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Distribution Shifts in Graph Machine Learning and Graph Domain Adaptation

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Graphs have been widely applied to model intricate relationships among entities. The application of Graph Machine Learning (GML) to enhance prediction capabilities for graph-structured data is prevalent in several scientific disciplines, such as particle physics, material science, and biology. However, applications in these domains often present challenges due to changes in data distributions due to the label collection process they employ. Specifically, the data used for model training often comes from the thoroughly investigated regimes, whose distributions often do not align well with the under-explored regime of scientific interest. Furthermore, the interconnected nature of entities in a graph presents an additional level of complexity, making current distributionally robust methods suboptimal when being applied to graph data.

This presentation will focus on our recent studies on GML under distribution shifts. Our studies are motivated by the observation of the data distribution shift in particle physics. We propose a method named graph structure alignment. The key idea of our approach is to estimate and quantify shifts in entity connection patterns from the training phase to real-world evaluation. Consequently, the influence of neighboring entities on a central node can be appropriately calibrated based on prior estimations, serving to mitigate the distribution shift in graph data.

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