A SIGNAL PROCESSING APPROACH TO INVARIANT REPRESENTATIONS OF GRAPH LAPLACIAN EIGENDATA

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The graph Laplacian is a central object in network science and related areas such as computational geometry and geometric deep learning. Most applications make use of the Laplacian's eigenvalues and eigenvectors (eigendata), which capture key features of the graph. However, when we use the eigendata as features for graph classification problems, we face several practical challenges. First, eigenvectors are only well-defined up to a choice of eigenbasis; second, only the first k eigenvectors are used as features in practice so as to compare graphs of different sizes [1]; and third, the eigenvalues and eigenvectors are often treated as separate features [1, 2], which ignores the association between an eigenvalue and its corresponding eigenvectors.

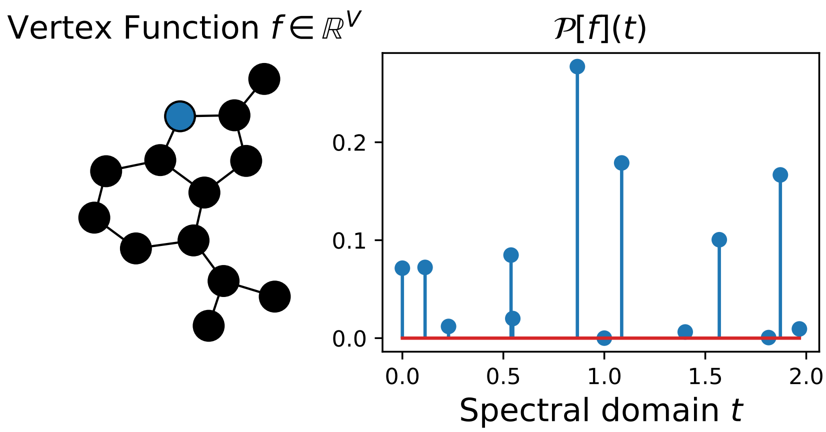

Figure 1. Left: A vertex function supported on a single vertex. Right: its corresponding power spectrum in the spectral domain.

Building on recent progress in addressing the first issue of basis invariance [2], we propose a procedure for encoding the Laplacian eigendata which addresses all three aforementioned issues. We leverage the role of the Laplacian in transforming vertex functions on a graph to its spectral domain, and represent a graph as a set of spectral power spectra. This encodes the eigendata in a basis invariant way without truncation of eigenvectors or decoupling of the eigenvalue-eigenvector associations. Applying the power spectra as features of graphs in benchmark graph classification problems, we show that our approach performs on par with state of the art graph neural networks, even without using any message passing scheme.

References

[1] Vijay Prakash Dwivedi et al. "Benchmarking graph neural networks". In: *arXiv preprint arXiv:2003.00982* (2020).

[2] Derek Lim et al. "Sign and Basis Invariant Networks for Spectral Graph Representation Learning". In: *arXiv preprint arXiv:2202.13013* (2022).