

BRIDGING SCIENTIFIC MACHINE LEARNING AND SCIENTIFIC DISCOVERY: NOVEL DEVELOPMENTS

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ABSTRACT

In recent literature, machine learning (ML) algorithms have made tremendous advances in accelerating computer simulations across various applications. Scientific ML (SciML) is a branch of ML that devises algorithms that are customized for scientific applications, for e.g., by imposing constraints and preserving symmetries. These are designed to bridge the gap between rigorous scientific computing, built on first-principles-based numerical modeling of various governing laws, and purely data-driven methods. In this minisymposium, we will showcase recent developments in an emergent but important application of SciML – where algorithms are designed not only to accelerate scientific computing, but also to discover some previously unknown underlying property of physical systems such as an invariant measure, a governing law, or a reward that engenders the observed behavior. Specifically, we wish to discuss how SciML algorithms can be devised to mature beyond simply reproducing observed data and simple extrapolation tasks.