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Augmenting Spectral Methods with Normalizing Flows and Application to Computing Molecular Excited States

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Abstract: (Pseudo)spectral methods are popular for solving a wide variety of differential equations and generic optimization problems. Due to favourable approximation properties, such as rapid convergence for smooth functions, they are particularly popular and effective for solving time-independent Schrödinger equations. For example, in the domain of molecular quantum physics, spectral and pseudospectral methods are the building blocks for a variety of variational techniques to solve nuclear Schrödinger equations. Despite their many favourable approximation properties, these methods suffer from the curse of dimensionality and have slow convergence rates for highly-oscillatory functions. This limits their applicability in a wide variety of fields. Moreover, their effectiveness is highly dependent on the initial choice of the basis.

In this talk I propose increasing the expressivity of (pseudo)spectral methods by composing a chosen orthonormal basis with an optimizable measurable mapping. This gives rise to an induced sequence. I characterize necessary and sufficient conditions for this sequence to inherit the completeness of the underlying orthonormal basis. Here, it is shown that the invertibility of the mapping is a necessary condition. Subsequently, I discuss the approximation of Schwartz functions in the linear span of Hermite functions that are composed with invertible mappings. To this end, I derive convergence guarantees and characterise the convergence order. Finally, I show numerical simulations for computing the vibrational spectra of polyatomic molecules. In these simulations, the invertible mapping was modelled using a normalizing flow, i.e., an invertible neural network to augment the expressivity of a given basis. Comparisons against the use of standard bases demonstrate orders-of-magnitude increased accuracy when using normalizing flows.