ETH
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Distributed Computing

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Learning Structural Representations in Graphs

Graphs are powerful tools for modeling relationships in diverse domains, from social networks to molecular biology. Many real-world graphs are not just random collections of connections—they have intricate structures. Nodes in graphs often play distinct *structural roles*. For example, in the food chain graphs shown in Figure 1, the orca and lynx both act as top predators in their respective ecosystems, making them structurally similar despite living in entirely different environments.

Message Passing Graph Neural Networks (MPNNs) are a popular approach for machine learning on graphs. They use the graph structure around each node to find an embedding, hence computing a kind of structural representation. However, these embeddings are typically trained for a specific task, and may not capture the full range of structural information present in the surrounding graph.

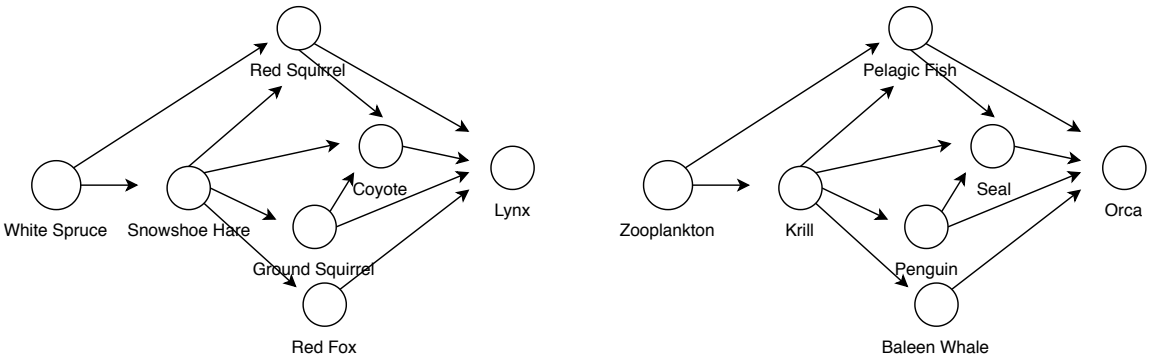

Figure 1: Food chain graphs, where nodes represent species and edges represent predator-prey relationships. [1]

This project aims to understand what structural information is actually included in the representations, and how to find better representations that capture the essence of the graph structure. Good node-level structural representations are also crucial for a graph-level structural representation. Potential applications include graph autoencoders, graph generation, and developing methods to explain what GNNs have learned.

Requirements: This project has a theoretical focus. A solid mathematical background – ideally including graph theory and linear algebra – is helpful. Python programming skills and some familiarity with machine learning are a plus. We can tune the project to be more theoretical or more practical, depending on your interests and background.

Interested? Please contact us for more details!

Contacts

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References

[1] Balasubramaniam Srinivasan and Bruno Ribeiro. On the equivalence between positional node embeddings and structural graph representations. In *International Conference on Learning Representations*, 2020.