PhD in Interdisciplinary Studies: physics, computer science and social sciences

Through Structure Alone. On the Geometry of Improvement in Physics-Informed and Graph Neural Networks

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Abstract

Improving neural networks often occurs through architectural interventions. This thesis therefore asks the question: *When does modifying a structural aspect of a problem improve learning, and how can we diagnose if it did?* We organise the answer around a coupling perspective, creating a distinction between separable interventions, which act only on the computational graph of a model, and entangled interventions, which alter computation and information content jointly. A recurring theme across this analysis is that of hyperparameters. This thesis therefore develops an approach to distinguishing genuine improvements from those that merely reflect a favourable point in configuration space.

Part II develops the separable case by showing that reformulating a differential equation improves the performance of Physics-Informed Neural Network when solving them. We demonstrate that the multi-task architecture developed to accommodate this also proves useful a completely different context of predicting cycling flows.

Part III addresses the entangled regime using Graph Neural Networks as a graph's topology determines both the computational graph and the information content of a task for these networks. In this context we reanalyse curvature-based rewiring and show that the observed accuracy gains are dominated by hyperparameter sensitivity. Additionally, we study curvature as a diagnostic tool to understand how topology and task intertwine. Our analysis demonstrates that this dependency is heavily task and architecture dependant.