordered* by eigenvalue. If we use $K = 1$, this is analogous to using a global term for graph-level communication [Gilmer et al., 2017, Battaglia et al., 2018].

Compared to other hierarchical GNN schemes [Mrowca et al., 2018, Li et al., 2018, Ying et al., 2018], Spectral GN uses the matrix of eigenvectors to exchange low- and high-level vertex information. Intuitively, the spectral augmentation can also be thought of as nonlinear low pass filtering on learned latents [Ortega et al., 2018]. Eigendecompositions can be expensive ($\mathcal{O}(N^3)$) to compute; however, approximations [Hammond et al., 2009] and learned models [Pfau et al., 2018] can help.

3 Experiments

We evaluated our models and baselines on three graph property prediction tasks: Graph-MNIST [Defferrard et al., 2016], MoleculeNet-HIV molecule classification [Wu et al., 2018], and QM9 quantum molecular property prediction [Ramakrishnan et al., 2014]. Across these benchmarks, we found that our hybrid spectral architectures yielded efficient training, were more robust to both missing vertices in the inputs and pruned edges during message passing, and in two cases (MNIST, MoleculeNet-HIV) yielded higher overall performance. For molecular tasks, the thresholded Spectral GNs were stronger while for MNIST, others the non-thresholded ones were. For all experiments, results tables, learning curves, and training details can be found in the Appendix.

3.1 Graph MNIST

MNIST handwritten digit classification [LeCun et al., 1998] can be adapted for graphs by treating each pixel as a vertex and placing an edge between neighboring pixels [Defferrard et al., 2016]. Each sample consists of a 28×28 grid and edges join the four axis-aligned neighbors (no superpixels). Vertex features were the pixels’ intensities and edge features contained the 2D displacement vector from sender to receiver vertex position. Under ‘‘uniform vertex dropout’’, vertices were uniformly randomly removed from each graph ($p_{\text{dropout}} \in [0, 0.1, 0.2]$). Under ‘‘shortest path vertex dropout’’, pairs of vertices were randomly selected, and all of the vertices along one of the shortest paths connecting them were removed ($n_{\text{paths}} \in [0, 1, 2, 3]$).

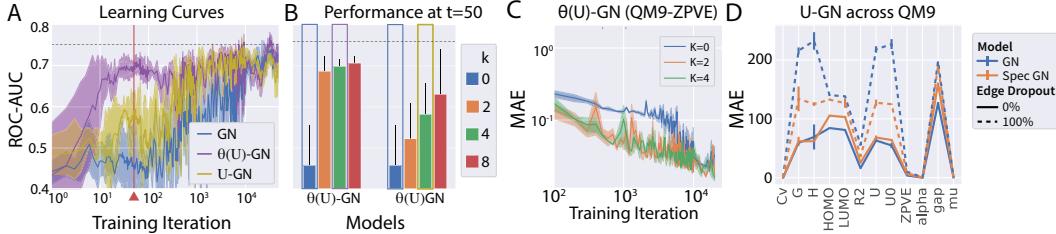


Figure 3: Molecular classification results. (A) Learning curves showing ROC-AUC (y -axis) across training iterations (x -axis) for GN, U -GN, and $\theta(U)$ -GN. Red line indicates $t = 50$ training iterations. (B) ROC-AUC across all spectral models, with U and $\theta(U)$ augmentation, sampled at $t = 50$ iterations. Models shown in (A) marked with boxes whose outline colors match their colors in (A). (C) Learning curves showing test loss early in training for an example QM9 target, ZPVE. Blue lines are networks without spectral information, Orange is $\theta(U)$ ($k = 2$) and Green is $\theta(U)$ ($k = 4$). Spectral models show better performance early on in training. (D) Final test MAE in target units, with best performing spectral model displayed per edge dropout value. Target units in Appendix.

Our U -GN reached the highest performance, trained more efficiently, and was more robust to vertex dropout (Figure 2). The U -GN spectral approach (0.992) outperformed GCN (0.8451), GN-GFT (0.925), and GCN-GFT (0.925) for 0 dropout, and outperformed thresholded $\theta(U)$ -GN (0.978). The GCNs deteriorated rapidly under dropout, while GN-GFTs deteriorated specifically under shortest path dropout. However, the vanilla GN showed a greatest decrement in performance compared with the Spectral GNNs under node dropout (Figure 2B). U -GN ($K = 4$ or $K = 8$) was the highest performing model under random shortest path vertex dropout (Figure 2C). However, increased dropout proportions appeared to weaken the U -GN and vanilla GN comparably, suggesting these perturbations to the global structure were harder for the Spectral GNNs to overcome.

3.2 Molecular Property Prediction (MoleculeNet-HIV and QM9)

MoleculeNet-HIV involves predicting if a molecule can inhibit HIV replication from its molecular graph [Wu et al., 2018, Hu et al., 2020]. QM9 is a quantum chemistry benchmark that that involves predicting 13 target properties from the annotated molecular graph [Ramakrishnan et al., 2014]. As is standard, we use separately trained models for each target and target whitening [Gilmer et al., 2017].

For both benchmarks, thresholded $\theta(U)$ augmented spectral models trained more efficiently than other models. The $\theta(U)$ -GNs ($k = 4$) reached 87% of state of the art in ~ 60 iterations (1920 samples), while GCN and GN took ~ 500 and $\sim 10,000$ iterations, respectively. For QM9, we found that the spectral models’ MAE was lower for the first $\sim 20K$ steps of training (Figure 3C).

Final performance on MoleculeNet-HIV was comparable to the top GNN methods on the Open Graph Benchmark leaderboard, GCN+GraphNorm (ROC-AUC=0.7883) [Hu et al., 2020, Dwivedi et al., 2020]. Our GNNs reached scores of 0.739 ± 0.029 , U -GN 0.753 ± 0.028 , and $\theta(U)$ -GN ($K = 4$) 0.769 ± 0.015 . For QM9, the vanilla GN was the top performing model among those were evaluated. Spectral GCNs did outperform vanilla GCNs. Our models were neither molecule-specific nor tailored to QM9, and did not reach state of the art performance, generally having $2\text{--}10\times$ SOTA MAE.

GNNs typically train more efficiently but perform worse with sparsified edges. We tested whether message passing over the spectral graph could potentially compensate for edge dropout of 50% and 100% to allow more efficient processesing. We found that spectral significantly outperformed their vanilla counterparts under 100% edge removal (Figure 3D, orange-dashed U -GN outperforming blue-dashed GN for 12/13 targets), but did not reach the solid lines denoting the non-sparsified graph. For 50% edge dropout: U -GN had lowest error for 5/13 targets, and for 0%, 2/13.

4 Conclusion

We introduce Spectral GraphNets, which combine spatial and spectral GNNs. Across our experiments, we find that the Spectral GNNs reach competitive performance, train efficiently, and compensate for missing vertices in the data and edge dropout in the GN.

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Appendices

A Implementation

Models were trained with learning rate of 10^{-4} for 250K steps (Graph MNIST), $5 \cdot 10^{-4}$ for 50K steps (MoleculeNet-HIV), or $5 \cdot 10^{-4}$ for 10^7 steps (QM9). The encoders, decoders, vertex, edge, and global updating functions all consisted of MLPs with 3 layers, 32 hidden units, and ReLU activation functions. Layer norm was applied to the output of the encoder and all message passing networks, and the activation function was not applied to the last layer of the networks performing message passing. The update functions were further modified to access the history of latents: at each round of message passing, initial, previous, and current latents were concatenated. Empty edge or node features in the input were initialized to 1.

The total number of parameters varies between GN, GCN, GN-GFT, and GCN-GFT because these MLPs are composed in different ways. GCNs do not have globals or edge updating functions. For the GFT (Graph Fourier Transform) spectral core, spectral vertices were ordered by eigenvalue index and reshaped into a $K \times n_{\text{latents}}$ vector, then fed processed by an MLP. Rather than repeating the same GN or GCN for each iteration of message passing, a unique core was used for each step. This permits each step of message passing to apply a different function.

B Dataset Overview

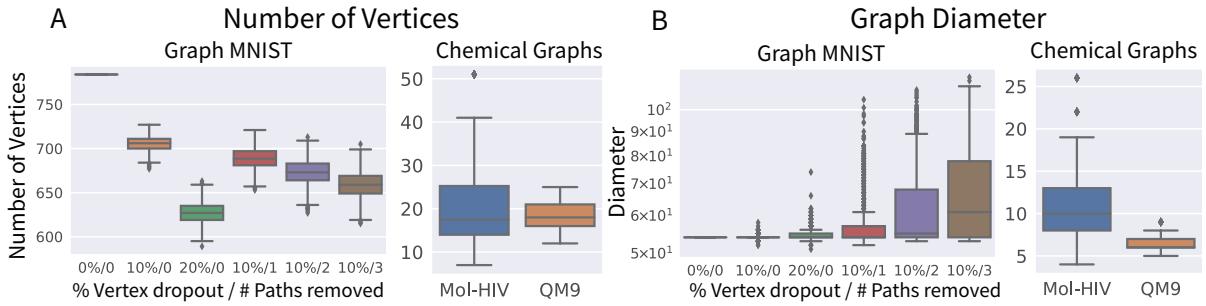


Figure B.1: (A) Distribution of number of vertices per graphs across tasks (B) Distribution of diameter per graphs across tasks

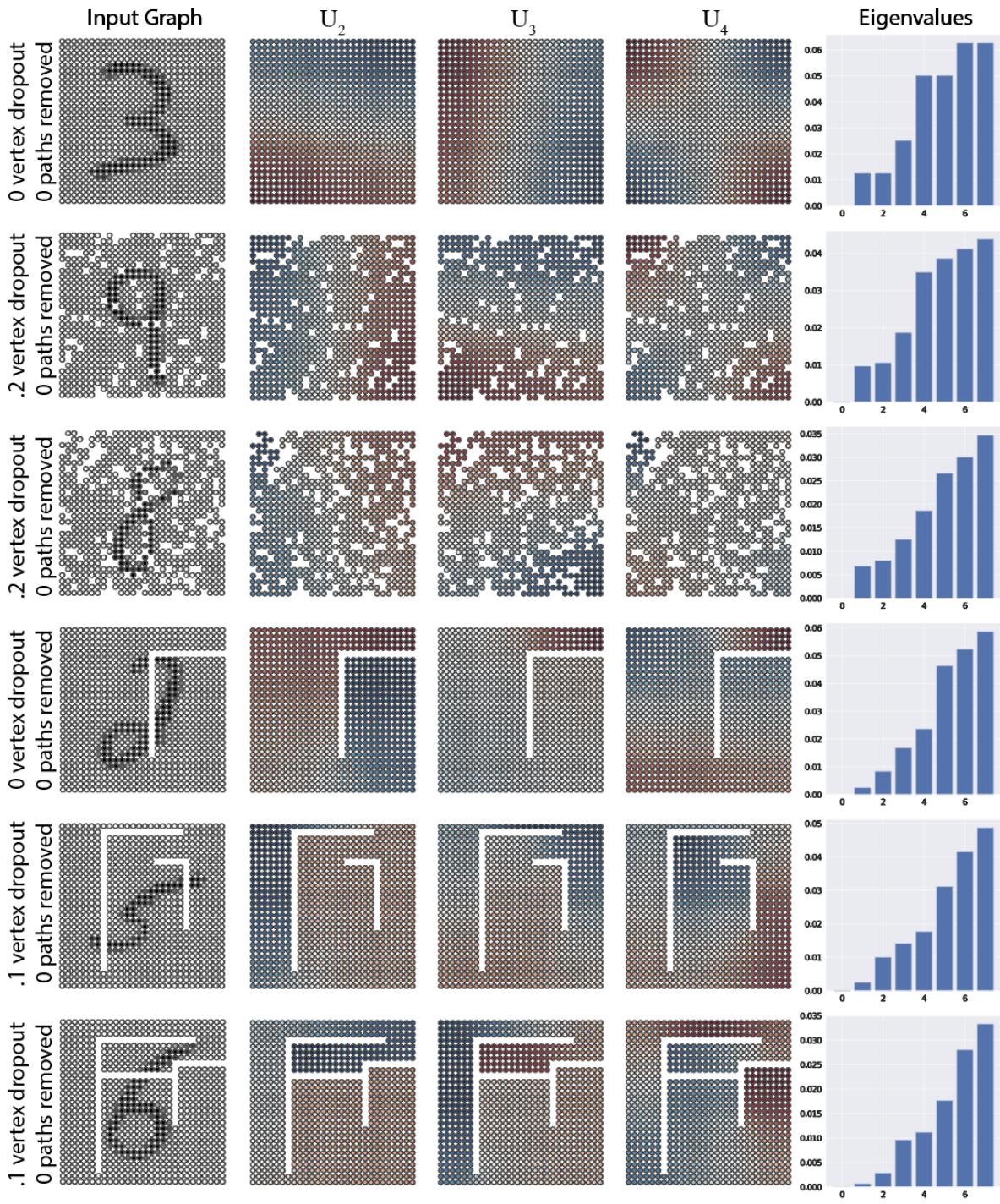


Figure B.2: Samples from Graph MNIST with various levels of dropout. First 4 Laplacian eigenvectors and eigenvalues are shown.

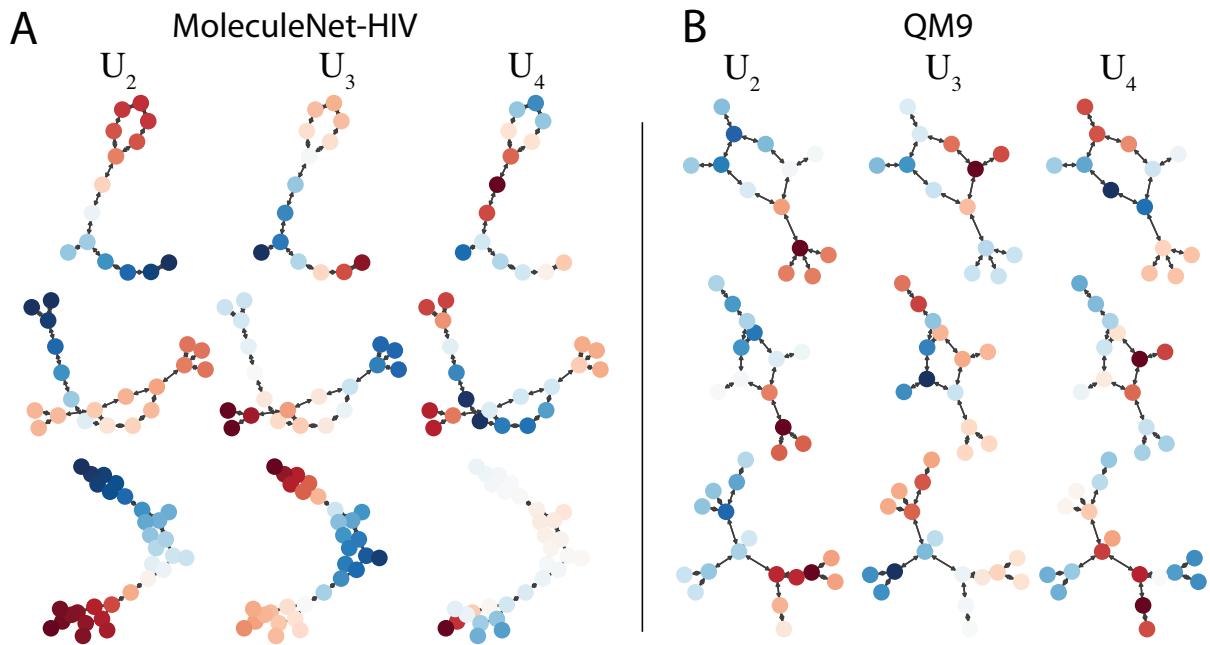


Figure B.3: Samples from (A) MoleculeNet-HIV and (B) QM9 with first 3 nontrivial Laplacian eigenvectors.

C MNIST

C.1 MNIST Learning Curves

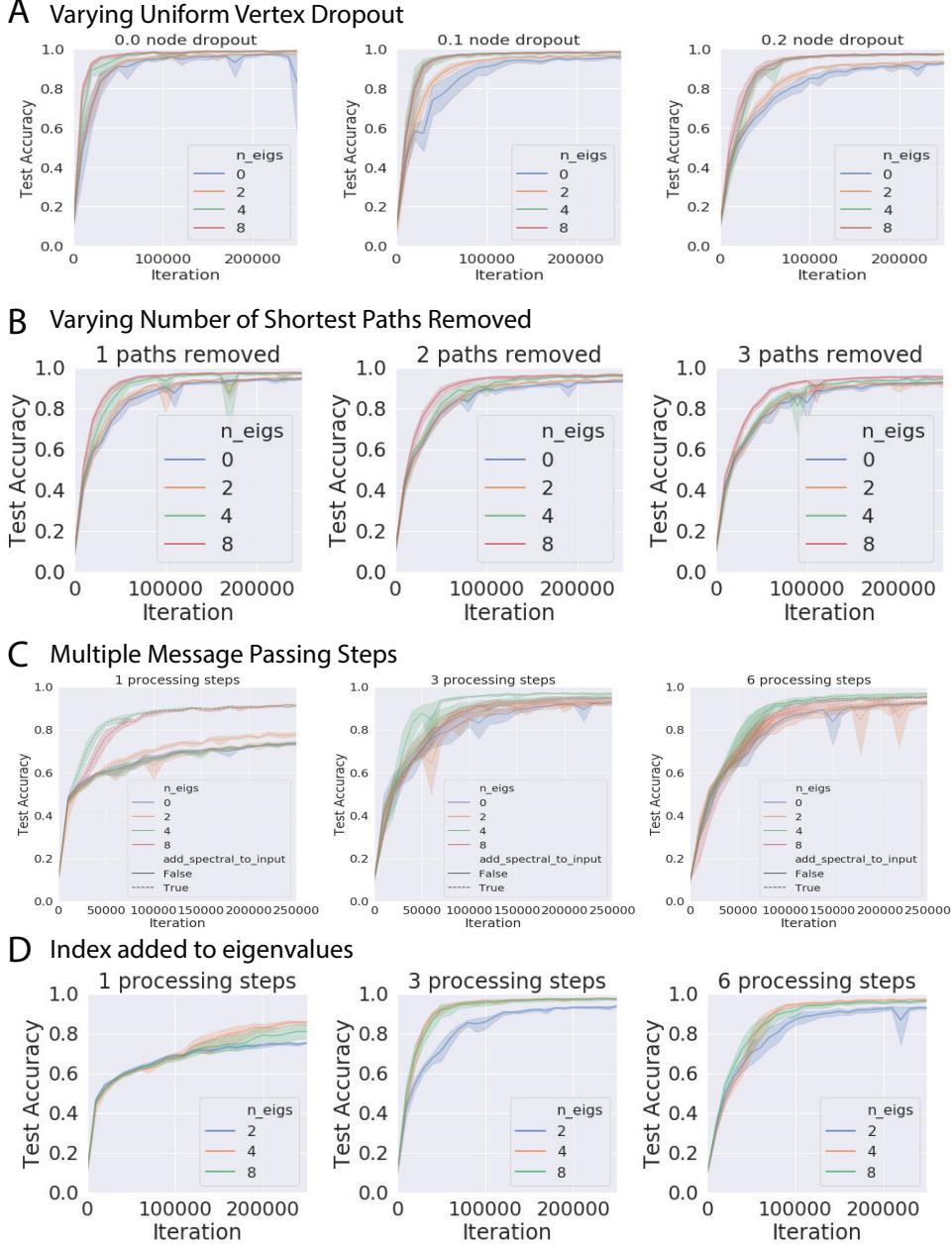


Figure C.4: Learning curves for GN and spectral U -GNs. Curves depict mean and standard deviation for each model type averaged over 5 seeds. Unless otherwise noted, runs have 0 shortest path dropout and 3 steps of message passing. **(A)** Varying rates of vertex dropout. **(B)** Varying numbers of shortest paths removed (vertex dropout rate = 0.1). **(C-D)** Varying numbers of message passing iterations (vertex dropout rate = 0.2). In (C), solid line indicates U -GN, dashed line GN+ U appended to vertex inputs. In (D), all runs use U -GN with eigenvalue index appended to eigenvalues in the inputted spectral graph.

MNIST: Message passing iterations Since the spectral models should, in principle, more easily aggregate information across large distances, we evaluated how the spectral models compared to simply increasing the number of message passing steps (using a uniform vertex dropout rate of 0.2).

As shown in Appendix Table C.3, and Figures C.4 and 2C,D, for 1 message passing step, the non-spectral GN, U -GN, and $\theta(U)$ -GN performed poorly, with accuracy of only 0.748 – 0.753 in 250K steps.

For 3 message passing steps, the spectral U_4 -GN and U_8 -GN had highest performance, with accuracy of 0.98 compared to the non-spectral GN's 0.94. We expected increasing the number of message passing steps to permit GN to approach the performance of U -GN. However, for 6 message passing steps, the U -GN still reached higher performance earlier in training than GN (see Appendix Figure C.4) and after 250K steps, the non-spectral GN was still behind with an accuracy of 0.938 compared to U -GN's 0.976 ($K = 4$). However, these models train considerably slower in terms of number of training iterations and wall clock time, so it is possible this may have changed with even more training time.

There were two experimental conditions under which a spectral model was able to excel with only 1 message passing iteration. The first was to simply append U to the inputted graph's vertex features. This suffers from degeneracies/instabilities since eigenvectors are ordered by index (Section ??) and does not permit the eigenvectors to explicitly route messages. However, this does permit vertices to access global information. Generally, integrating the eigenvectors via spectral message passing had better performance than providing the eigenvectors as input (Appendix Table C.3; Figures ??C-D). However, for only 1 message passing step, the appended eigenvectors significantly outperformed the spectral message passing model.

The other condition was to append vertex index information to the incoming spectral graph. Typically, the vertex latents of the spectral graph are set to the eigenvalue corresponding to each vertex. We also experimented with appending a one-hot indicating the index of that eigenvector. In theory, this should be easy for the spectral graph to deduce with a small number of message passing iterations. However, in the absence of a large number of message passing steps, appending eigenvalue index boosted learning for 1 but had no discernible effect for 3 or 6 message passing iterations (Appendix Table C.3).

C.2 MNIST Tables

		0% Vertex Dropout			
	K	0	2	4	8
U	GCN	0.846±0.010	0.849±0.007	0.851±0.004	0.851±0.005
	GCN-GFT	0.846±0.010	0.882±0.009	0.925±0.007	0.867±0.023
	GN	0.979±0.002	0.983±0.002	0.991±0.001	0.992±0.001
	GN-GFT	0.979±0.002	0.984±0.002	0.987±0.002	0.985±0.002
$\theta(U)$	GCN	0.846±0.010	0.571±0.022	0.561±0.019	0.564±0.010
	GCN-GFT	0.846±0.010	0.551±0.013	0.599±0.028	0.580±0.005
	GN	0.979±0.002	0.977±0.003	0.978±0.003	0.947±0.045
	GN-GFT	0.979±0.002	0.935±0.010	0.951±0.011	0.923±0.029
10% Vertex Dropout					
U	GCN	0.694±0.007	0.696±0.006	0.694±0.006	0.691±0.009
	GCN-GFT	0.694±0.007	0.730±0.007	0.782±0.028	0.638±0.040
	GN	0.968±0.003	0.973±0.002	0.987±0.004	0.987±0.002
	GN-GFT	0.968±0.003	0.973±0.004	0.982±0.004	0.977±0.003
$\theta(U)$	GCN	0.694±0.007	0.467±0.006	0.467±0.009	0.466±0.005
	GCN-GFT	0.694±0.007	0.425±0.013	0.442±0.016	0.439±0.019
	GN	0.968±0.003	0.967±0.004	0.967±0.011	0.974±0.009
	GN-GFT	0.968±0.003	0.915±0.045	0.905±0.058	0.828±0.030
20% Vertex Dropout					
U	GCN	0.566±0.008	0.567±0.007	0.561±0.010	0.566±0.011
	GCN-GFT	0.566±0.008	0.565±0.016	0.605±0.014	0.456±0.024
	GN	0.940±0.005	0.950±0.004	0.977±0.002	0.980±0.005
	GN-GFT	0.940±0.005	0.946±0.004	0.970±0.008	0.948±0.007
$\theta(U)$	GCN	0.566±0.008	0.424±0.017	0.419±0.008	0.406±0.021
	GCN-GFT	0.566±0.008	0.358±0.012	0.351±0.023	0.372±0.009
	GN	0.940±0.005	0.940±0.004	0.941±0.020	0.945±0.015
	GN-GFT	0.940±0.005	0.874±0.060	0.817±0.060	0.738±0.063

Table C.1: (Above) Overall best test classification accuracy across 5 seeds given 2.5e5 training steps for different GraphNet architectures.

		0 paths removed, 10% Vertex dropout			
	K	0	2	4	8
U	GCN	0.694±0.007	0.696±0.006	0.694±0.006	0.691±0.009
	GCN-GFT	0.694±0.007	0.730±0.007	0.782±0.028	0.638±0.040
	GN	0.968±0.003	0.973±0.002	0.987±0.004	0.987±0.002
	GN-GFT	0.968±0.003	0.973±0.004	0.982±0.004	0.977±0.003
$\theta(U)$	GCN	0.694±0.007	0.467±0.006	0.467±0.009	0.466±0.005
	GCN-GFT	0.694±0.007	0.425±0.013	0.442±0.016	0.439±0.019
	GN	0.968±0.003	0.967±0.004	0.967±0.011	0.974±0.009
	GN-GFT	0.968±0.003	0.915±0.045	0.905±0.058	0.828±0.030
1 path removed, 10% Vertex dropout					
U	GCN	0.625±0.019	0.646±0.001	0.641±0.003	0.631±0.015
	GCN-GFT	0.625±0.019	0.632±0.009	0.599±0.018	0.511±0.011
	GN	0.957±0.006	0.960±0.005	0.981±0.000	0.981±0.004
	GN-GFT	0.957±0.006	0.956±0.007	0.973±0.001	0.954±0.006
$\theta(U)$	GCN	0.625±0.019	0.446±0.006	0.436±0.005	0.446±nan
	GCN-GFT	0.625±0.019	0.362±0.034	0.397±0.032	0.400±0.018
	GN	0.957±0.006	0.914±0.052	0.941±nan	0.955±0.012
	GN-GFT	0.957±0.006	0.844±0.085	0.862±0.088	0.762±0.032
2 path removed, 10% Vertex dropout					
U	GCN	0.595±0.009	0.605±0.004	0.595±0.006	0.593±0.008
	GCN-GFT	0.595±0.009	0.583±0.002	0.525±0.005	0.470±0.014
	GN	0.945±0.006	0.949±0.005	0.969±0.001	0.971±0.005
	GN-GFT	0.945±0.006	0.952±0.001	0.957±0.007	0.934±0.010
$\theta(U)$	GCN	0.595±0.009	0.438±0.015	0.430±nan	0.423±0.004
	GCN-GFT	0.595±0.009	0.385±0.013	0.353±0.021	0.365±0.023
	GN	0.945±0.006	0.943±0.002	0.837±0.205	0.936±0.014
	GN-GFT	0.945±0.006	0.788±0.007	0.768±0.023	0.748±0.009
3 path removed, 10% Vertex dropout					
	K	0	2	4	8
U	GCN	0.567±0.007	0.579±nan	0.559±0.014	0.568±0.009
	GCN-GFT	0.567±0.007	0.559±0.005	0.483±0.007	0.427±0.020
	GN	0.942±0.003	0.939±0.003	0.953±0.005	0.964±0.007
	GN-GFT	0.942±0.003	0.936±nan	0.949±0.006	0.922±0.009
$\theta(U)$	GCN	0.567±0.007	0.414±0.007	0.407±nan	0.408±0.001
	GCN-GFT	0.567±0.007	0.366±0.008	0.340±0.010	0.343±0.015
	GN	0.942±0.003	0.936±nan	0.951±nan	0.918±0.024
	GN-GFT	0.942±0.003	0.945±nan	0.816±0.104	0.822±0.099

Table C.2: (Above) Overall best test classification accuracy across 5 seeds given 2.5e5 training steps for different GraphNet architectures. Left column specifies the rate of random vertex dropout. Varying levels numbers of shortest paths removed.

1 processing steps, 20% Vertex Dropout						
		K	0	2	4	8
U	GN	spectral MP	0.746±0.003	0.749±0.007	0.748±0.004	nan±nan
		as input	0.746±0.003	0.795±0.005	0.915±0.004	0.921±0.006
	GN	index eigvals	0	0.764±nan	0.877±nan	0.864±0.023
3 processing steps, 20% Vertex Dropout						
U	GN	spectral MP	0.940±0.005	0.950±0.004	0.977±0.002	0.980±0.005
		U as input	0.940±0.005	0.937±0.009	0.964±0.003	0.961±0.011
		index eigvals	0.940±0.005	0.948±0.001	0.982±0.001	0.985±0.001
6 processing steps, 20% Vertex Dropout						
U	GN	spectral MP	0.938±0.008	0.943±0.006	0.976±0.005	nan±nan
		U as input	0.938±0.008	0.946±0.008	0.963±0.007	0.963±0.005
		index eigvals	938±0.008	0.956±0.001	0.979±0.002	0.971±0.008

Table C.3: Overall best test classification accuracy across 5 seeds given 2.5e5 training steps for different GraphNet architectures. Left column specifies the rate of random vertex dropout. Varying levels numbers of message passing steps.

D OGB-MOLHIV

D.1 Supplementary Methods

MoleculeNet consists of a set of molecular property prediction benchmarks [2]. One of the largest datasets within MoleculeNet is the HIV dataset, in which the challenge is to predict a binary target indicating whether a molecule has an experimentally measured ability to inhibit HIV replication. This benchmark allows us to assess the benefits of spectral augmentation on chemical graph property prediction, a dataset with very different structure to images. The input data consists of a molecular graph in which vertices are atoms and edges bonds, and vertex and edge features identify key properties of the atoms and bonds. Both atoms and bonds were encoded as 100 dimensional feature vectors using Open Graph Benchmark’s atom and bond encoders, respectively. The dataset consists of 41,127 small, sparse molecular graphs (on average, #vertices=25.5, #edges=27.7, diameter=12.0) and is skewed such that 2.7% of the dataset is labelled positive (see Appendix Figure B.1 for statistics across datasets). This dataset is available on Open Graph Benchmark [1].

D.2 Tables and Figures

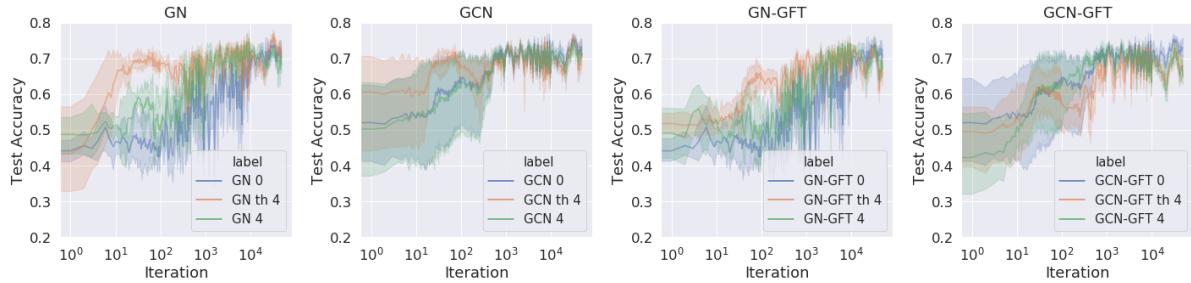


Figure D.5: Model performance over time for GN, GCN, GN-GFT, and GCN-GFT, and their spectral variants, U and $\theta(U)$, on MoleculeNet-HIV.

MoleculeNet HIV Results					
	K	0	2	4	8
U	GCN	0.755 ± 0.015	0.751 ± 0.019	0.743 ± 0.021	0.761 ± 0.030
	GCN-GFT	0.755 ± 0.015	0.743 ± 0.017	0.736 ± 0.017	0.741 ± 0.014
	GN	0.739 ± 0.029	0.753 ± 0.028	0.747 ± 0.023	0.746 ± 0.019
	GN-GFT	0.739 ± 0.029	0.748 ± 0.024	0.743 ± 0.024	0.742 ± 0.020
$\theta(U)$	GCN	0.755 ± 0.015	0.755 ± 0.020	0.759 ± 0.020	0.750 ± 0.032
	GCN-GFT	0.755 ± 0.015	0.754 ± 0.024	0.734 ± 0.018	0.744 ± 0.014
	GN	0.739 ± 0.029	0.764 ± 0.016	0.769 ± 0.015	0.748 ± 0.018
	GN-GFT	0.739 ± 0.029	0.758 ± 0.015	0.745 ± 0.025	0.734 ± 0.014

Table D.4: Best performances of each model on MoleculeNet-HIV in terms of ROC-AUC.

Literature Leaderboard	
GatedGCN	0.7765±0.0050
GIN+virtual vertex	0.7707±0.0149
GCN	0.7606±0.0097
GCN+virtual vertex	0.7599±0.0119
GIN	0.7558±0.0140
Graph-agnostic MLP	0.6819±0.0071

Table D.5: Leaderboard showing the performance of various literature models on MoleculeNet-HIV [1]

E QM9

E.1 Supplementary Methods

Molecules within the dataset consist of Hydrogen, Carbon, Oxygen, Nitrogen and Fluorine atoms and contain up to 9 heavy (non Hydrogen) atoms. The dataset consists of 134k molecules, of which 10k are randomly selected for validation and test sets. The vertex features in our input graph consist of atom coordinates, atomic number, formal charge, hybridization, Mulliken particle charge and whether it is aromatic. Edges are defined by the chemical graph, and where applicable edge features of bond type, bond length and bond vector are provided. For targets U0, U, H and G, the reference energy is subtracted. For this task, we train for 5 million steps with a latent size of 32.

E.2 Tables and Figures

Edge Dropout = 0.0						
	Unit	GN	GN-U (n=2)	GN-U (n=4)	GN-U _{thresh} (n=2)	GN-U _{thresh} (n=4)
Cv	cal/(mol K)	0.07±0.0	0.15±0.0	0.15±0.0	0.10±0.0	0.11±0.0
G	meV	59.35±0.3	90.27±27.8	61.77±7.8	63.81±9.0	63.18±6.2
H	meV	69.24±21.2	73.89±3.8	62.10±0.4	79.64±21.8	67.03±0.4
HOMO	meV	84.38±0.9	109.77±6.4	105.53±1.3	93.83±1.9	101.17±1.0
LUMO	meV	81.19±0.4	98.06±1.4	103.09±1.9	93.16±2.9	102.01±6.5
R2	Bohr ²	16.33±0.3	27.13±1.3	25.78±1.4	17.47±0.1	17.23±0.1
U	meV	63.28±2.7	97.43±23.2	68.28±3.5	61.79±1.4	90.42±6.4
U0	meV	54.81±4.4	84.96±3.7	64.16±1.7	63.19±9.3	70.73±17.2
ZPVE	meV	3.79±0.1	6.11±0.3	5.85±0.4	4.12±0.3	4.08±0.1
alpha	Bohr ³	0.23±0.0	0.39±0.0	0.34±0.0	0.28±0.0	0.28±0.0
gap	meV	126.72±1.8	156.22±2.4	160.22±0.4	145.29±1.9	151.85±5.4
mu	D	0.38±0.0	0.46±0.0	0.47±0.0	0.45±0.0	0.51±0.0
Edge Dropout = 0.5						
	Unit	GN	GN-U (n=2)	GN-U (n=4)	GN-U _{thresh} (n=2)	GN-U _{thresh} (n=4)
Cv	cal/(mol K)	0.12±0.0	0.15±0.0	0.13±0.0	0.14±0.0	0.12±0.0
G	meV	127.54±16.7	110.92±17.6	80.57±4.7	119.07±18.4	115.22±13.9
H	meV	122.17±6.8	118.39±39.6	98.61±13.3	106.03±1.6	124.93±19.0
HOMO	meV	108.92±5.4	121.44±6.7	114.68±5.0	123.66±6.0	131.34±1.9
LUMO	meV	107.12±0.3	112.95±2.8	110.66±0.7	115.74±6.1	120.44±2.5
R2	Bohr ²	26.70±0.2	31.51±0.6	28.14±0.1	29.18±0.2	31.26±0.6
U	meV	118.52±4.4	98.12±12.8	95.11±9.7	113.11±3.2	157.62±80.5
U0	meV	124.08±6.8	105.79±5.6	93.70±3.7	121.12±15.8	107.42±10.1
ZPVE	meV	5.85±0.2	6.31±0.7	5.78±0.6	5.00±0.4	5.25±0.2
alpha	Bohr ³	0.35±0.0	0.42±0.0	0.41±0.0	0.39±0.0	0.39±0.0
gap	meV	142.50±1.8	179.66±6.4	171.94±9.6	180.77±1.7	185.96±2.3
mu	D	0.46±0.0	0.60±0.0	0.56±0.0	0.59±0.0	0.59±0.0
Edge Dropout = 1.0						
	Unit	GN	GN-U (n=2)	GN-U (n=4)	GN-U _{thresh} (n=2)	GN-U _{thresh} (n=4)
Cv	cal/(mol K)	0.28±0.0	0.21±0.0	0.17±0.0	0.20±0.0	0.21±0.0
G	meV	215.91±5.5	168.73±1.2	133.99±21.0	163.65±22.2	145.04±12.4
H	meV	232.32±14.9	179.32±1.8	125.08±3.2	172.41±26.4	150.03±2.8
HOMO	meV	140.23±1.1	150.29±1.0	132.69±1.6	146.81±1.4	158.18±5.2
LUMO	meV	138.37±0.6	134.81±1.2	126.81±7.8	140.53±4.9	141.94±0.0
R2	Bohr ²	56.08±1.0	40.89±1.2	36.79±2.0	45.20±3.1	41.28±1.0
U	meV	217.95±5.4	166.49±3.6	127.26±5.5	176.89±30.1	152.18±16.9
U0	meV	226.98±8.5	170.18±6.6	124.98±0.9	175.25±1.6	150.29±14.8
ZPVE	meV	10.19±0.5	8.61±0.0	7.51±0.6	8.29±0.7	7.87±0.3
alpha	Bohr ³	0.58±0.0	0.53±0.0	0.49±0.0	0.52±0.0	0.51±0.0
gap	meV	197.88±0.4	211.70±2.7	189.59±5.6	211.23±2.2	211.32±9.4
mu	D	0.59±0.0	0.66±0.0	0.63±0.0	0.68±0.0	0.65±0.0

Table E.6: Mean Absolute Error across U and $\theta(U)$ -GN on QM9 targets with varying rates of edge dropout.

Edge Dropout = 0.0						
	Unit	GCN	GCN- U ($n=2$)	GCN- U ($n=4$)	GCN- U_{thresh} ($n=2$)	GCN- U_{thresh} ($n=4$)
Cv	cal/(mol K)	0.14±0.0	0.15±0.0	0.15±0.0	0.12±0.0	0.12±0.0
G	meV	132.11±11.4	110.24±1.8	111.65±9.0	96.79±6.0	99.05±7.6
H	meV	142.37±14.1	125.69±14.0	116.03±3.7	100.51±5.3	112.59±7.9
HOMO	meV	107.71±2.3	117.86±1.8	120.90±2.9	109.94±1.1	113.43±0.5
LUMO	meV	99.75±3.0	109.97±2.6	110.31±1.7	100.01±1.6	107.60±1.2
R2	Bohr ²	27.32±1.0	30.12±0.1	32.37±0.4	25.44±0.0	27.07±1.0
U	meV	133.49±2.8	131.09±12.5	143.50±26.4	95.45±1.1	100.23±3.0
U0	meV	128.15±6.8	133.82±23.0	112.08±1.6	101.20±8.3	99.07±13.7
ZPVE	meV	5.60±0.0	5.67±0.2	5.59±0.2	5.42±0.9	5.11±0.2
alpha	Bohr ³	0.37±0.0	0.39±0.0	0.40±0.0	0.36±0.0	0.35±0.0
gap	meV	143.96±0.6	167.64±2.8	166.84±3.4	153.15±0.7	155.86±0.9
mu	D	0.43±0.0	0.53±0.0	0.53±0.0	0.50±0.0	0.52±0.0
Edge Dropout = 0.5						
	Unit	GCN	GCN- U ($n=2$)	GCN- U ($n=4$)	GCN- U_{thresh} ($n=2$)	GCN- U_{thresh} ($n=4$)
Cv	cal/(mol K)	0.32±0.0	0.25±0.0	0.24±0.0	0.20±0.0	0.18±0.0
G	meV	330.67±8.2	282.96±16.0	272.90±2.4	166.69±12.9	167.59±3.5
H	meV	370.21±5.8	280.86±13.6	287.68±7.8	164.55±2.1	161.74±0.7
HOMO	meV	151.60±0.7	153.27±0.8	154.42±2.8	139.58±1.8	142.35±3.4
LUMO	meV	144.57±1.8	143.03±0.2	148.15±0.5	131.56±1.2	133.95±2.3
R2	Bohr ²	54.69±0.6	40.99±1.6	41.43±0.3	43.90±1.6	44.19±2.4
U	meV	365.30±40.5	279.27±1.8	293.47±15.6	167.70±7.9	168.76±20.7
U0	meV	340.62±0.7	273.01±0.9	280.44±13.9	164.54±3.3	146.67±0.3
ZPVE	meV	14.79±0.3	10.43±0.3	11.15±0.1	7.45±0.2	7.35±0.3
alpha	Bohr ³	0.70±0.0	0.60±0.0	0.61±0.0	0.48±0.0	0.48±0.0
gap	meV	198.23±2.8	202.46±5.3	205.60±1.0	186.78±0.4	188.60±2.8
mu	D	0.54±0.0	0.61±0.0	0.62±0.0	0.59±0.0	0.59±0.0
Edge Dropout = 1.0						
	Unit	GCN	GCN- U ($n=2$)	GCN- U ($n=4$)	GCN- U_{thresh} ($n=2$)	GCN- U_{thresh} ($n=4$)
Cv	cal/(mol K)	0.31±0.0	0.26±0.0	0.26±0.0	0.23±0.0	0.22±0.0
G	meV	237.48±7.2	191.62±3.5	217.30±29.4	166.32±14.8	147.05±1.7
H	meV	239.66±3.6	197.13±1.8	202.01±7.5	170.63±5.6	157.53±1.1
HOMO	meV	148.98±0.6	157.66±3.0	162.34±0.4	140.05±1.0	142.38±1.1
LUMO	meV	146.83±3.4	156.96±2.5	167.63±1.4	138.35±1.3	138.26±0.6
R2	Bohr ²	58.94±0.5	42.20±0.7	47.38±0.1	46.61±1.4	45.23±0.4
U	meV	251.92±5.7	197.72±4.3	203.85±2.5	169.65±2.1	172.10±18.7
U0	meV	249.59±7.0	208.01±24.1	197.44±3.0	166.86±10.5	154.57±15.7
ZPVE	meV	11.42±0.0	8.84±0.2	9.35±0.2	9.87±0.6	7.92±0.4
alpha	Bohr ³	0.60±0.0	0.56±0.0	0.62±0.0	0.51±0.0	0.49±0.0
gap	meV	202.90±1.6	225.53±1.9	235.63±5.7	198.51±3.8	194.22±4.3
mu	D	0.57±0.0	0.65±0.0	0.69±0.0	0.60±0.0	0.60±0.0

Table E.7: Mean Absolute Error across U and $\theta(U)$ -GN on QM9 targets with varying rates of edge dropout.

	Unit	PPGN	SchNet	PhysNet	MEGNet-s	Comorant	DimeNet
Cv	cal/(mol K)	0.055	0.033	0.0529	0.05	0.13	0.0286
G	meV	36.4	14	9.40	12	-	8.98
H	meV	36.3	14	8.42	12	-	8.11
HOMO	meV	40.3	41	32.9	43	36	27.8
LUMO	meV	32.7	34	24.7	44	36	19.7
R2	Bohr ²	0.592	0.073	0.765	0.302	0.673	0.331
U	meV	36.8	14	8.15	12	-	7.89
U0	meV	36.8	14	8.15	12	-	8.02
ZPVE	meV	3.12	1.7	1.39	1.43	1.98	1.29
alpha	Bohr ³	0.131	0.235	0.0615	0.081	0.092	0.0469
gap	meV	60.0	63	42.5	66	60	34.8
mu	D	0.047	0.033	0.0529	0.05	0.13	0.0286

Table E.8: Reported Results on QM9 in Literature

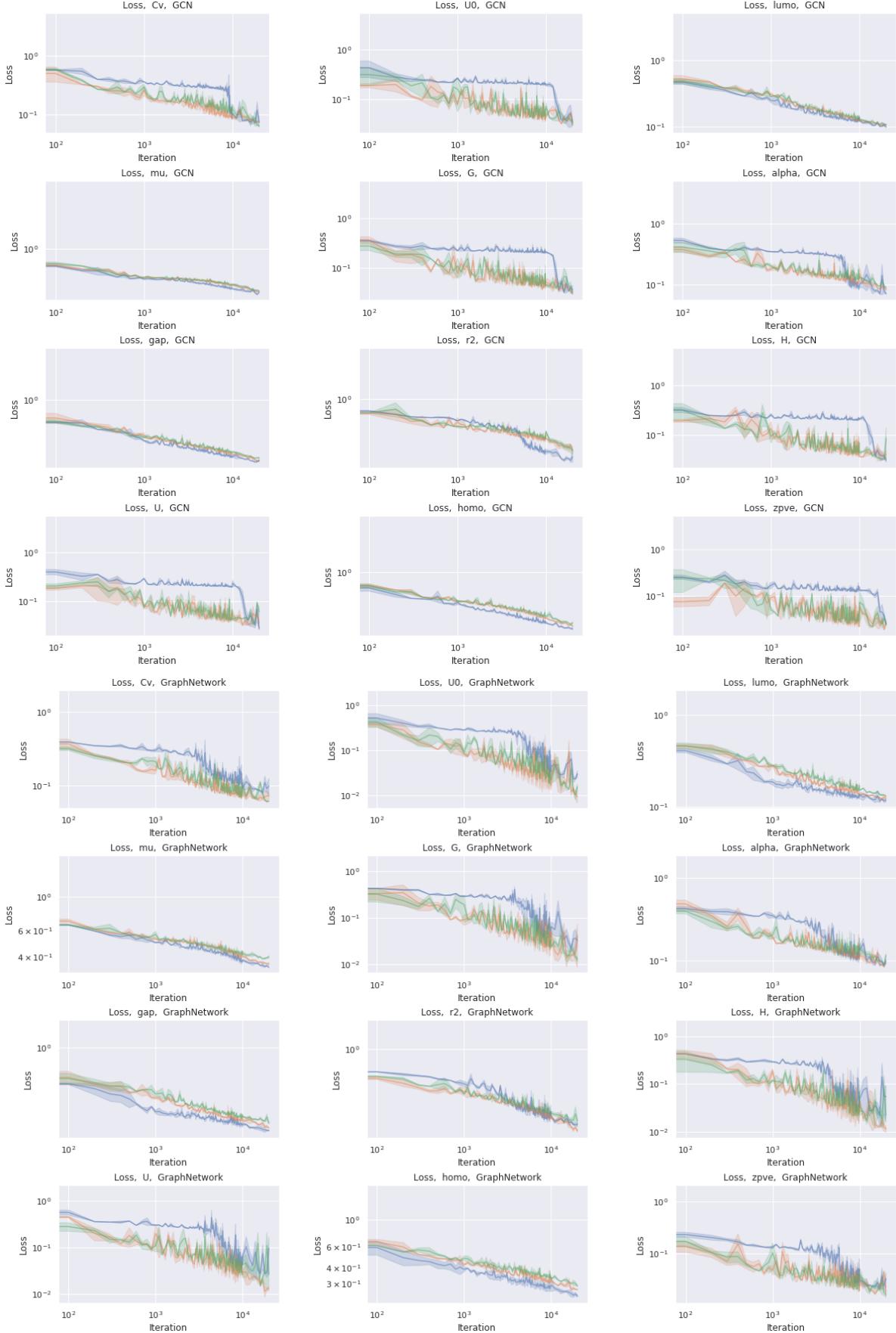


Figure E.6: Early training curves for $\theta(U)$ -GCN and $\theta(U)$ -GN, with $K = 0$ (blue), $K = 2$ (orange), and $K = 4$ (green).

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