

Abstract

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This thesis studies novel approaches to learning of physical models, incorporating constraints and optimizing path dependent loss functions. Recent advances in deep learning and artificial intelligence are connected with established knowledge about dynamical and chemical systems, offering new synergies and improving upon existing methodologies. We present significant contributions to simulation techniques that utilize automatic differentiation to propagate through the dynamics, showing not only their promising use case but also formulating new theoretical results about the gradient behavior in long evolutions controlled by neural networks. All the tools are carefully tested and evaluated on examples from physics and chemistry, thus proposing and promoting their further applications.