Appendix for: Chemical Language Meets Geometric Graphs: A Multimodal Fusion Approach for Molecular Properties

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Appendix

Hyperparameter optimization

The tables below contain the hyperparameters which were optimized as the adapter layers for the LM (Table A1) and the LM+GNN approach (Table A2).

Hyperparameter	Search Range	Data Type
Dropout Rate	$[0.1, 0.5]$	Float
Learning Rate	$[10^{-6}, 10^{-1}]$	Float
Number of Layers	$[1, 5]$	Integer
ExponentialLR Gamma	$[0.9, 0.999]$	Float

Table A1: LM Adapter search space.

Hyperparameter	Search Range	Data Type
Hidden Dimension	$[50, 150]$ or $[50, 300]$ (QM9)	Integer
Number of Convolutional Layers	$[1, 5]$	Integer
Number of Head Layers	$[1, 2]$ or $[1, 3]$ (QM9)	Integer
Number of Shared Layers	$[1, 3]$ or $[1, 5]$ (QM9)	Integer
Dimension of Shared Layers	$[32, 100]$	Integer
Dimension of Head Layers	$[50, 100]$ (per layer)	Integer (multiple)
ExponentialLR Gamma	$[0.9, 0.999]$	Float
Learning Rate	$[10^{-6}, 10^{-2}]$ (log scale)	Float

Table A2: GNN and LM+GNN search space. On columns with another search range, the dataset which used the alternative search range is specified in parentheses.

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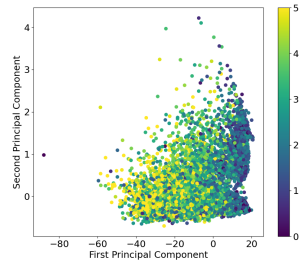
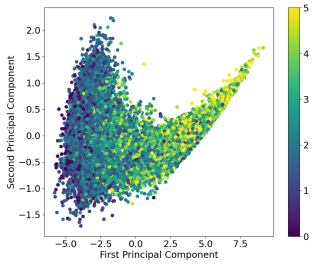
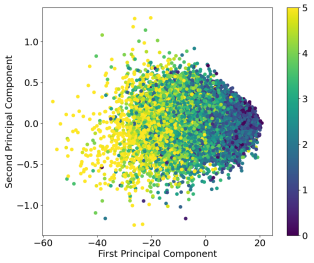
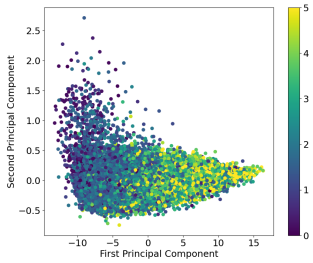
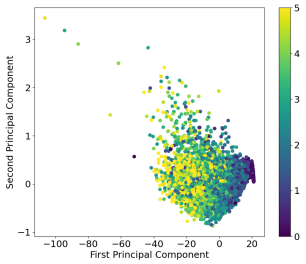
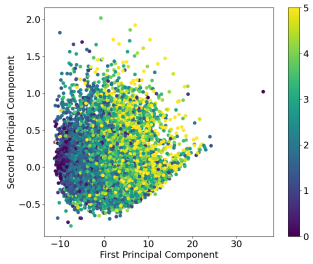
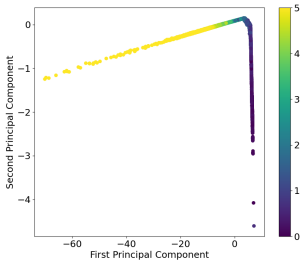
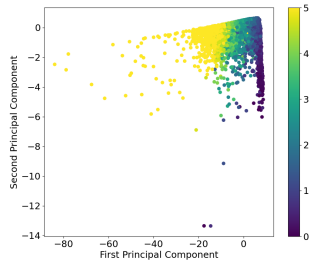
Subset size	GNN	LM+GNN
500		
750		
1000		
111206		

Table A3: Dimensionality reduction of embeddings for GNN and LM+GNN on the QM9 dipole moment task. Uses a randomly selected model from the 8 trials used in the scaling tests and runs PCA on test set embeddings. Colorbar corresponds to the dipole moment of the molecule of the test set.