SIGN AND BASIS INVARIANT NETWORKS FOR SPECTRAL GRAPH REPRESENTATION LEARNING

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ABSTRACT

Many machine learning tasks involve processing eigenvectors derived from data. Especially valuable are Laplacian eigenvectors, which capture useful structural information about graphs and other geometric objects. However, ambiguities arise when computing eigenvectors: for each eigenvector $v$, the sign flipped $-v$ is also an eigenvector. More generally, higher dimensional eigenspaces contain infinitely many choices of basis eigenvectors. These ambiguities make it a challenge to process eigenvectors and eigenspaces in a consistent way. In this work we introduce SignNet and BasisNet — new neural architectures that are invariant to all requisite symmetries and hence process collections of eigenspaces in a principled manner. Our networks are universal, i.e., they can approximate any continuous function of eigenvectors with the proper invariances. They are also theoretically strong for graph representation learning — they can approximate any spectral graph convolution, can compute spectral invariants that go beyond message passing neural networks, and can provably simulate previously proposed graph positional encodings. Experiments show the strength of our networks for learning spectral graph filters and learning graph positional encodings.

1 INTRODUCTION

Numerous machine learning models process eigenvectors, which arise in various scenarios including principal component analysis, matrix factorizations, and operators associated to graphs or manifolds. An important example is the use of graph Laplacian eigenvectors to encode information about the structure of a graph (Belkin & Niyogi, 2003). Positional encodings that involve Laplacian eigenvectors have recently been used to generalize Transformers to graphs (Kreuzer et al., 2021; Dwivedi & Bresson, 2021), and to improve the expressive power and empirical performance of graph neural networks (GNNs) (Dwivedi et al., 2022). Furthermore, these eigenvectors are crucial for defining spectral operations on graphs, which form foundations for graph signal processing and spectral GNNs (Ortega et al., 2018; Bruna et al., 2014).

However, there are nontrivial symmetries that should be accounted for when processing eigenvectors. If $v$ is a unit-norm eigenvector, then so is $-v$, with the same eigenvalue. More generally, if an eigenvalue has higher multiplicity, then there are infinitely many unit-norm eigenvectors that can be chosen. Indeed, a full set of orthonormal eigenvectors is only defined up to a change of basis in each eigenspace. In the case of sign invariance, for any $k$ eigenvectors there are $2^k$ possible choices of sign. Accordingly, prior works randomly flip eigenvector signs during training in order to approximately learn sign invariance (Kreuzer et al., 2021; Dwivedi et al., 2020). However, learning all $2^k$ invariances is challenging and limits the effectiveness of Laplacian eigenvectors for encoding positional information. Sign invariance is a special case of basis invariance when all eigenvalues are distinct, but higher dimensional basis invariance is even more difficult to deal with, and we show that these higher dimensional eigenspaces are abundant in real datasets (see Appendix D.2).

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This work solves the sign and basis ambiguity problems by developing new neural networks, SignNet and BasisNet, with sign invariance and basis invariance built-in. Our networks are universal and can approximate any continuous function of eigenvectors with the proper invariances. Moreover, our networks are theoretically powerful for graph representation learning — they can approximate spectral graph convolutions and compute powerful spectral invariants, which allows our networks to express graph properties like subgraph counts that message passing neural networks cannot. Finally, Laplacian eigenvectors with SignNet and BasisNet can approximate previously proposed graph positional encodings, including those based on random walks (Li et al., 2020; Dwivedi et al., 2022) and heat kernels (Mialon et al., 2021; Feldman et al., 2022). We experimentally demonstrate the strength of SignNet and BasisNet for learning spectral graph convolutions and graph positional encodings.

2 SIGN AND BASIS IN Variant NETWORKS

For an $n \times n$ symmetric matrix, let $\lambda_1 \leq \ldots \leq \lambda_n$ be eigenvalues and $v_1, \ldots , v_n$ the corresponding eigenvectors, which we may assume form an orthonormal basis. For instance, we could consider the normalized graph Laplacian $L = I - D^{-1/2}AD^{-1/2}$, where $A \in \mathbb{R}^{n \times n}$ is the adjacency matrix and $D$ is the diagonal degree matrix of some underlying graph. For undirected graphs, $L$ is symmetric. Our goal is to parameterize a class of models $f(v_1, \ldots , v_k)$ taking $k$ eigenvectors as input that respects the eigenvector symmetries. For instance, $-v_i$ is also an eigenvector for any $v_i$, so a well-defined function $f$ should be sign invariant:

$$f(v_1, \ldots , v_k) = f(s_1v_1, \ldots , s_kv_k) \quad (1)$$

for all sign choices $s_i \in \{-1, 1\}$. That is, we want $f$ to be invariant to the product group $\{-1, 1\}^k$. This captures all eigenvector symmetries if the $\lambda_i$ are distinct. However, if the eigenvalues have higher multiplicity, then there are further symmetries to consider. Let $V_1, \ldots , V_l$ be bases of eigenspaces — i.e. $V_i = [v_{i1} | \ldots | v_{id_i}] \in \mathbb{R}^{n \times d_i}$ has orthonormal columns and spans the eigenspace associated with the shared eigenvalue $\mu_i = \lambda_{i1} = \ldots = \lambda_{id_i}$.

Any other orthonormal basis that spans the eigenspace is of the form $V_iQ$ for some orthogonal $Q \in O(d_i) \subseteq \mathbb{R}^{d_i \times d_i}$ (see Appendix A.2). Thus, a function $f$ that is invariant to changes of basis in each eigenspace satisfies

$$f(V_1, \ldots , V_l) = f(V_1Q_1, \ldots , V_lQ_l), \quad Q_i \in O(d_i). \quad (2)$$

In other words, $f$ is invariant to the product group $O(d_1) \times \ldots \times O(d_l)$. The $l$ and $d_i$ may vary between matrices, so we show below that our architectures can handle this. Note that $O(1) = \{-1, 1\}$, so sign invariance is a special case of this basis invariance when all eigenvalues are distinct.

We often further desire such a function $f$ to be invariant or equivariant to permutation along the entries (or rows) of each vector, since natural functions on graphs that output node features or node predictions are permutation equivariant. Thus, we typically additionally require $f(PV_1, \ldots , PV_l) = Pf(V_1, \ldots , V_l)$ for any permutation matrix $P \in \mathbb{R}^{n \times n}$. Figure 1 illustrates the full setup.

2.1 WARMUP: NEURAL NETWORKS ON ONE EIGENSPACE

Before considering the general setting, we design neural networks that take a single eigenvector or eigenspace as input and are sign or basis invariant. These single space architectures will become building blocks for the general architectures. For one subspace, a sign invariant function is merely an even function, and is easily parameterized.
Proposition 1. A continuous function \( h : \mathbb{R}^n \rightarrow \mathbb{R}^s \) is sign invariant if and only if
\[
h(v) = \phi(v) + \phi(-v)
\]
for some continuous \( \phi : \mathbb{R}^n \rightarrow \mathbb{R}^s \). A continuous \( h : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is sign invariant and permutation equivariant if and only if equation 3 holds for a continuous permutation equivariant \( \phi : \mathbb{R}^n \rightarrow \mathbb{R}^n \).

In practice, \( \phi \) is parameterized by a neural network — any architecture choice will ensure sign invariance, whilst permutation equivariance can be achieved using DeepSets or most GNNs.

Switching focus to basis invariance for a single eigenspace. Then we parameterize our \( \text{IGN}(V V^\top) \) — a neural network mapping to and from tensors of arbitrary order \( \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times d} \) that has the desired permutation equivariance. We thus parameterize a family with the requisite invariance and equivariance as follows:
\[
f(V) = \text{IGN}(V V^\top).
\]
The following proposition shows that this architecture universally approximates \( O(d) \) invariant and permutation equivariant functions; though this requires high order tensors to be used for the IGN.

Proposition 2. Any continuous, \( O(d) \) invariant \( h : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^s \) is of the form \( h(V) = \varphi(V V^\top) \) for a continuous \( \varphi \). For a compact domain \( Z \subseteq \mathbb{R}^{n \times d} \), maps of the form \( V \mapsto \text{IGN}(V V^\top) \) universally approximate continuous \( h : Z \subseteq \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^n \) that are \( O(d) \) invariant and permutation equivariant.

2.2 Neural Networks on Multiple Eigenspaces

Our fully general sign invariant and basis invariant networks are built on top of the single eigenspace case. Eigenspaces are first independently processed using the models introduced in Section 2.1, then the processed eigenspaces are aggregated into a single embedding. This approach is motivated by the general decomposition theorem we prove for product spaces in Section 3, which in our setting essentially says that it suffices to decompose along these single subspace cases.

SignNet. We parameterize our unconstrained SignNet \( f : \mathbb{R}^{n \times k} \rightarrow \mathbb{R}^s \) on eigenvectors \( v_1, \ldots, v_k \) in the form:
\[
f(v_1, \ldots, v_k) = \rho \left( [\phi(v_i) + \phi(-v_i)]_{i=1}^k \right),
\]
where \( \phi \) and \( \rho \) are generally unrestricted neural networks, and \([\cdot]_i\) denotes concatenation of vectors.

BasisNet. We take a similar approach for basis invariance. Let \( V_i \in \mathbb{R}^{n \times d_i} \) be an orthonormal basis of a \( d_i \) dimensional eigenspace. Then we parameterize our unconstrained BasisNet \( f \) by
\[
f(V_1, \ldots, V_l) = \rho \left( [\phi_{d_i}(V_i V_i^\top)]_{i=1}^l \right),
\]
where each \( \phi_{d_i} \) is shared amongst all subspaces of the same dimension \( d_i \), and \( l \) is the number of eigenspaces (i.e., number of distinct eigenvalues, which can differ from the number of eigenvectors \( k \)). As \( l \) differs between different graphs, we may use zero-padding or a sequence model like a
Theorem 1 (Decomposition Theorem). Let $X_1, \ldots, X_k$ be topological spaces, and let $G_i$ be a group acting on $X_i$ for each $i$. We assume mild topological conditions on $X_i$ and $G_i$ hold. For any continuous $f : X = X_1 \times \ldots \times X_k \to \mathbb{R}^a$ that is invariant to the action of $G = G_1 \times \ldots \times G_k$, there exists continuous $\phi_i$ and a continuous $\rho$ such that

$$f(v_1, \ldots, v_k) = \rho(\phi_1(v_1), \ldots, \phi_k(v_k)).$$

Furthermore: (1) each $\phi_i$ can be taken to be invariant to $G_i$, (2) the domain $Z$ of $\rho$ is compact if each $X_i$ is compact, (3) if $X_i = X_j$ and $G_i = G_j$, then $\phi_i$ can be taken to be equal to $\phi_j$.

This result says that when a product of groups $G$ acts on a product of spaces $X$, for invariance to the product group $G$ it suffices to individually process each smaller group $G_i$ on $X_i$ and then aggregate the results. Along with the proof of Theorem 1, the mild topological assumptions are explained in Appendix B.1. The assumptions hold for sign invariance and basis invariance (when not requiring permutation equivariance). By applying this theorem, we can prove universality of our networks.

Corollary 1. Unconstrained SignNet can represent any sign invariant function and unconstrained BasisNet can represent any basis invariant function. Expressive-BasisNet is a universal approximator of functions that are both basis invariant and permutation equivariant.

3 Universality

Whilst the networks introduced in the previous section have the requisite invariances, it is not immediately obvious whether they are powerful enough to express all possible functions with these invariances. The universality of all three architectures introduced in Section 2.2 follow as corollaries of the following general decomposition result.

Theorem 2 (Universal Approximation). Consider the same setup as Theorem 1, where each $X_i$ is additionally compact. Let $\Phi_i$ be a family of functions that universally approximate $G_i$-invariant continuous functions $X_i \to \mathbb{R}^{a_i}$, and let $\mathcal{R}$ be a family of continuous functions that universally approximate continuous functions $Z \subseteq \mathbb{R}^a \to \mathbb{R}^a$ where $a = \sum a_i$ for every compact $Z$. Then the functions $\rho(\phi_1(x_1), \ldots, \phi_k(x_k))$ for $\rho \in \mathcal{R}$, $\phi_i \in \Phi_i$ universally approximate continuous functions $f : X_1 \times \ldots \times X_k \to \mathbb{R}^a$ that are invariant to the action of $G_1 \times \ldots \times G_k$.

4 Theoretical Power for Graph Representation Learning

Here, we prove that our SignNets and BasisNets can compute useful basis invariant and permutation equivariant functions on Laplacian eigenvectors for graph representation learning, including: spectral graph convolutions, spectral invariants, and existing graph positional encodings. Of course, our Expressive-BasisNets can compute these functions, as they are universal, but the takeaway of this section is that our practical SignNets and BasisNets can also compute them.
4.1 SignNets and BasisNets Generalize Spectral Graph Convolution

For node features $X \in \mathbb{R}^{n \times d}$ and an eigendecomposition $V \Lambda V^T$, a spectral graph convolution takes the form $f(V, \Lambda, X) = \sum_{i=1}^{n} \theta_i \phi(\lambda_i, X)$, for some parameters $\theta_i$, that may optionally be continuous functions $h(\lambda_i) = \theta_i$ of the eigenvalues (Bruna et al., 2014; Defferrard et al., 2016). This family includes important functions like heat kernels and generalized PageRanks on graphs (Li et al., 2019). It can be seen (in Appendix C.1) that spectral graph convolutions are permutation equivariant and sign invariant, and if $\theta_i = h(\lambda_i)$ (i.e. the spectral graph convolution is parametric) they are additionally invariant to change of bases in each eigenspace.

Our SignNet and BasisNet can be viewed as generalizations of spectral graph convolutions, as our networks can universally approximate all spectral graph convolutions of the above form. For sign invariance, our network with $\rho = \sum_{i=1}^{n} \phi(\lambda_i, X) = \theta_i \nu_i \nu_i^\top X$ directly gives the spectral graph convolution. This is captured in the below proposition. In fact, our architecture is very natural for learning these functions, so one might expect learning spectral graph convolutions to be easy; this is theoretically justified by the principle of algorithmic alignment (Xu et al., 2020), and empirically justified by our experiments in Section 5.

**Proposition 3.** SignNet universally approximates all spectral graph convolutions. BasisNet universally approximates all parametric spectral graph convolutions.

4.2 BasisNets can Compute Spectral Invariants

Many works compare the expressive power of graph neural networks by comparing their power for testing graph isomorphism (Xu et al., 2019; Sato, 2020), or by comparing their ability to compute certain functions on graphs like subgraph counts (Chen et al., 2020; Tahmasebi et al., 2020). These works often compare GNNs to combinatorial invariants on graphs, especially the $k$-Weisfeiler-Lehman ($k$-WL) tests of graph isomorphism.

While we may also compare with these combinatorial invariants, as other GNN works that use spectral information have done (Beaini et al., 2021), we argue that it is more natural to analyze our methods in terms of spectral invariants, which are computed from the eigenvalues and eigenvectors of graphs. There is a rich literature of spectral invariants from the fields of spectral graph theory and complexity theory (Cvetković et al., 1997). A spectral invariant must be invariant to permutations and changes of basis in each eigenspace, so our networks indeed compute spectral invariants.

The most obvious spectral invariant is the multiset of eigenvalues, which we give as input to our networks. Another widely studied spectral invariant is the collection of graph angles, which are defined as the values $\alpha_{ij} = \|V_i V_j^\top e_j\|_2$, where $V_i \in \mathbb{R}^{n \times d}$ is an orthonormal basis for the $i$th adjacency matrix eigenspace, and $e_j$ is the $j$th standard basis vector, which is zero besides a one in the $j$th component. These are easily computed by our networks, and thus our networks inherit the strength of these invariants for learning functions on graphs; we capture these results in the following proposition, which also lists a few properties that graph angles determine (Cvetković, 1991).

**Proposition 4.** BasisNet universally approximates the graph angles $\alpha_{ij}$. The eigenvalues and graph angles (and thus BasisNets) can determine the number of length 3, 4, or 5 cycles, whether a graph is connected, and the number of length $k$ closed walks from any vertex to itself.

In contrast to this result, message passing GNNs are not able express any of these properties (Arvind et al., 2020; Chen et al., 2020). Although spectral invariants are strong, Fürer (2010) shows that the eigenvalues and graph angles — as well as some strictly stronger spectral invariants — are not stronger than the 3-WL test (sometimes denoted the 2-FWL test). Future work could study the combination of spectral invariants or spectral graph positional encodings with combinatorial algorithms and graph neural networks.

4.3 SignNets and BasisNets Generalize Existing Graph Positional Encodings

Since Expressive-BasisNet is universal, we can view it as parameterizing a maximally expressive spectral positional encoding on graphs. Also, we are able to show that our efficient SignNets and BasisNets can universally approximate previously used graph positional encodings, as captured in the following proposition. This is because these positional encodings can be expressed as spectral graph convolution matrices, or the diagonal of a spectral graph convolution matrix.
Proposition 5. SignNets and BasisNets universally approximate heat kernel positional encodings (Feldman et al., 2022) and random walk node positional encodings (RWPE) (Dwivedi et al., 2022). BasisNets universally approximate diffusion and $p$-step random walk relative positional encodings (Mialon et al., 2021), as well as generalized PageRank and landing probability distance encodings (Li et al., 2020).

5 Experiments

5.1 Graph Regression

Table 1: Results on the ZINC dataset with 500k parameter budget. All models use edge features. Numbers are the mean and standard deviation over 4 runs, each with different seeds.

| Base model | Positional encoding | $k$ | #param | Test MAE (↓) |
|------------|---------------------|-----|--------|--------------|
| GatedGCN   | No PE               | N/A | 492k   | 0.252±0.007 |
|            | LapPE (flip)        | 8   | 492k   | 0.198±0.011 |
|            | LapPE (abs.)        | 8   | 492k   | 0.204±0.009 |
|            | LapPE (can.)        | 8   | 492k   | 0.298±0.019 |
|            | SignNet             | 8   | 405k   | 0.121±0.005 |
| Sparse Transformer | No PE               | N/A | 473k   | 0.258±0.030 |
|            | LapPE (flip)        | 16  | 487k   | 0.223±0.007 |
|            | SignNet             | 16  | 479k   | 0.115±0.008 |
| PNA        | No PE               | N/A | 474k   | 0.128±0.000 |
|            | LapPE (flip)        | 8   | 474k   | 0.139±0.000 |
|            | SignNet             | 8   | 476k   | 0.105±0.007 |
| GINE       | No PE               | N/A | 470k   | 0.170±0.002 |
|            | LapPE (flip)        | 16  | 470k   | 0.178±0.004 |
|            | SignNet             | 16  | 470k   | 0.147±0.005 |
|            | SignNet All         | 417 | 470k   | 0.102±0.002 |

We study the effectiveness of our sign invariant networks in learning positional encodings (PEs) from the eigenvectors of the graph Laplacian on the ZINC dataset. We consider three settings: 1) No positional encoding, 2) Laplacian PE (LapPE) – the $k$ eigenvectors of the graph Laplacian with smallest eigenvalue are concatenated with existing node features, 3) SignNet positional features – passing the eigenvectors through a SignNet and concatenating the output with node features. We parameterize the SignNet by taking $\phi$ to be a GIN (Xu et al., 2019) and $\rho$ to be an MLP (see Appendix E.2 for further details). We consider four different base models: GatedGCN (Bresson & Laurent, 2017), a Transformer with sparse attention only over neighbours as introduced by Kreuzer et al. (2021), PNA (Corso et al., 2020), and GIN (Xu et al., 2019) with edge features (i.e. GINE) (Hu et al., 2020b). The combined total number of parameters of the SignNet and the base model is kept within a 500k budget by adjusting network width.

Results comparing different positional encoding methods are displayed in Table 1. For all 4 base model, the PE learned with SignNet yields the best test MAE (lower is better). Notably, this includes the cases of PNA and GINE, for which Laplacian PE with simple random sign flipping was unable to improve performance over using no PE at all. Besides SignNet, we consider two non-learned approaches to resolving eigenvector sign ambiguity — canonicalization and taking element-wise absolute values (see Appendix E.2 for details). Results with GatedGCN show that these alternatives are not more effective than random sign flipping for learning positional encodings. Finally, we experimented with using all available eigenvectors in SignNet (in this case the aggregation function $\rho$ is taken to be a Transformer to handle variable length inputs). Results on GINE suggest that using all available eigenvectors is preferable.

5.2 Learning Spectral Graph Convolutions

To numerically test the ability of our basis invariant networks for learning spectral graph convolutions, we follow the experimental setups of Balcilar et al. (2020); He et al. (2021). We take the
dataset of 50 images in He et al. (2021) (originally from the Image Processing Toolbox of MATLAB), and resize them from $100 \times 100$ to $32 \times 32$. Then we apply the same spectral graph convolutions on them as in He et al. (2021), and train neural networks to learn these as regression targets. As in prior work, we report sum of squared errors on the training set to test expressivity.

We compare against message passing GNNs (Kipf & Welling, 2017; Veličković et al., 2018) and spectral GNNs (Chien et al., 2021; Bianchi et al., 2021; Defferrard et al., 2016; He et al., 2021). Also, we consider standard Transformers with only node features, with eigenvectors and sign flip augmentation, and with absolute values of eigenvectors. These models are all approximately sign invariant (they either use eigenvectors in a sign invariant way or do not use eigenvectors). We use DeepSets (Zaheer et al., 2017) in SignNet and 2-IGN (Maron et al., 2018) in BasisNet for $\phi$, use a DeepSets for $\rho$ in both cases, and then feed the features into another DeepSets or a standard Transformer (Vaswani et al., 2017) to make the final predictions. That is, we are only given graph information through the eigenvectors and eigenvalues, and we do not use message passing.

Table 2 displays the results. SignNet and BasisNet allow DeepSets and Transformers to perform strongly, beating the spectral GNNs GPR-GNN and ARMA on all tasks. Also, our networks outperform all other methods on the band-rejection and comb filters, and they are close to the best model on the other filters. Hence, our theoretical results in Section 4.1 are validated in these experiments.

### 5.3 Counting Substructures and Regressing Graph Properties

Substructure counts (e.g. of cycles) and global graph properties (e.g. connectedness, diameter, radius) are important graph features that are known to be informative for problems in bio- and chemoinformatics (Chen et al., 2020; Corso et al., 2020). Following the setting in Zhao et al. (2022), we show that SignNet with Laplacian positional encodings boosts the ability of simple GNNs to count substructures and regress graph properties. We take a 4-layer GIN as the base model for all settings, and for SignNet we use GIN as $\phi$ and a Transformer as $\rho$ to handle variable numbers of eigenvectors (see Appendix. E.3 for details). As shown in Table 3, Laplacian PEs with flip-
based data augmentation improves performance in counting substructures but not in regressing graph properties, while Laplacian PEs processed by SignNet significantly boost performance on all tasks.

6 RELATED WORK

6.1 GRAPH POSITIONAL ENCODINGS

Various graph positional encodings have been proposed, which have been motivated for increasing expressive power or practical performance of graph neural networks, and for generalizing Transformers to graphs. Positional encodings are related to so-called position-aware network embeddings (Chami et al., 2020), which capture distances between nodes in graphs. These include network embedding methods like Deepwalk (Perozzi et al., 2014) and node2vec (Grover & Leskovec, 2016), which have been recently integrated into GNNs that respect their invariances by Wang et al. (2022). Further, Li et al. (2020) studies the theoretical and practical benefits of incorporating distance features into graph neural networks. Dwivedi et al. (2022) proposes a method to inject learnable positional encodings into each layer of a graph neural network, and uses a simple random walk based node positional encoding. You et al. (2021) proposes a node positional encoding \( \text{diag}(A^k) \), which captures the number of closed walks from a node to itself. Dwivedi et al. (2020) propose to use Laplacian eigenvectors as positional encodings in graph neural networks, with sign ambiguities alleviated by sign flipping data augmentation.

While positional encodings in sequences as used for Transformers (Vaswani et al., 2017) are able to leverage the canonical order in sequences, there is no such useful canonical order for nodes in a graph, due in part to permutation symmetries. Thus, different permutation equivariant positional encodings have been proposed to help generalize Transformers to graphs. Dwivedi & Bresson (2021) directly adds in linearly projected Laplacian eigenvectors to node features before processing these features with a Transformer. Kreuzer et al. (2021) propose an architecture that uses attention over Laplacian eigenvectors and eigenvalues to learn node or edge positional encodings. Mialon et al. (2021) uses spectral kernels such as the diffusion kernel to define relative positional encodings that modulate the attention matrix. Ying et al. (2021) achieve state-of-the-art empirical performance with simple Transformers that incorporate shortest-path based relative positional encodings. Zhang et al. (2021) also utilizes shortest-path distances for positional encodings in their graph Transformer.

6.2 EIGENVECTOR SYMMETRIES IN GRAPH REPRESENTATION LEARNING

Many works that attempt to respect the invariances of eigenvectors solely focus on sign invariance (Dwivedi et al., 2020; Dwivedi & Bresson, 2021; Dwivedi et al., 2022; Kreuzer et al., 2021). This may be reasonable for continuous data, where eigenvalues of associated matrices may be usually distinct and separated (e.g. Puny et al. (2022) finds that this empirically holds for covariance matrices of \( n \)-body problems). However, discrete graph Laplacians are known to have higher multiplicity eigenvalues in many cases, and in Appendix D.2 we find this to be true in various types of real-world graph data. Graphs without higher multiplicity eigenspaces are easier to deal with; in fact, graph isomorphism can be tested in polynomial time on graphs of bounded multiplicity for adjacency matrix eigenvalues (Babai et al., 1982), with a time complexity that is lower for graphs with lower maximum multiplicities.

A recent work of Wang et al. (2022) proposes full orthogonal group invariance for functions that process positional encodings. In particular, for positional encodings \( Z \in \mathbb{R}^{n \times k} \), they parameterize functions \( f(Z) \) such that \( f(Z) = f(ZQ) \) for all \( Q \in O(k) \). This indeed makes sense for network embeddings like node2vec (Grover & Leskovec, 2016), as their objective functions are based on inner products and are thus orthogonally invariant. While they prove stability results when enforcing full orthogonal invariance for eigenvectors, this is too strict of a constraint compared to our basis invariance. For instance, when \( k = n \) and all eigenvectors are used in \( V \), the condition \( f(V) = f(VQ) \) implies that \( f \) is a constant function on orthogonal matrices, since any orthogonal matrix \( W \) can be obtained as \( W = VQ \) for \( Q = V^{-1}W \in O(n) \). In other words, for bases of eigenspaces \( V_1, \ldots, V_l \) and \( V = [V_1 \ldots V_l] \), Wang et al. (2022) enforces \( VQ \cong V \), while we enforce \( V \text{Diag}(Q_1, \ldots, Q_l) \cong V \). While the columns of \( V \text{Diag}(Q_1, \ldots, Q_l) \) are still eigenvectors, the columns of \( VQ \) generally are not.
6.3 Graph Spectra and Learning on Graphs

More generally, graph spectra is widely used in analyzing graphs, and spectral graph theory (Chung, 1997) studies the connection between graph properties and graph spectra. Different graph kernels have been defined based on graph spectra, which use robust and discriminative notions of generalized spectral distance (Verma & Zhang, 2017), the spectral density of states (Huang et al., 2021), random walk return probabilities (Zhang et al., 2018), or the trace of the heat kernel (Tsitsulin et al., 2018). Graph signal processing relies on spectral operations to define Fourier transforms, frequencies, convolutions, and other useful concepts for processing data on graphs (Ortega et al., 2018). The closely related spectral graph neural networks (Wu et al., 2020; Balcilar et al., 2020) parameterize neural architectures that are based on similar spectral operations.

7 Conclusion

SignNet and BasisNet are novel architectures for processing eigenvectors that are invariant to sign flips and choices of eigenspace bases, respectively. Both architectures are provably universal: they can represent any function with the corresponding invariances. When used with Laplacian eigenvectors as inputs they can approximate spectral graph convolutions, can compute spectral invariants and graph properties such as subgraph counts, and can approximate a number of other graph positional encoding approaches. These theoretical results on the power of SignNet and BasisNet for graph representation learning are supported by experiments showing that SignNet and BasisNet are highly expressive in practice, and learn effective graph positional encodings that improve the performance of message passing graph neural networks.

Acknowledgments Stefanie Jegelka and Suvrit Sra acknowledge support from NSF CCF-2112665 (TILOS AI Research Institute). Stefanie Jegelka also acknowledges support from NSF Award 2134108 and NSF Convergence Accelerator Track D 2040636. Suvrit Sra acknowledges support from NSF CAREER grant (IIS-1846088). Joshua Robinson is partially supported by a Two Sigma fellowship.

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A DEFINITIONS, NOTATIONS, AND BACKGROUND

A.1 BASIC TOPOLOGY AND ALGEBRA DEFINITIONS

We will use some basic topology and algebra for our theoretical results. A topological space \((X, \tau)\) is a set \(X\) along with a family of subsets \(\tau \subseteq 2^X\) satisfying certain properties, which gives useful notions like continuity and compactness. From now on, we will omit mention of \(\tau\), and refer to a topological space as the set \(X\) itself. For topological spaces \(X\) and \(Y\), we write \(X \cong Y\) and say that \(X\) is homeomorphic to \(Y\) if there exists a continuous bijection with continuous inverse from \(X\) to \(Y\). We will say \(X = Y\) if the underlying sets and topologies are equal as sets (we will often use this notion of equality for simplicity, even though it can generally be substituted with homeomorphism).

For a function \(f : X \to Y\) between topological spaces \(X\) and \(Y\), the image \(\text{im} f\) is the set of values that \(f\) takes, \(\text{im} f = \{f(x) : x \in X\}\). This is also denoted \(f(X)\). A function \(f : X \to Y\) is called a topological embedding if it is a homeomorphism from \(X\) to its image.

A group \(G\) is a set along with a multiplication operation \(G \times G \to G\), such that multiplication is associative, there is a multiplicative identity \(e \in G\), and each \(g \in G\) has a multiplicative inverse \(g^{-1}\). A topological group is a group that is also a topological space such that the multiplication and inverse operations are continuous.

A group \(G\) may act on a set \(X\) by a function \(\cdot : G \times X \to X\). We usually denote \(g \cdot x\) as \(gx\). A topological group is said to act continuously on a topological space \(X\) if \(\cdot\) is continuous. For any group \(G\) and topological space \(X\), we define the coset \(Gx = \{gx : x \in X\}\), which can be viewed as an equivalence class of elements that can be transformed from one to another by a group element. The quotient space \(X/G\) is the set of all such equivalence classes, with a topology induced by \(X\).

For \(x \in \mathbb{R}^s\), \(|x|_2\) denotes the standard Euclidean norm. By the \(\infty\) norm of functions \(f : Z \to \mathbb{R}^s\) from a compact \(Z\) to a Euclidean space \(\mathbb{R}^s\), we mean \(\|f\|_\infty = \sup_{z \in Z} |f(z)|_2\).

A.2 BACKGROUND ON EIGENSPACE INVARIANCES

Let \(V = [v_1 \ldots v_d]\) and \(W = [w_1 \ldots w_d] \in \mathbb{R}^{n \times d}\) be two orthonormal bases for the same \(d\) dimensional subspace of \(\mathbb{R}^n\). Define a linear map \(T : \mathbb{R}^d \to \mathbb{R}^d\) by mapping \(T(v_i) = w_i\). This map is orthogonal, because for any \(v = \sum_i a_i v_i\) and \(v' = \sum_i a'_i v_i\) in \(\mathbb{R}^d\), we have

\[
T(v)^\top T(v) = \sum_i a_i a'_i w_i^\top w_i = \sum_i a_i a'_i = v^\top v. \tag{10}
\]

Thus, \(T\) can be written as an orthogonal matrix \(Q\) such that \(V Q = W\). This means that any two orthonormal bases of the same subspace can be mapped to each other by right multiplication by an orthogonal matrix.

For another perspective on this, define the Grassmannian \(\text{Gr}(d, n)\) as the smooth manifold consisting of all \(d\) dimensional subspaces of \(\mathbb{R}^n\). Further define the Stiefel manifold \(\text{St}(d, n)\) as the set of all orthonormal tuples \([v_1 \ldots v_d] \in \mathbb{R}^{n \times d}\) of \(d\) vectors in \(\mathbb{R}^n\). Letting \(O(d)\) act by right multiplication, it holds that \(\text{St}(d, n)/O(d) \cong \text{Gr}(d, n)\). This implies that any \(O(d)\) invariant function on \(\text{St}(d, n)\) can be viewed as a function on subspaces. See e.g. Gallier & Quaintance (2020) Chapter 5 for more information on this. We will use this relationship in our proofs of universal representation.

When we consider permutation invariance or equivariance, the permutation acts on dimensions of size \(n\). Then a tensor \(X \in \mathbb{R}^{n \times d}\) is called an order \(k\) tensor with respect to this permutation symmetry, where order 0 are called scalars, order 1 tensors are called vectors, and order 2 tensors are called matrices. Note that this does not depend on \(d\); in this work, we only ever consider vectors and scalars with respect to the \(O(d)\) action.

B PROOFS OF UNIVERSALITY

We begin by proving the two propositions for the single subspace case from Section 2.1.

**Proposition 1.** A continuous function \(h : \mathbb{R}^n \to \mathbb{R}^s\) is sign invariant if and only if

\[
h(v) = \phi(v) + \phi(-v) \tag{3}
\]
for some continuous \( \phi : \mathbb{R}^n \to \mathbb{R}^s \). A continuous \( h : \mathbb{R}^n \to \mathbb{R}^n \) is sign invariant and permutation equivariant if and only if equation 3 holds for a continuous permutation equivariant \( \phi : \mathbb{R}^n \to \mathbb{R}^n \).

**Proof.** If \( h(v) = \phi(v) + \phi(-v) \), then \( h \) is obviously sign invariant. On the other hand, if \( h \) is sign invariant, then letting \( \phi(v) = h(v)/2 \) gives that \( h(v) = \phi(v) + \phi(-v) \), and \( \phi \) is of course continuous.

If \( h(v) = \phi(v) + \phi(-v) \) for a permutation equivariant \( \phi \), then \( h(-Pv) = \phi(-Pv) + \phi(Pv) = P\phi(-v) + P\phi(v) = P(\phi(v) + \phi(-v)) = Ph(v) \), so \( h \) is permutation equivariant and sign invariant.

If \( h \) is permutation equivariant and sign invariant, then define \( \phi(v) = h(v)/2 \) again; it is clear that \( \phi \) is continuous and permutation equivariant.

**Proposition 2.** Any continuous, \( O(d) \) invariant \( h : \mathbb{R}^{n \times d} \to \mathbb{R}^s \) is of the form \( h(V) = \varphi(VV^T) \) for a continuous \( \varphi \). For a compact domain \( Z \subseteq \mathbb{R}^{n \times d} \), maps of the form \( V \mapsto \text{IGN}(VV^T) \) universally approximate continuous functions \( h : Z \subseteq \mathbb{R}^{n \times d} \to \mathbb{R}^n \) that are \( O(d) \) invariant and permutation equivariant.

**Proof.** The case without permutation equivariance holds by the First Fundamental Theorem of \( O(d) \) (Lemma 2).

For the permutation equivariant case, let \( Z' = \{ VV^T : V \in Z \} \) and let \( \epsilon > 0 \). Note that \( Z' \) is compact, as it is the continuous image of a compact set. Since \( h \) is \( O(d) \) invariant, the first fundamental theorem of \( O(d) \) shows that there exists a continuous function \( \varphi : Z' \subseteq \mathbb{R}^{n \times n} \to \mathbb{R}^n \) such that \( h(V) = \varphi(VV^T) \). Since \( h \) is permutation equivariant, for any permutation matrix \( P \) we have that

\[
\begin{align*}
    h(PV) &= P \cdot h(V) \\
    \varphi(PVV^TP^T) &= P \cdot \varphi(VV^T),
\end{align*}
\]

so \( \varphi \) is a continuous permutation equivariant function from matrices to vectors. Then note that Keriven & Peyré (2019) show that invariant graph networks (of generally high tensor order in hidden layers) universally approximate continuous permutation equivariant functions from matrices to vectors on compact sets of matrices. Thus, an IGN can \( \epsilon \)-approximate \( \varphi \), and hence \( V \mapsto \text{IGN}(VV^T) \) can \( \epsilon \)-approximate \( h \).

**B.1 Proof of Decomposition Theorem**

\[
\begin{align*}
    \phi &= \psi \circ \pi \\
    \pi &= \pi_1 \times \ldots \times \pi_k \\
    f &= \tilde{f} \circ \pi \\
    \psi &= \psi_1 \times \ldots \times \psi_k \\
    \rho &= f \circ \psi^{-1}
\end{align*}
\]

Figure 2: Commutative diagram for our proof of Theorem 1. Black arrows denote functions from topological constructions, and red dashed lines denote functions that we parameterize by neural networks (\( \phi = \phi_1 \times \ldots \times \phi_k \) and \( \rho \)).

Here, we give the formal statement of Theorem 1, which provides the necessary topological assumptions for the theorem to hold. In particular, we only require the \( G_i \) be a topological group that acts continuously on \( \mathcal{X}_i \) for each \( i \), and that there exists a topological embedding of each quotient space into some Euclidean space. The first assumption is very mild, and it holds for any finite or compact
matrix group, which all of the invariances we consider in this paper can be represented as. Also, many different conditions can guarantee existence of a topological embedding of the quotient space in a Euclidean space. For instance, if the quotient space is a smooth manifold, then the Whitney Embedding Theorem (Lemma 5) guarantees such an embedding. Also, if the base space $X_i$ is a Euclidean space and $G_i$ is a finite or compact matrix Lie group, then a map built from $G$-invariant polynomials gives such an embedding (González & de Salas (2003) Lemma 11.13).

Figure 2 provides a commutative diagram representing the constructions in our proof.

**Theorem 1** (Decomposition Theorem). Let $X_1, \ldots, X_k$ be topological spaces, and let $G_i$ be a topological group acting continuously on $X_i$ for each $i$. Assume that there is a topological embedding $\psi_i : X_i/G_i \to \mathbb{R}^{a_i}$ of each quotient space into a Euclidean space $\mathbb{R}^{a_i}$ for some dimension $a_i$. Then, for any continuous function $f : X = X_1 \times \ldots \times X_k \to \mathbb{R}^s$ that is invariant to the action of $G = G_1 \times \ldots \times G_k$, there exists continuous functions $\phi_i : X_i \to \mathbb{R}^{a_i}$ and a continuous function $\rho : Z \subseteq \mathbb{R}^a \to \mathbb{R}^s$, where $a = \sum a_i$, such that

$$f(v_1, \ldots, v_k) = \rho(\phi_1(v_1), \ldots, \phi_k(v_k)).$$

Furthermore: (1) each $\phi_i$ can be taken to be invariant to $G_i$; (2) the domain $Z$ is compact if each $X_i$ is compact, (3) if $X_i = X_j$ and $G_i = G_j$, then $\phi_i$ can be taken to be equal to $\phi_j$.

**Proof.** Let $\pi_i : X_i \to X_i/G_i$ denote the quotient map for $X_i/G_i$. Since each $G_i$ acts continuously, Lemma 3 gives that the quotient of the product space is the product of the quotient spaces, i.e. that

$$(X_1 \times \ldots \times X_k)/(G_1 \times \ldots \times G_k) \cong (X_1/G_1) \times \ldots \times (X_k/G_k),$$

and the corresponding quotient map $\pi : X/G$ is given by

$$\pi = \pi_1 \times \ldots \times \pi_k, \quad \pi(x_1, \ldots, x_k) = (\pi_1(x_1), \ldots, \pi_k(x_k)).$$

By passing to the quotient (Lemma 1), there exists a continuous $\tilde{f} : X/G \to \mathbb{R}^s$ on the quotient space such that $f = \tilde{f} \circ \pi$. By Lemma 4, each $X_i/G_i$ is compact if $X_i$ is compact. Defining the image $Z_i = \psi_i(X_i/G_i) \subseteq \mathbb{R}^{a_i}$, we thus know that $Z_i$ is compact if $X_i$ is compact.

Moreover, as $\psi_i$ is a topological embedding, it has a continuous inverse $\psi_i^{-1}$ on its image $Z_i$. Further, we have a topological embedding $\psi : X/G \to Z = Z_1 \times \ldots \times Z_k$ given by $\psi = \psi_1 \times \ldots \times \psi_k$, with continuous inverse $\psi^{-1} = \psi_1^{-1} \times \ldots \times \psi_k^{-1}$.

Note that

$$f = \tilde{f} \circ \pi = (\tilde{f} \circ \psi^{-1}) \circ (\psi \circ \pi).$$

So we define

$$\rho = \tilde{f} \circ \psi^{-1}, \quad \rho : Z \to \mathbb{R}^s \quad (17)$$
$$\phi_i = \psi_i \circ \pi_i, \quad \phi_i : X_i \to Z_i \quad (18)$$
$$\phi = \psi \circ \pi = \phi_1 \times \ldots \times \phi_k, \quad \phi : X \to Z \quad (19)$$

Thus, $f = \rho \circ \phi = \rho \circ (\phi_1 \times \ldots \times \phi_k)$, so equation 9 holds. Moreover, the $\rho$ and $\phi_i$ are continuous, as they are compositions of continuous functions. Furthermore, (1) holds as each $\phi_i$ is invariant to $G_i$ because each $\pi_i$ is invariant to $G_i$. Since each $Z_i$ is compact if $X_i$ is compact, the product $Z = Z_1 \times \ldots \times Z_k$ is compact if each $X_i$ is compact, thus proving (2).

To show the last statement (3), note simply that if $X_i = X_j$ and $G_i = G_j$, then the quotient maps are equal, i.e. $\pi_i = \pi_j$. Moreover, we can choose the embeddings to be equal, so say $\psi_i = \psi_j$. Then, $\phi_i = \psi_i \circ \pi_i = \psi_j \circ \pi_j = \phi_j$, so we are done.

**B.2 Universality of SignNet and BasisNet**

Here, we prove Corollary 1 on the universal representation and approximation capabilities of our unconstrained SignNets, unconstrained BasisNets, and Expressive-BasisNets. We proceed in several steps, first proving universal representation of continuous functions when we do not require permutation equivariance, then proving universal approximation when we do require permutation equivariance.
B.2.1 Sign Invariant Universal Representation

Recall that $S^{n-1}$ denotes the unit sphere in $\mathbb{R}^n$. As we normalize eigenvectors to unit norm, the domain of our functions on $k$ eigenvectors are on the compact space $(S^{n-1})^k$.

**Corollary 2** (Universal Representation for SignNet). A continuous function $f : (S^{n-1})^k \to \mathbb{R}^n$ is sign invariant, i.e. $f(s_1v_1, \ldots, s_kv_k) = f(v_1, \ldots, v_k)$ for any $s_i \in \{1, -1\}$, if and only if there exists a continuous $\phi : \mathbb{R}^n \to \mathbb{R}^{2n-2}$ and a continuous $\rho : \mathbb{R}^{(2n-2)k} \to \mathbb{R}^n$ such that

$$f(v_1, \ldots, v_k) = \rho \left( \left[ \phi(v_i) + \phi(-v_i) \right]_{i=1}^k \right).$$

**Proof.** It can be directly seen that any $f$ of the above form is sign invariant.

Thus, we show that any sign invariant $f$ can be expressed in the above form. First, we show that we can apply the general Theorem 1. The group $G_i = \{1, -1\}$ acts continuously and satisfies that $S^{n-1}/\{1, -1\} = \mathbb{R}P^{n-1}$, where $\mathbb{R}P^{n-1}$ is the real projective space of dimension $n - 1$. Since $\mathbb{R}P^{n-1}$ is a smooth manifold of dimension $n - 1$, Whitney’s embedding theorem states that there exists a (smooth) topological embedding $\psi : \mathbb{R}P^{n-1} \to \mathbb{R}^{2n-2}$ (Lemma 5).

Thus, we can apply the general theorem to see that $f = \rho \circ \tilde{\phi}^k$ for some continuous $\rho$ and $\tilde{\phi}^k$. Note that each $\tilde{\phi}_i = \phi$ is the same, as each $X_i = S^{n-1}$ and $G_i = \{1, -1\}$ is the same. Also, Theorem 1 says that we may assume that $\tilde{\phi}$ is sign invariant, so $\tilde{\phi}(x) = \phi(-x)$. Letting $\phi(x) = \phi(x)/2$, we are done with the proof.

B.2.2 Sign Invariant Universal Representation with Extra Features

Recall that we may want our sign invariant functions to process other data besides eigenvectors, such as eigenvalues or node features associated to a graph. Here, we show universal representation for when we have this other data that does not possess sign symmetry. The proof is a simple extension of Corollary 2, but we provide the technical details for completeness.

**Corollary 3** (Universal Representation for SignNet with features). For a compact space of features $\Omega \subseteq \mathbb{R}^d$, let $f(v_1, \ldots, v_k, x_1, \ldots, x_k)$ be a continuous function $f : (S^{n-1} \times \Omega)^k \to \mathbb{R}^n$.

Then $f$ is sign invariant for the inputs on the sphere, i.e.

$$f(s_1v_1, \ldots, s_kv_k, x_1, \ldots, x_k) = f(v_1, \ldots, v_k, x_1, \ldots, x_k) \quad s_i \in \{1, -1\},$$

if and only if there exists a continuous $\psi : \mathbb{R}^{n+d} \to \mathbb{R}^{2n-2+d}$ and a continuous $\rho : \mathbb{R}^{(2n-2+d)k} \to \mathbb{R}^n$ such that

$$f(v_1, \ldots, v_k) = \rho \left( \varphi(v_1, x_1) + \varphi(-v_1, x_1), \ldots, \varphi(v_k, x_k) + \varphi(-v_k, x_k) \right).$$

**Proof.** Once again, the sign invariance of any $f$ in the above form is clear.

We follow very similar steps to the proof of Corollary 2 to show that we may apply Theorem 1. We can view $\Omega$ as a quotient space, after quotienting by the trivial group that does nothing, $\Omega \cong \Omega/\{1\}$. The corresponding quotient map is $id_\Omega$, the identity map. Also, $\Omega$ trivially topologically embeds in $\mathbb{R}^d$ by the inclusion map.

As $G_i = \{1, -1\} \times \{1\}$ acts continuously, by Lemma 3 we have that

$$(S^{n-1} \times \Omega)/\{(1, -1) \times \{1\}\} \cong (S^{n-1}/\{1, -1\}) \times (\Omega/\{1\}) \cong \mathbb{R}P^{n-1} \times \mathbb{R},$$

with corresponding quotient map $\pi \times id_\Omega$, where $\pi$ is the quotient map to $\mathbb{R}P^{n-1}$.

Letting $\tilde{\psi}$ be the embedding of $\mathbb{R}P^{n-1} \to \mathbb{R}^{2n-2}$ guaranteed by Whitney’s embedding theorem (Lemma 5), we have that $\psi = \tilde{\psi} \times id_\Omega$ is an embedding of $\mathbb{R}P^{n-1} \times \Omega \to \mathbb{R}^{2n-2+d}$. Thus, we can apply Theorem 1 to write $f = \rho \circ \tilde{\phi}^k$ for $\phi = (\psi \times id_\Omega) \circ (\pi \times id_\Omega)$, so

$$\tilde{\phi}(v_i, x_i) = (\psi(v_i), x_i),$$

where $\tilde{\phi}(v_i, x_i) = \tilde{\phi}(-v_i, x_i)$. Letting $\phi(v_i, x_i) = \tilde{\phi}(v_i, x_i)/2$, we are done.

\[ \square \]
B.2.3 Basis Invariant Universal Representation

Recall that \( \text{St}(d, n) \) is the Stiefel manifold of \( k \)-tuples of vectors \((v_1, \ldots, v_k)\) where \( v_i \in \mathbb{R}^n \) and \( v_1, \ldots, v_k \) are orthonormal. This is where our inputs lie, as our eigenvectors are unit norm and orthogonal. We will also make use of the Grassmannian \( \text{Gr}(d, n) \), which consists of all \( d \)-dimensional subspaces in \( \mathbb{R}^n \). This is because the Grassmannian is the quotient space for the group action we want, \( \text{Gr}(d, n) \cong \text{St}(d, n)/O(d) \), where \( Q \in O(d) \) acts on \( V \in \text{St}(d, n) \subseteq \mathbb{R}^{n \times d} \) by mapping \( V \) to \( VQ \) (Gallier & Quaintance, 2020).

**Corollary 4** (Universal Representation for BasisNet). *For dimensions \( d_1, \ldots, d_l \leq n \) let \( f \) be a continuous function on \( \text{St}(d_1, n) \times \ldots \times \text{St}(d_l, n) \). Further assume that \( f \) is invariant to \( O(d_1) \times \ldots \times O(d_l) \), where \( O(d_i) \) acts on \( \text{St}(d_i, n) \) by multiplication on the right.*

Then there exist continuous \( \rho : \mathbb{R}^{\sum_{i=1}^{l} 2d_i(n-d_i)} \rightarrow \mathbb{R}^n \) and continuous \( \phi_i : \text{St}(d_i, n) \rightarrow \mathbb{R}^{2d_i(n-d_i)} \) such that

\[
 f(V_1, \ldots, V_l) = \rho (\phi_1(V_1), \ldots, \phi_l(V_l)),
\]

where the \( \phi_i \) are \( O(d_i) \) invariant functions, and we can take \( \phi_i = \phi_j \) if \( d_i = d_j \).

**Proof.** Letting \( X_i = \text{St}(d_i, n) \) and \( G_i = O(d_i) \), it can be seen that \( G_i \) acts continuously on \( X_i \). Also, we have that the quotient space \( \text{St}(d_i, n)/O(d_i) = \text{Gr}(d_i, n) \) is the Grassmannian of \( d_i \)-dimensional subspaces in \( \mathbb{R}^n \), which is a smooth manifold of dimension \( d_i(n-d_i) \). Thus, the Whitney embedding theorem (Lemma 5) gives a topological embedding \( \psi_i : \text{Gr}(d_i, n) \rightarrow \mathbb{R}^{2d_i(n-d_i)} \).

Hence, we may apply Theorem 1 to obtain continuous \( O(d_i) \) invariant \( \phi_i : \text{St}(d_i, n) \rightarrow \mathbb{R}^{2d_i(n-d_i)} \) and continuous \( \rho : \mathbb{R}^{\sum_{i=1}^{l} 2d_i(n-d_i)} \rightarrow \mathbb{R}^n \) such that \( f = \rho \circ (\phi_1 \times \ldots \times \phi_l) \). Also, if \( d_i = d_j \), then \( X_i = X_j \) and \( G_i = G_j \), so we can take \( \phi_i = \phi_j \).

\( \Box \)

B.2.4 Basis Invariant and Permutation Equivariant Universal Approximation

With the restriction that \( f(V_1, \ldots, V_l) : \mathbb{R}^{n \times \sum_{i=1}^{l} d_i} \rightarrow \mathbb{R}^n \) be permutation equivariant and basis invariant, we need to use the impractically expensive Expressive-BasisNet to approximate \( f \). Universality of permutation invariant or equivariant functions from matrices to scalars or matrices to vectors is difficult to achieve in a computationally tractable manner (Maron et al., 2019; Keriven & Peyré, 2019). One intuitive reason to expect this is that universally approximating such functions allows solution of the graph isomorphism problem (Chen et al., 2019), which is a computationally difficult problem. While we have exact representation of basis invariant functions by continuous \( \rho \) and \( \phi \) when there is no permutation equivariance constraint, we can only achieve approximation up to an arbitrary \( \epsilon > 0 \) when we require permutation equivariance.

**Corollary 5** (Universal Approximation for Expressive-BasisNet). *Let \( f(V_1, \ldots, V_l) : \text{St}(d_1, n) \times \ldots \times \text{St}(d_l, n) \rightarrow \mathbb{R}^n \) be continuous, \( O(d_1) \times \ldots \times O(d_l) \) invariant, and permutation equivariant. Then \( f \) can be \( \epsilon \)-approximated by an Expressive-BasisNet.*

**Proof.** By invariance, Corollary 4 of the decomposition theorem shows that \( f \) can be written as

\[
 f(V_1, \ldots, V_l) = \rho (\phi_{d_1}(V_1), \ldots, \phi_{d_l}(V_l))
\]

for some continuous \( O(d_i) \) invariant \( \phi_{d_i} \) and continuous \( \rho \). By the first fundamental theorem of \( O(d) \) (Lemma 2), each \( \phi_{d_i} \) can be written as \( \phi_{d_i}(V_i) = \varphi_{d_i}(V_i V_i^\top) \) for some continuous \( \varphi_{d_i} \). Let

\[
 Z = \{(V_1 V_1^\top, \ldots, V_l V_l^\top) : V_i \in \text{St}(d_i, n)\} \subseteq \mathbb{R}^{n^2 \times l},
\]

which is compact as it is the image of the compact space \( \text{St}(d_1, n) \times \ldots \times \text{St}(d_l, n) \) under a continuous function. Define \( h : Z \subseteq \mathbb{R}^{n^2 \times l} \rightarrow \mathbb{R}^n \) by

\[
 h(V_1 V_1^\top, \ldots, V_l V_l^\top) = \rho (\varphi_{d_1}(V_1 V_1^\top), \ldots, \varphi_{d_l}(V_l V_l^\top)).
\]

Then note that \( h \) is continuous and permutation equivariant from matrices to vectors, so it can be \( \epsilon \)-approximated by an invariant graph network (Keriven & Peyré, 2019), call it IGN. If we define
\( \tilde{\rho} = \text{IGN} \) and \( \text{IGN}_{d_i}(V_i V_i^T) = V_i V_i^T \) (this identity operation is linear and permutation equivariant, so it can be exactly expressed by an IGN), then we have \( \epsilon \)-approximation of \( f \) by
\[
\tilde{\rho} \left( \text{IGN}_{d_1}(V_1 V_1^T), \ldots, \text{IGN}_{d_n}(V_n V_n^T) \right).
\]

(29)

### B.3 Proof of Universal Approximation for General Decompositions

**Theorem 2** (Universal Approximation). Consider the same setup as Theorem 1, where \( \mathcal{X}_i \) are also compact. Let \( \Phi_i \) be a family of \( G_i \)-invariant functions that universally approximate \( G_i \)-invariant continuous functions \( \mathcal{X}_i \rightarrow \mathbb{R}^{a_i} \), and let \( \mathcal{R} \) be a set of continuous function that universally approximate continuous functions \( Z \subseteq \mathbb{R}^a \rightarrow \mathbb{R}^s \) where \( a = \sum_i a_i \) for every compact \( Z \). Then for any \( \epsilon > 0 \) and any \( G \)-invariant continuous function \( f : \mathcal{X}_1 \times \ldots \mathcal{X}_k \rightarrow \mathbb{R}^s \) there exists \( \phi \in \Phi \) and \( \rho \in \mathcal{R} \) such that \( \| f - \rho(\phi_1, \ldots, \phi_k) \|_\infty < \epsilon \).

**Proof.** Consider a particular \( G \)-invariant continuous function \( f : \mathcal{X}_1 \times \ldots \mathcal{X}_k \rightarrow \mathbb{R}^s \). By Theorem 1 there exists \( G_i \)-invariant continuous functions \( \phi'_i : \mathcal{X}_i \rightarrow \mathbb{R}^{a_i} \) and a continuous function \( \rho' : Z \subseteq \mathbb{R}^a \rightarrow \mathbb{R}^s \) (where \( a = \sum_i a_i \)) such that
\[
f(v_1, \ldots, v_k) = \rho'(\phi'_1(v_1), \ldots, \phi'_k(v_k)).
\]

Now fix an \( \epsilon > 0 \). For any \( \rho \in \mathcal{R} \) and any \( \phi_i \in \Phi_i \) \((i = 1, \ldots, k)\) we may bound the difference from \( f \) as follows (suppressing the \( v_i \)'s for brevity),
\[
\| f - \rho(\phi_1, \ldots, \phi_k) \|_\infty
= \| \rho'(\phi'_1, \ldots, \phi'_k) - \rho(\phi_1, \ldots, \phi_k) \|_\infty
\leq \| \rho'(\phi'_1, \ldots, \phi'_k) - \rho(\phi'_1, \ldots, \phi'_k) \|_\infty + \| \rho(\phi'_1, \ldots, \phi'_k) - \rho(\phi_1, \ldots, \phi_k) \|_\infty
= I + II
\]

Now let \( K' = \prod_{i=1}^k \text{im} \phi'_i \). Since each \( \phi'_i \) is continuous and defined on a compact set \( \mathcal{X}_i \) we know that \( \text{im} \phi'_i \) is compact, and so the product \( K' \) is also compact. Since \( K' \) is compact, it is contained in a closed ball \( B(\rho) \) of radius \( \rho > 0 \) centered at the origin. Let \( K \) be the closed ball \( B(\rho + 1) \) of radius \( \rho + 1 \) centered at the origin, so \( K' \) contains \( K' \) and a ball of radius 1 around each point of \( K' \). We may extend \( \rho' \) continuously to \( K' \) as needed, so assume \( \rho' : K \rightarrow \mathbb{R}^s \). By universality of \( \mathcal{R} \) we may pick a particular \( \rho : K \rightarrow \mathbb{R}^s \), \( \rho \in \mathcal{R} \) such that
\[
I = \sup_{\{v_i \in \mathcal{X}_i\}_{i=1}^k} \| \rho'(\phi'_1, \ldots, \phi'_k) - \rho(\phi'_1, \ldots, \phi'_k) \|_\infty \leq \sup_{z \in K} \| \rho'(z) - \rho(z) \|_2 < \epsilon / 2.
\]

Keeping this choice of \( \rho \), it remains only to bound \( II \). As \( \rho \) is continuous on a compact domain, it is in fact uniformly continuous. Thus, we can choose a \( \delta' > 0 \) such that if \( \| y - z \|_2 < \delta' \), then \( \| \rho(y) - \rho(z) \|_\infty < \epsilon / 2 \), and then we define \( \delta = \min(\delta', 1) \).

Since \( \Phi_i \) universally approximates \( \phi'_i \) we may pick \( \phi_i \in \Phi_i \) such that \( \| \phi_i - \phi'_i \|_\infty < \delta / \sqrt{k} \), and thus \( \| (\phi_1, \ldots, \phi_k) - (\phi'_1, \ldots, \phi'_k) \|_\infty \leq \delta \). With this choice of \( \phi_i \), we know that \( \prod_{i=1}^k \text{im} \phi_i \subseteq K \) (because each \( \phi_i(x_i) \) is within distance 1 of \( \phi'_i(x_i) \)). Thus, \( \rho(\phi_1(x_1), \ldots, \phi_k(x_k)) \) is well-defined, and we have
\[
II = \| \rho(\phi'_1, \ldots, \phi'_k) - \rho(\phi_1, \ldots, \phi_k) \|_\infty
= \sup_{\{x_i \in \mathcal{X}_i\}_{i=1}^k} \| \rho(\phi'_1(x_1), \ldots, \phi'_k(x_k)) - \rho(\phi_1(x_1), \ldots, \phi_k(x_k)) \|_2
< \epsilon / 2
\]
due to our choice of \( \delta \), which completes the proof.

### C Basis Invariance for Graph Representation Learning

#### C.1 Spectral Graph Convolution

In this section, we consider spectral graph convolutions, which for node features \( X \in \mathbb{R}^{n \times q} \) take the form \( f(V, \Lambda, X) = \sum_{i=1}^n \theta_i v_i v_i^T X \) for some parameters \( \theta_i \). We can optionally take \( \theta_i = h(\lambda_i) \) for
some continuous function $h : \mathbb{R} \rightarrow \mathbb{R}$ of the eigenvalues. This form captures most popular spectral graph convolutions in the literature (Bruna et al., 2014; Hamilton, 2020; Bronstein et al., 2017); often, such convolutions are parameterized by taking $h$ to be some analytic function such as a simple affine function (Kipf & Welling, 2017), a linear combination in a polynomial basis (Defferrard et al., 2016; Chien et al., 2021), or a parameterization of rational functions (Levie et al., 2018; Bianchi et al., 2021).

First, it is well known and easy to see that spectral graph convolutions are permutation equivariant, as for a permutation matrix $P$ we have

$$f(PV, \Lambda, PX) = \sum_i \theta_i P_{ii} v_i^T P^T PX = \sum_i \theta_i P_{ii} v_i^T X = Pf(V, \Lambda, X).$$

(30)

Also, it is easy to see that they are sign invariant, as $(-v_i)(-v_i)^T = v_i v_i^T$. However, if the $\theta_i$ do not depend on the eigenvalues, then the spectral graph convolution is not necessarily basis invariant. For instance, if $v_1$ and $v_2$ are in the same eigenspace, and we change basis by permuting $v_1' = v_2$ and $v_2' = v_1$, then if $\theta_1 \neq \theta_2$ the spectral graph convolution will generally change as well.

On the other hand, if $\theta_i = h(\lambda_i)$ for some function $h : \mathbb{R} \rightarrow \mathbb{R}$, then the spectral graph convolution is basis invariant. This is because if $v_1$ and $v_2$ belong to the same eigenspace, then $\lambda_i = \lambda_j$ so $h(\lambda_i) = h(\lambda_j)$. Thus, if $v_1, \ldots, v_d$ are eigenvectors of the same eigenspace with eigenvalue $\lambda$, we have that $\sum_{i=1}^d h(\lambda_i) v_i v_i^T = h(\lambda) \sum_{i=1}^d v_i v_i^T$. Now, note that $\sum_{i=1}^d v_i v_i^T$ is the orthogonal projector onto the eigenspace (Trefethen & Bau III, 1997). A change of basis does not change this orthogonal projector, so such spectral graph convolutions are basis invariant.

Another way to see this basis invariance is through basic algebra. Let $V_1, \ldots, V_l$ be the eigenspaces of dimension $d_1, \ldots, d_l$, where $V_l \in \mathbb{R}^{n \times d_l}$. Let the corresponding eigenvalues be $\mu_1, \ldots, \mu_l$. Then for any orthogonal matrices $Q_i \in O(d_i)$, we have

$$h(\lambda_i) v_i v_i^T = \sum_{j=1}^l V_j h(\mu_j) I_{d_j} V_j^T$$

(31)

$$= \sum_{j=1}^l V_j h(\mu_j) I_{d_j} Q_j Q_j^T V_j^T$$

(32)

$$= \sum_{j=1}^l (V_j Q_j) h(\mu_j) I_{d_j} (V_j Q_j)^T,$$

(33)

so the spectral graph convolution is invariant to substituting $V_j Q_j$ for $V_j$.

Now, we give the proof that shows SignNet and BasisNet can universally approximate spectral graph convolutions.

**Proposition 3** (Learning Spectral Graph Convolutions). Suppose the node features $X \in \mathbb{R}^{n \times q}$ take values in compact sets. Then SignNet can universally approximate any spectral graph convolution, and both BasisNet and Expressive-BasisNet can universally approximate any parametric spectral graph convolution.

**Proof.** Note that eigenvectors and eigenvalues of normalized Laplacian matrices take values in compact sets, since the eigenvalues are in $[0, 2]$ and we take eigenvectors to have unit-norm. Thus, the whole domain of the spectral graph convolution is compact.

Let $\varepsilon > 0$. First, consider a spectral graph convolution $f(V, \Lambda, X) = \sum_{i=1}^n \theta_i v_i v_i^T X$. For SignNet, let $\phi(v_i, \lambda_i, X)$ approximate the function $\phi(v_i, \lambda_i, X) = \theta_i v_i v_i^T$ to within $\varepsilon/n$ error, which DeepSets can do since this is a continuous permutation equivariant function from vectors to vectors (Segol & Lipman, 2019) (note that we can pass $\lambda_i$ as a vector in $\mathbb{R}^n$ by instead passing $\lambda_i 1$, where $1$ is the all ones vector). Then $\rho = \sum_{i=1}^n$ is a linear permutation equivariant operation that can be exactly expressed by DeepSets, so the total error is within $\varepsilon$. The same argument applies when $\theta_i = h(\lambda_i)$ for some continuous function $h$.

For the basis invariant case, consider a parametric spectral graph convolution $f(V, \Lambda, X) = \sum_{i=1}^n h(\lambda_i) v_i v_i^T X$. Note that if the eigenspace bases are $V_1, \ldots, V_l$ with eigenvalues $\mu_1, \ldots, \mu_l$,
we can write the \( f(V, \Lambda, X) = \sum_{i=1}^{l} h(\mu_i) V_i V_i^T X \). Again, we will let \( \rho = \sum_{i=1}^{l} \) be a sum function, which can be expressed exactly by DeepSets. Thus, it suffices to show that \( h(\mu_i) V_i V_i^T X \) can be \( \epsilon/n \) approximated by a 2-IGN (i.e., an IGN that only uses vectors and matrices).

Note that since \( h \) is continuous, we can use an elementwise MLP (which IGNs can learn) to approximate \( f_1(\mu \mathbf{1} \mathbf{1}^T, V V^T, X) = (h(\mu) \mathbf{1} \mathbf{1}^T, V V^T, X) \) to arbitrary precision (note that we represent the eigenvalue \( \mu \) as a constant matrix \( \mu \mathbf{1} \mathbf{1}^T \)). Also, since a 2-IGN can learn matrix vector multiplication (Cai & Wang (2022) Lemma 10), we can approximate \( f_2(h(\mu) \mathbf{1} \mathbf{1}^T, V V^T, X) = (h(\mu) \mathbf{1} \mathbf{1}^T, V V^T, X) \), as \( V_i V_i^T \in \mathbb{R}^{n \times q} \) is a matrix and \( X \in \mathbb{R}^{n \times q} \) is a vector with respect to permutation symmetries. Finally, we use an elementwise MLP to approximate the scalar-vector multiplication \( f_3(h(\mu) \mathbf{1} \mathbf{1}^T, V V^T, X) = h(\mu) V V^T X \). Since \( f_3 \circ f_2 \circ f_1(\mu \mathbf{1} \mathbf{1}^T, V V^T, X) = h(\mu) V V^T X \), and since 2-IGNs universally approximate each \( f_i \), applying Lemma 6 shows that a 2-IGN can approximate \( h(\mu) V V^T X \) to \( \epsilon/n \) accuracy, so we are done. Since Expressive-BasisNet is stronger than BasisNet, it can also universally approximate these functions.

From the proof, we can see that SignNet and BasisNet need only learn simple functions for the \( \rho \) and \( \phi \) when \( h \) is simple, or when the filter is non-parametric and we need only learn \( \theta_i \). Xu et al. (2020) propose the principle of algorithmic alignment, and show that if separate modules of a neural network each need only learn simple functions (that is, functions that are well-approximated by low-order polynomials with small coefficients), then the network may be more sample efficient. If we do not require permutation equivariance, and parameterize SignNet and BasisNet with simple MLPs, then algorithmic alignment may suggest that our models are sample efficient. Indeed, \( \rho = \sum_{i} \) is a simple linear function with coefficients 1, and \( \phi(V, \lambda, X) = h(\lambda) V V^T X \) is quadratic in \( V \) and linear in \( X \), so it is simple if \( h \) is simple.

### C.2 Existing Positional Encodings

Here, we show that our SignNets and BasisNets universally approximate various types of existing graph positional encodings. The key is to show that these positional encodings are related to spectral graph convolution matrices and diagonals, and to show that our networks can approximate these matrices and diagonals.

**Proposition 6.** SignNets and BasisNets universally approximate the diagonal of any spectral graph convolution matrix \( f(V, \Lambda) = \text{diag} \left( \sum_{i=1}^{n} h(\lambda_i) v_i v_i^T \right) \). BasisNets can additionally universally approximate any spectral graph convolution matrix \( f(V, \Lambda) = \sum_{i=1}^{n} h(\lambda_i) v_i v_i^T \).

**Proof.** Note that \( v_i \) and \( \lambda_i \) come from compact sets, as \( \lambda_i \in [0, 2] \) for the normalize Laplacian and \( v_i \) is of unit norm. Also, as \( \text{diag} \) is linear, the spectral graph convolution diagonal can be written \( \sum_{i=1}^{n} h(\lambda_i) \text{diag}(v_i v_i^T) \).

Let \( \epsilon > 0 \). For SignNet, let \( \rho = \sum_{i=1}^{n} \), which can be exactly expressed as it is a permutation equivariant linear operation from vectors to vectors. Then \( \phi(v_i, \lambda_i) \) can approximate the function \( \lambda_i \text{diag}(v_i v_i^T) \) to arbitrary precision, as it is a permutation equivariant function from vectors to vectors (Segol & Lipman, 2019). Thus, letting \( \phi \) approximate the function to \( \epsilon/n \) accuracy, SignNet can approximate \( f \) to \( \epsilon \) accuracy.

Let \( l \) be the number of eigenspaces \( V_1, \ldots, V_l \), so \( f(V, \Lambda) = \sum_{i=1}^{l} h(\mu_i) V_i V_i^T \). For BasisNet, we need only show that it can approximate the spectral graph convolution matrix to \( \epsilon/l \) accuracy, as a 2-IGN can exactly express the \( \text{diag} \) function in \( \rho \), since it is a linear permutation equivariant function from matrices to vectors. A 2-IGN can universally approximate the function \( f_1(\mu_i, V_i V_i^T) = (h(\mu_i), V_i V_i^T) \), as it can express any elementwise MLP. Also, a 2-IGN can universally approximate the scalar-matrix multiplication \( f_2(h(\mu_i), V_i V_i^T) = h(\mu_i) V_i V_i^T \) by another elementwise MLP. Since \( h(\mu_i) V_i V_i^T = f_2 \circ f_1(\mu_i, V_i V_i^T) \), Lemma 6 shows that a single 2-IGN can approximate this composition to \( \epsilon/l \) accuracy, so we are done.
Here, we consider the graph angles $\alpha_{ij} = \|V_i V_j^T e_j\|_2$, for $i = 1, \ldots, l$ where $l$ is the number of eigenspaces, and $j = 1, \ldots, n$. It is clear that graph angles are permutation invariant and basis invariant. These graph angles have been extensively studied, so we simply cite a number of interesting properties of them. That graph angles determine the number of length 3, 4 and 5 cycles, the connectivity of a graph, and the number of length $k$ closed walks is all shown in Chapter 4 of Cvetković et al. (1997). Other properties may be of use for graph representation learning as well. For instance, the eigenvalues of node-deleted subgraphs of a graph $G$ are determined by the eigenvalues and graph
angles of $G$; this may be useful in extending recent graph neural networks that are motivated by node deletion and the reconstruction conjecture (Cotta et al., 2021; Bevilacqua et al., 2022; Papp et al., 2021; Tahmasebi et al., 2020).

Now, we prove that BasisNet can universally approximate the graph angles. The graph properties we consider in the proposition are all integer valued (e.g. the number of cycles of length 3 in a graph is an integer). Thus, any two graphs that differ in these properties will differ by at least 1, so as long as we have universal approximation to $\varepsilon < 1/2$, we can distinguish any two graphs that differ in these properties. Recall the statement of Proposition 4.

**Proposition 4.** BasisNet can universally approximate the graph angles $\alpha_{ij}$. The eigenvalues and graph angles (and thus BasisNets) can determine the number of length 3, 4, and 5 cycles, whether a graph is connected, and the number of length $k$ closed walks from any vertex to itself.

**Proof.** Note that the graph angles satisfy

$$\alpha_{ij} = \|V_i V_i^\top e_j\|_2 = \sqrt{e_j^\top V_i V_i^\top V_i V_i^\top e_j} = \sqrt{e_j^\top V_i V_i^\top e_j},$$

where $V_i$ is a basis for the $i$th adjacency matrix eigenspace, and $e_j^\top V_i V_i^\top e_j$ is the $(j,j)$-entry of $V_i V_i^\top$. These graph angles are just the elementwise square roots of the diagonals of the matrices $V_i V_i^\top$. As $f_1(V_i V_i^\top) = \text{diag}(V_i V_i^\top)$ is a permutation equivariant linear function from matrices to vectors, 2-IGN on $V_i V_i^\top$ can exactly compute this with 0 error. Then a 2-IGN can learn an elementwise MLP to approximate the elementwise square root $f_2(\text{diag}(V_i V_i^\top)) = \sqrt{\text{diag}(V_i V_i^\top)}$ to arbitrary precision. Finally, there may be remaining operations $f_3$ that are permutation invariant or permutation equivariant from vectors to vectors; for instance, the $\alpha_{ij}$ are typically gathered into a matrix of size $l \times n$ where the columns are lexicographically sorted ($l$ is the number of eigenspaces) (Cvetović et al., 1997), or we may have a permutation invariant readout to compute a subgraph count. A DeepSets can approximate $f_3$ without any higher order tensors besides vectors (Zaheer et al., 2017; Segol & Lipman, 2019).

As 2-IGNs can approximate each $f_i$ individually, a single 2-IGN can approximate $f_1 \circ f_2 \circ f_3$ by Lemma 6. Also, since the graph properties considered in the proposition are integer-valued, BasisNet can distinguish any two graphs that differ in one of these properties. \qed

### D Eigenvectors and Eigenvalues in Practice

In this section, we study the properties of eigenvalues and eigenvectors computed by numerical algorithms on real-world data.

#### D.1 Sign and Basis Ambiguities in Numerical Eigensolvers

When learning from real-world data, we use eigenvectors that are computed by numerical algorithms. These algorithms return specific eigenvectors for each eigenspace, so there is some theoretically arbitrary choice of sign or basis of each eigenspace. The general symmetric matrix eigensolvers `numpy.linalg.eigh` and `scipy.linalg.eigh` both call LAPACK routines. They both proceed as follows: for a symmetric matrix $A$, they first decompose it as $A = QTQ^\top$ for orthogonal $Q$ and tridiagonal $T$, then they compute the eigendecomposition of $T = W\Lambda W^\top$, so the eigendecomposition of $A$ is $A = (QW)\Lambda(W^\top Q^\top)$. There are multiple ambiguities here: for diagonal sign matrices $S = \text{Diag}(s_1, \ldots, s_n)$ and $S' = \text{Diag}(s'_1, \ldots, s'_n)$, where $s_i, s'_i \in \{-1, 1\}$, we have that $A = QS(STS)SQ^\top$ is also a valid tridiagonalization, as $QS$ is still orthogonal, $SS = I$, and $STS$ is still tridiagonal. Also, $T = (WS')\Lambda(S'W^\top)$ is a valid eigendecomposition of $T$, as $WS'$ is still orthogonal.

In practice, the general symmetric matrix eigensolvers `numpy.linalg.eigh` and `scipy.linalg.eigh` differ between frameworks but are consistent with the same framework. More specifically, for a symmetric matrix $A$, we find that the eigenvectors computed with the default settings in numpy tend to differ by a choice of sign or basis from those that are computed with the default settings in scipy. On the other hand, the called LAPACK routines are deterministic, so the eigenvectors returned by numpy are the same in each call, and the eigenvectors returned by scipy are likewise the same in each call.
Table 4: Eigenspace statistics for datasets of multiple graphs. From left to right, the columns are: dataset name, number of graphs, range of number of nodes per graph, largest multiplicity, and percent of graphs with an eigenspace of dimension > 1.

| Dataset     | Graphs | # Nodes | Max. Mult | % Graphs mult. > 1 |
|-------------|--------|---------|-----------|-------------------|
| ZINC        | 12,000 | 9-37    | 9         | 64.1              |
| ogbg-molhiv | 41,127 | 2-222   | 42        | 68.0              |
| IMDB-M      | 1,500  | 7-89    | 37        | 99.9              |
| COLLAB      | 5,000  | 32-492  | 238       | 99.1              |
| PROTEINS    | 1,113  | 4-620   | 20        | 77.3              |
| COIL-DEL    | 3,900  | 3-77    | 4         | 4.00              |

Eigenvalues for sparse symmetric matrices like `scipy.linalg.eigsh` are required for large scale problems. This function calls ARPACK, which uses an iterative method that starts with a randomly sampled initial vector. Due to this stochasticity, the sign and basis of eigenvectors returned differs between each call.

Bro et al. (2008) develops a data-dependent method to choose signs for each singular vector of a singular value decomposition. Still, in the worst case the signs chosen will be arbitrary, and they do not handle rotational ambiguities in higher dimensional eigenspaces. Other works have made choices of sign, such as by picking the sign so that the eigenvector’s entries are in the largest lexicographic order (Tam & Dunson, 2022). This choice of sign may work poorly for learning on graphs, as it is sensitive to permutations on nodes. For some graph regression experiments in Section 5.1, we try a choice of sign that is permutation invariant, but we find it to work poorly.

D.2 Higher Dimensional Eigenspaces in Real Graphs

Here, we investigate the normalized Laplacian eigenspace statistics of real world graph data. For any graph that has distinct Laplacian eigenvalues, only sign invariance is required in processing eigenvectors. However, we find that graph data tends to have higher multiplicity eigenvalues, so basis invariance would be required for learning symmetry-respecting functions on eigenvectors.

Indeed, we show statistics for multi-graph datasets in Table 4 and for single-graph datasets with more nodes per graph in Table 5. For multi-graph datasets, we consider:

- Molecule graphs: ZINC (Irwin et al., 2012; Dwivedi et al., 2020), ogbg-molhiv (Wu et al., 2018; Hu et al., 2020a)
- Social networks: IMDB-M, COLLAB (Yanardag & Vishwanathan, 2015; Morris et al., 2020),
- Bioinformatics graphs: PROTEINS (Morris et al., 2020)
- Computer vision graphs: COIL-DEL (Riesen & Bunke, 2008; Morris et al., 2020).

For single-graph datasets, we consider:

- The 32 × 32 image grid as in Section 5.2
- Citation networks: Cora, Citeseer (Sen et al., 2008)
- Co-purchasing graphs with Amazon Photo (McAuley et al., 2015; Shchur et al., 2018).

We see that these datasets all contain higher multiplicity eigenspaces, so sign invariance is insufficient for fully respecting symmetries. The majority of graphs in each multi-graph dataset besides COIL-DEL contain higher multiplicity eigenspaces. Also, the dimension of these eigenspaces can be quite large compared to the size of the graphs in the dataset. The single-graph datasets have a large proportion of their eigenvectors belonging to higher dimensional eigenspaces. Thus, basis invariance may play a large role in processing spectral information from these graph datasets.
Table 5: Eigenspace statistics for single graphs. From left to right, the columns are: dataset name, number of nodes, distinct eigenvalues (i.e. distinct eigenspaces), number of unique multiplicities, largest multiplicity, and percent of eigenvectors belonging to an eigenspace of dimension $\geq 1$.

| Dataset       | Nodes | Distinct $\lambda$ | # Mult. | Max Mult. | % Vecs mult. $\geq 1$ |
|---------------|-------|--------------------|---------|-----------|-----------------------|
| $32 \times 32$ image | 1,024 | 513 | 3 | 32 | 96.9 |
| Cora          | 2,708 | 2,187 | 11 | 300 | 19.7 |
| Citeseer      | 3,327 | 1,861 | 12 | 491 | 44.8 |
| Amazon Photo  | 7,650 | 7,416 | 8 | 136 | 3.71 |

E further experimental details

E.1 Spectral Graph Convolution Details

In Section 5.2, we conduct node regression experiments for learning spectral graph convolutions. The experimental setup is mostly taken from He et al. (2021). However, we resize the 100 × 100 images to $32 \times 32$. Thus, each image is viewed as a 1024-node graph. The node features $X \in \mathbb{R}^n$ are the grayscale pixel intensities of each node. Just as in He et al. (2021), we only train and evaluate on nodes that are not connected to the boundary of the grid (that is, we only evaluate on the $28 \times 28$ middle section). For all experiments we limit each model to 50,000 parameters. For each of the GNN baselines (GCN, GAT, GPR-GNN, ARMA, ChebNet, BernNet), we select the best performing out of 4 hyperparameter settings: either 2 or 4 convolution layers, and a hidden dimension of size 32 or $D$, where $D$ is just large enough to stay with 50,000 parameters (for instance, $D = 128$ for GCN, GPR-GNN, and BernNet).

We use DeepSets or standard Transformers as our prediction network. This takes in the output of SignNet or BasisNet and concatenates it with the node features, then outputs a scalar prediction. We use a 3 layer output network for DeepSets SignNet, and 2 layer output networks for all other configurations. All networks use ReLU activations.

For SignNet, we use DeepSets for both $\phi$ and $\rho$. Our $\phi$ takes in eigenvectors only, then our $\rho$ takes the outputs of $\phi$ and the eigenvalues. We use three layers for $\phi$ and $\rho$.

For BasisNet, we use the same DeepSets for $\rho$ as in SignNet, and 2-IGNs for the $\phi_{d_i}$. There are three distinct multiplicities for the grid graph (1, 2, and 32), so we only need 3 separate IGNs. Each IGN consists of an $\mathbb{R}^{n^2 \times 1} \rightarrow \mathbb{R}^{n \times d'''}$ layer and two $\mathbb{R}^{n \times d''} \rightarrow \mathbb{R}^{n \times d''''}$ layers, where the $d'$ are hidden dimensions. There are no matrix to matrix operations used, as the memory requirements are intensive for these $\geq 1000$ node graphs. The $\phi_{d_i}$ only take in $V_i V_i^\top$ from the eigenspaces, and the $\rho$ takes the output of the $\phi_{d_i}$ as well as the eigenvalues.

E.2 Graph Regression Details

In Section 5.1 we study the effectiveness of SignNet for learning positional encodings to boost the expressive power, and thereby generalization, on the graph regression problem ZINC. In all cases we take our $\phi$ encoder to be an 8 layer GIN with ReLU activation. The input eigenvector $v_i \in \mathbb{R}^n$, where $n$ is the number of nodes in the graph, is treated as a single scalar feature for each node. In the case of using a fixed number of eigenvectors $k$, the aggregator $\rho$ is taken to be an 8 layer MLP with batch normalization and ReLU activation. The aggregator $\rho$ is applied separately to the concatenation of the $k$ different embeddings for each node in a graph, resulting in one single embedding per node. This embedding is concatenated to the node features for that node, and the result passed as input to the base (predictor) model. The final row of Table 1 also considers using all available eigenvectors instead of a fixed number $k$. Since the total number of eigenvectors is a variable quantity, equal to the number of nodes in the underlying graph, an MLP cannot be used for $\rho$. To handle the variable sized input in this case we take $\rho$ to be a single layer Transformer with 4 heads.

As well as testing SignNet, we also checked whether simple transformations that resolve the sign ambiguity of the Laplacian eigenvectors $p = (v_1, \ldots, v_k)$ could serve as effective positional encoding. We considered three options. First is to randomly flip the sign of each $\pm v_i$ during training. This is a common heuristic used in prior work on Laplacian positional encoding (Kreuzer et al., 2021;
Table 6: Results on the ZINC dataset with 500k parameter budget and no edge features. Numbers are the mean and standard deviation over 4 runs each with different seeds.

| Base model | Positional encoding | $k$ | #params | Test MAE ($\downarrow$) |
|------------|---------------------|-----|---------|------------------------|
| GIN        | No PE               | 16  | 497k    | 0.348±0.014            |
|            | LapPE (flip)        | 16  | 498k    | 0.341±0.011            |
| SignNet    |                     | 16  | 500k    | 0.238±0.012            |
| GAT        | No PE               | 16  | 501k    | 0.464±0.011            |
|            | LapPE (flip)        | 16  | 502k    | 0.462±0.013            |
| SignNet    |                     | 16  | 499k    | 0.243±0.008            |

Dwivedi et al., 2020). Second, take the element-wise absolute value $|v_i|$. This is a non-injective map, creating sign invariance at the cost of destroying positional information. Third is a different canonicalization that avoids stochasticity and use of absolute values by selecting the sign of each $v_i$ so that the majority of entries are non-negative, with ties broken by comparing the $\ell_1$-norm of positive and negative parts. When the tie-break also fails, the sign is chosen randomly. Results for GatedGCN base model on ZINC in Table 1 show that all three of these approaches are significantly poorer positional encodings compared to SignNet.

Our training pipeline largely follows that of Dwivedi et al. (2022), and we use the GatedGCN and PNA base models from the accompanying implementation (see https://github.com/vijaydwivedi75/gnn-lspe). The Sparse Transformer base model architecture we use, which like GAT computes attention only across neighbouring nodes, is introduced by Kreuzer et al. (2021). Finally, the GINE implementation is based on the PyTorch Geometric implementation (Fey & Lenssen, 2019).

All models in Table 1 use edge features for learning and inference. To show that SignNet is also useful when no edge features are available, we ran ZINC experiments without edge features as well. The results are displayed in Table 6.

E.3 Substructures and Graph Properties Regression Details

We use the random graph dataset from Chen et al. (2020) for counting substructures and the synthetic dataset from Corso et al. (2020) for regressing graph properties. To keep fair comparison we fix the base model as a 4-layer GIN model with hidden size 128. As graphs can have different number of nodes, the number of Laplacian eigenvectors is the same as the number of nodes and hence is different across graphs. One can truncate it to keep the top $k$ most important eigenvectors but this loses information. We may instead use all eigenvectors by designing the model to handle positional encodings of varying sizes. SignNet can accept varying numbers of Laplacian eigenvectors as input by choosing $\rho$ and $\phi$ to be neural networks allowing variable-size input. Specifically, we choose $\phi$ as 4-layer GIN (independently applied to every eigenvector) and $\rho$ as 1-layer Transformer (independently applied to every node). Combined with proper batching and masking, we have a SignNet that takes Laplacian eigenvectors $V \in \mathbb{R}^{n \times n}$ and outputs fixed size sign-invariant encoding node features $f(V, \Lambda, X) \in \mathbb{R}^{n \times d}$, where $n$ varies between graphs but $d$ is fixed. We use this SignNet in our experiments and compare with other methods of handling PEs.

F Useful Lemmas

In this section, we collect useful lemmas for our proofs. These lemmas generally only require basic tools to prove. Our first lemma is a crucial property of quotient spaces.

**Lemma 1** (Passing to the quotient). Let $\mathcal{X}$ and $\mathcal{Y}$ be topological spaces, and let $\mathcal{X}/G$ be a quotient space, with corresponding quotient map $\pi$. Then for every continuous $G$-invariant function $f : \mathcal{X} \to \mathcal{Y}$, there is a unique continuous $\bar{f} : \mathcal{X}/G \to \mathcal{Y}$ such that $f = \bar{f} \circ \pi$.

**Proof.** For $z \in \mathcal{X}/G$, by surjectivity of $\pi$ we can choose an $x_z \in \mathcal{X}$ such that $\pi(x_z) = z$. Define $\bar{f} : \mathcal{X}/G \to \mathcal{Y}$ by $\bar{f}(z) = f(x_z)$. This is well-defined, since if $\pi(x_z) = \pi(x)$ for any other $x \in \mathcal{X}$,
then \( gx_2 = x \) for some \( g \in G \), so
\[
f(x) = f(gx_2) = f(x_2) = \tilde{f}(z),
\]
where the second equality uses the \( G \)-invariance of \( f \). Note that \( \tilde{f} \) is continuous by the universal property of quotient spaces. Also, \( \tilde{f} \) is the unique function such that \( f = \tilde{f} \circ \pi \); if there were another function \( h : \mathcal{X}/G \to \mathcal{Y} \) with \( h(z) \neq \tilde{f}(z) \), then \( h(z) \neq f(x_2) \), so \( h(\pi(x_2)) = h(z) \neq f(x_2) \).

Next, we give the First Fundamental Theorem of \( O(d) \), a classical result that has been recently used for machine learning by Villar et al. (2021). This result shows that an orthogonally invariant function \( f(V) \) can be expressed as a function \( h(VV^\top) \). We give a proof that if \( f \) is continuous, then \( h \) is also continuous.

**Lemma 2** (First Fundamental Theorem of \( O(d) \)). A continuous function \( f : \mathbb{R}^{n \times d} \to \mathbb{R}^s \) is orthogonally invariant, i.e. \( f(QV) = f(V) \) for all \( Q \in O(d) \), if and only if \( f(V) = h(VV^\top) \) for some continuous \( h \). 

**Proof.** If \( f(V) = h(VV^\top) \), then we have \( f(VQ) = h(VQQ^\top V^\top) = h(VV^\top) \) so \( f \) is orthogonally invariant.

For the other direction, invariant theory shows that the \( O(d) \) invariant polynomials are generated by the inner products \( v_i^\top v_j \), where \( v_i \in \mathbb{R}^d \) are the rows of \( V \) (Kraft & Procesi, 1996). Let \( p : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times n} \) be the map \( p(V) = V V^\top \). Then González & de Salas (2003) Lemma 11.13 shows that the quotient space \( \mathbb{R}^{n \times d}/O(d) \) is homeomorphic to a closed subset \( p[\mathbb{R}^{n \times d}] = \mathcal{Z} \subseteq \mathbb{R}^{n \times n} \), so \( p \) refers to this homeomorphism, and note that \( \tilde{p} \circ \pi = p \) by passing to the quotient (Lemma 1). Then any continuous \( O(d) \) invariant \( f \) passes to a unique continuous \( \tilde{f} : \mathbb{R}^{n \times d}/O(d) \to \mathbb{R}^s \) (Lemma 1), so \( f = \tilde{f} \circ \pi \) where \( \pi \) is the quotient map. Define \( h : \mathcal{Z} \to \mathbb{R}^s \) by \( h = \tilde{f} \circ \tilde{p}^{-1} \), and note that \( h \) is a composition of continuous functions and hence continuous. Finally, we have that \( h(VV^\top) = h(\tilde{p} \circ \pi(V)) = \tilde{f} \circ \pi(V) = f(V) \), so we are done.

The next lemma allows us to decompose a quotient of a product space into a product of smaller quotient spaces.

**Lemma 3.** Let \( \mathcal{X}_1, \ldots, \mathcal{X}_k \) be topological spaces and \( G_1, \ldots, G_k \) be topological groups such that each \( G_i \) acts continuously on \( \mathcal{X}_i \). Denote the quotient maps by \( \pi_i : \mathcal{X}_i \to \mathcal{X}_i/G_i \). Then the quotient of the product is the product of the quotient, i.e.
\[
(\mathcal{X}_1 \times \cdots \times \mathcal{X}_k)/(G_1 \times \cdots \times G_k) \cong (\mathcal{X}_1/G_1) \times \cdots \times (\mathcal{X}_k/G_k), \tag{40}
\]
and \( \pi_1 \times \cdots \times \pi_k : \mathcal{X}_1 \times \cdots \times \mathcal{X}_k \to (\mathcal{X}_1/G_1) \times \cdots \times (\mathcal{X}_k/G_k) \) is quotient map.

**Proof.** First, we show that \( \pi_1 \times \cdots \times \pi_k \) is a quotient map. This is because 1. the quotient map of any continuous group action is an open map, so each \( \pi_i \) is an open map, 2. the product of open maps is an open map, so \( \pi_1 \times \cdots \times \pi_k \) is an open map and 3. a continuous surjective open map is a quotient map, so \( \pi_1 \times \cdots \times \pi_k \), which is continuous and surjective, is a quotient map.

Now, we need only apply the theorem of uniqueness of quotient spaces to show 40 (see e.g. Lee (2013), Theorem A.31). Letting \( q : \mathcal{X}_1 \times \cdots \times \mathcal{X}_k \to (\mathcal{X}_1 \times \cdots \times \mathcal{X}_k)/(G_1 \times \cdots \times G_k) \) denote the quotient map for this space, it is easily seen that \( q(x_1, \ldots, x_k) = q(y_1, \ldots, y_k) \) if and only if \( \pi_1 \times \cdots \times \pi_k(x_1, \ldots, x_k) = \pi_1 \times \cdots \times \pi_k(y_1, \ldots, y_k) \), since either of these is true if and only if there exist \( g_i \in G_i \) such that \( x_i = y_i g_i \) for each \( i \). Thus, we have an isomorphism of these quotient spaces.

The following lemma shows that quotients of compact spaces are also compact, which is useful for universal approximation on quotient spaces.

**Lemma 4** (Compactness of quotients of compact spaces). Let \( \mathcal{X} \) be a compact space. Then the quotient space \( \mathcal{X}/G \) is compact.

**Proof.** Denoting the quotient map by \( \pi : \mathcal{X} \to \mathcal{X}/G \) and letting \( \{U_\alpha\}_\alpha \) be an open cover of \( \mathcal{X}/G \), we have that \( \{\pi^{-1}(U_\alpha)\}_\alpha \) is an open cover of \( \mathcal{X} \). By compactness of \( \mathcal{X} \), we can choose a finite subcover \( \{\pi^{-1}(U_\alpha)\}_{i=1,\ldots,n} \). Then \( \pi(\pi^{-1}(U_\alpha)) \{i=1,\ldots,n = \{U_\alpha\}_{i=1,\ldots,n} \) by surjectivity, and \( \{U_\alpha\}_{i=1,\ldots,n} \) is thus an open cover of \( \mathcal{X}/G \).
The Whitney embedding theorem gives a nice condition that we apply to show that the quotient spaces $X/G$ that we deal with embed into Euclidean space. It says that when $X/G$ is a smooth manifold, then it can be embedded into a Euclidean space of double the dimension of the manifold. The proof is outside the scope of this paper.

**Lemma 5** (Whitney Embedding Theorem (Whitney, 1944)). Every smooth manifold $M$ of dimension $n > 0$ can be smoothly embedded in $\mathbb{R}^{2n}$.

Finally, we give a lemma that helps prove universal approximation results. It says that if functions $f$ that we want to approximate can be written as compositions $f = f_L \circ \ldots \circ f_1$, then it suffices to universally approximate each $f_i$ and compose the results to universally approximate the $f$. This is especially useful for proving universality of neural networks, as we may use some layers to approximate each $f_i$, then compose these layers to approximate the target function $f$.

**Lemma 6** (Layer-wise universality implies universality). Let $\mathcal{Z} \subseteq \mathbb{R}^{d_0}$ be a compact domain, let $\mathcal{F}_1, \ldots, \mathcal{F}_L$ be families of continuous functions where $\mathcal{F}_i$ consists of functions from $\mathbb{R}^{d_{i-1}} \to \mathbb{R}^{d_i}$ for some $d_1, \ldots, d_L$. Let $\mathcal{F}$ be the family of functions $\{f_L \circ \ldots \circ f_1 : Z \to \mathbb{R}^{d_L}, f_i \in \mathcal{F}_i\}$ that are compositions of functions $f_i \in \mathcal{F}_i$.

For each $i$, let $\Phi_i$ be a family of continuous functions that universally approximates $\mathcal{F}_i$. Then the family of compositions $\Phi = \{\phi_L \circ \ldots \circ \phi_1 : \phi_i \in \Phi_i\}$ universally approximates $\mathcal{F}$.

**Proof.** Let $f = f_L \circ \ldots \circ f_1 \in \mathcal{F}$. Let $\tilde{Z}_1 = Z$, and then for $i \geq 2$ let $\tilde{Z}_i = f_{i-1}(\tilde{Z}_{i-1})$. Then each $\tilde{Z}_i$ is compact by continuity of the $f_i$. For $1 \leq i < L$, let $Z_i = \tilde{Z}_i$, and for $i = L$ let $Z_L$ be a compact set containing $\tilde{Z}_L$ such that every ball of radius one centered at a point in $\tilde{Z}_L$ is still contained in $\tilde{Z}_L$.

Let $\epsilon > 0$. We will show that there is a $\phi \in \Phi$ such that $\|f - \phi\|_\infty < \epsilon$ by induction on $L$. This holds trivially for $L = 1$, as then $\Phi = \Phi_1$.

Now, let $L \geq 2$, and suppose it holds for $L - 1$. By universality of $\Phi_L$, we can choose a $\phi_L : Z_L \to \mathbb{R}^{d_L} \in \Phi_L$ such that $\|\phi_L - f_L\|_\infty < \epsilon/2$. As $\phi_L$ is continuous on a compact domain, it is also uniformly continuous, so we can choose a $\delta > 0$ such that $\|y - z\|_2 < \delta \implies \|\phi_L(y) - \phi_L(z)\|_2 < \epsilon/2$.

Let $\delta = \min(\delta, 1)$. By induction, we can choose $\phi_{L-1} \circ \ldots \circ \phi_1, \phi_i \in \Phi_i$ such that

$$\|\phi_{L-1} \circ \ldots \circ \phi_1 - f_{L-1} \circ \ldots \circ f_1\|_\infty < \delta. \quad (41)$$

Note that $\phi_{L-1} \circ \ldots \circ \phi_1(Z) \subseteq Z_L$, because for each $x \in Z$, $\phi_{L-1} \circ \ldots \circ \phi_1(x)$ is within $\delta \leq 1$ Euclidean distance to $f_{L-1} \circ \ldots \circ f_1(x) \in \tilde{Z}_L$, so it is contained in $Z_L$ by construction. Thus, we may define $\phi = \phi_L \circ \ldots \circ \phi_1 : Z \to \mathbb{R}^{d_L}$, and compute that

$$\|\phi - f\|_\infty \leq \|\phi - \phi_L \circ f_{L-1} \circ \ldots \circ f_1\|_\infty + \|\phi_L \circ f_{L-1} \circ \ldots \circ f_1 - f\|_\infty \quad (42)$$

$$< \|\phi - \phi_L \circ f_{L-1} \circ \ldots \circ f_1\|_\infty + \epsilon/2, \quad (43)$$

since $\|\phi_L - f_L\|_\infty < \epsilon/2$. To bound this other term, let $x \in Z$, and for $y = \phi_{L-1} \circ \ldots \circ \phi_1(x)$ and $z = f_{L-1} \circ \ldots \circ f_1(x)$, we know that $\|y - z\|_2 < \delta$, so $\|\phi_L(y) - \phi_L(z)\|_2 < \epsilon/2$ by uniform continuity. As this holds for all $x$, we have $\|\phi - \phi_L \circ f_{L-1} \circ \ldots \circ f_1\|_\infty \leq \epsilon/2$, so $\|\phi - f\|_\infty < \epsilon$ and we are done. \qed