model to effectively incorporate more global topological information, demonstrating the significance of the proposed global topological representation learning module for graph classification, and (iv) Wit-TopoPool consistently outperforms Wit-TopoPool w/o Attention Mechanism on all 3 datasets, indicating the attention mechanism can successfully extract the most correlated information and, hence, improves the generalization of unseen graph structures. Moreover, we also compare Wit-TopoPool with VR-TopoPool (i.e., replacing witness complex in global information learning with Vietoris-Rips complex) (see Appendix B for a discussion).

	Architecture	Accuracy mean±std
COX2	**Wit-TopoPool**	***87.24±3.15**
	W/o TPGCL	82.67±3.26
	W/o Wit-TL	85.21±3.20
	W/o Attention mechanism	85.58±3.53
PTC_MM	**Wit-TopoPool**	**76.76±5.78**
	W/o TPGCL	67.38±5.33
	W/o Wit-TL	70.58±5.29
	W/o Attention mechanism	75.12±5.59
IMDB-B	**Wit-TopoPool**	****78.40±1.50**
	W/o TPGCL	73.93±1.83
	W/o Wit-TL	77.00±1.69
	W/o Attention mechanism	76.20±1.98

Table 3: Ablation study of the Wit-TopoPool architecture.

Sensitivity Analysis We perform sensitivity analysis of (i) landmark set selection and (ii) topological score function to explore the effect of above two components on our Wit-TopoPool performance. The optimal choice of landmark set selection and topological score function can be obtained via cross-validation. We first explore the effect of landmark set selection. We consider 3 types of landmark set selections, i.e., (i) randomly ($\mathfrak{L}_r$), (ii) node betweenness centrality ($\mathfrak{L}_b$), and (iii) node degree centrality ($\mathfrak{L}_d$), and report results on COX2 and PTC_MM datasets. As Table 4 shows, we observe that the landmark set selection based on either node betweenness or degree centrality helps to improve the graph classification performance, whereas the landmark set based on randomly results in the performance drop. We also explore the effect of topological score function for the importance measurement of the persistence diagram (see Eq. 2). As the results in Table 5 suggest, summing over lifespans of topological features (points) in persistence diagrams can significantly improve performance, but applying piecewise linear weighting function on topological features may result in deterioration of performance.

Computational Complexity Computational complexity of the standard persistent homology matrix reduction algorithm (**?**) (i.e., based on column operations over boundary matrix of the complex) runs in cubic time in the worst case, i.e., $\mathcal{O}(m^3)$, where m is the number of simplices in the filtration. For 0-dimensional PH, it can be computed efficiently using disjoint sets with complexity $\mathcal{O}(m\alpha^{-1}m)$, where $\alpha^{-1}(\cdot)$ is the inverse Ackermann function (**?**). Computational complexity of the witness complex construction is $\mathcal{O}(\mathfrak{L}\log(n))$ (where n is the number of data points and $\mathfrak{L}$ is the landmark set), involving calculating the distance between data points and landmark points.

Dataset	Landmark set	Accuracy mean±std
COX2	$\mathfrak{L}_r$	82.98±3.88
	$\mathfrak{L}_b$	85.10±2.52
	$\mathfrak{L}_d$	**87.24±3.15**
PTC_MM	$\mathfrak{L}_r$	71.53±6.17
	$\mathfrak{L}_b$	**79.12±4.45**
	$\mathfrak{L}_d$	76.76±5.78

Table 4: Sensitivity analysis with respect to the landmark set selection for Wit-TopoPool on COX2 and PTC_MM.

Dataset	Weighting function	Accuracy mean±std
COX2	$d_\rho - b_\rho$	*****87.24±3.15**
	$\arctan\left(C \times ((d_\rho - b_\rho)^\eta)\right)$	79.78±1.06
PTC_MM	$d_\rho - b_\rho$	***79.12±4.45**
	$\arctan\left(C \times ((d_\rho - b_\rho)^\eta)\right)$	76.18±5.00

Table 5: Sensitivity analysis with respect to selection of weighting functions within the topological score for Wit-TopoPool on COX2 and PTC_MM.

Conclusion

In this paper, we have proposed Wit-TopoPool, a differentiable and comprehensive pooling operator for graph classification that simultaneously extracts the key topological characteristics of graphs at both local and global levels, using the notions of persistence, landmarks, and witnesses. In the future, we will expand the ideas of learnable topological representations and adaptive similarity learning among nodes to dynamic and multilayer networks.

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