Teaching Computers to be Physicists: Machine Learning with Network Functions

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It is often the case that a physicist must find a mathematical relationship between a set of independent variables and some observable. This can be carried out by fitting the data to some assumed form, but machine learning techniques can be used to carry out the same task with more generality. Network functions are computational networks designed to allow the techniques of machine learning to be used to find mathematical relationships buried in a set of data. Network functions use composition of fundamental mathematical operations, to represent complex analytical functions. This is done through a continuously variable functional form, governed by a set of trainable parameters. The precise form taken on by a network can be learned using simple training algorithms. Unlike neural networks, many target functions can be learned *exactly* over their entire domain by a finite—and often small—network. In the worst case, a network can learn to approximate a target function to arbitrary precision within some range of inputs. There are many uses for network functions, including searching for a kinetic energy density functional or an improved exchange-correlation functional within density functional theory.

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