A Persistent Weisfeiler–Lehman Procedure for Graph Classification

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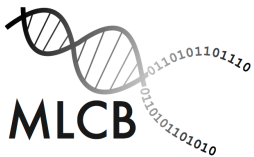
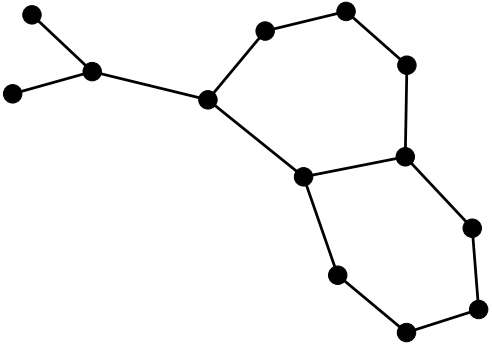
ETH zürich



Graph classification

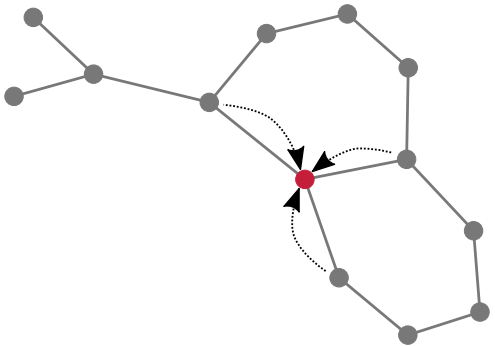


Graph

Potential labels

Graph classification

Neighbourhood aggregation

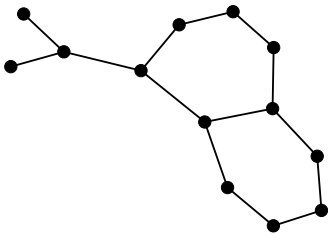


Our proposed method

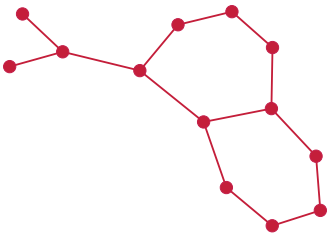
"P-WL = WL + TDA"

Topological features in graphs

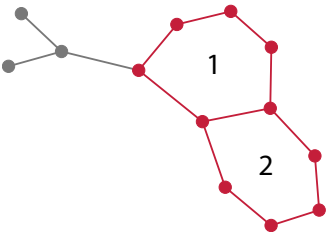
Connected components and cycles



Graph



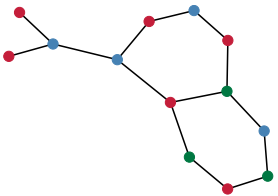
A connected component



Cycles

Finding topological features

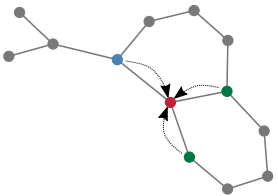
Calculating the persistent homology of a weighted graph



Labelled graph

Finding topological features

Calculating the persistent homology of a weighted graph



Weisfeiler–Lehman aggregation

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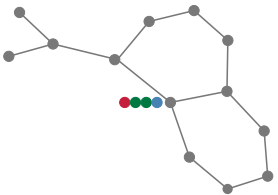
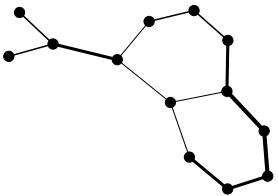
Calculating the persistent homology of a weighted graph



Label multisets

Finding topological features

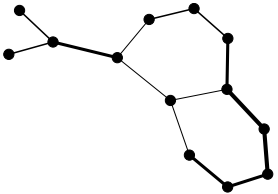
Calculating the persistent homology of a weighted graph



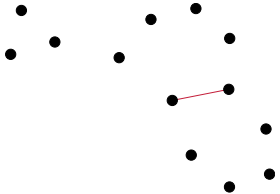
Weighted graph

Finding topological features

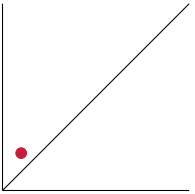
Calculating the persistent homology of a weighted graph



Weighted graph



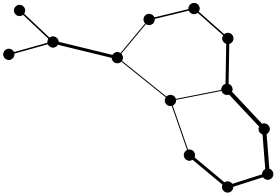
Graph filtration



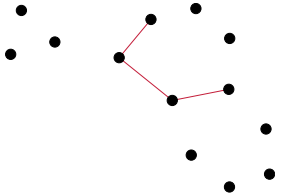
Topological feature descriptor

Finding topological features

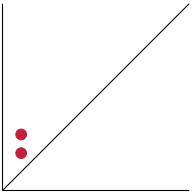
Calculating the persistent homology of a weighted graph



Weighted graph



Graph filtration



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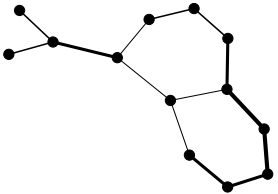
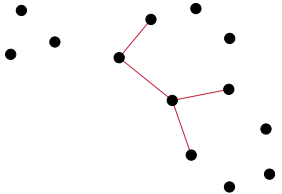


Weighted graph



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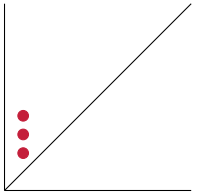

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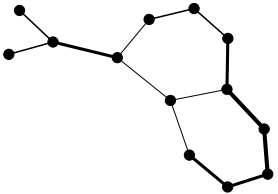
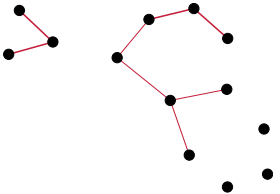
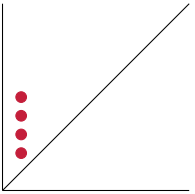


Weighted graph



Graph filtration



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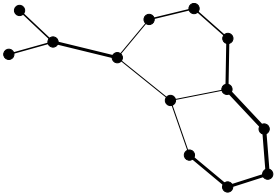
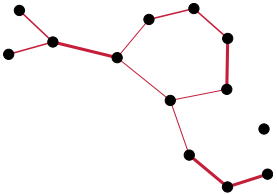


Weighted graph



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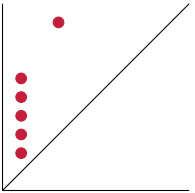

Topological feature descriptor

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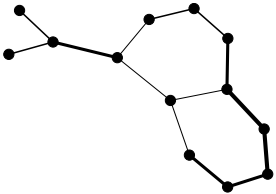
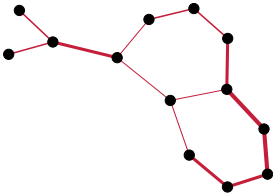


Weighted graph



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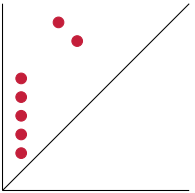

Topological feature descriptor

Conclusion

P-WL…

- …is almost as efficient as the Weisfeiler–Lehman kernel
- …exhibits favourable performance
- …outperforms “deep” graph kernels
- …shows the potential of *topological data analysis* (TDA)

Poster #224