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	authors	<ul style="list-style-type: none">Scherbela, M.Reisenhofer, R.Gerard, L.Marquetand, P.Grohs, P.	authors	<ul style="list-style-type: none">Michael ScherbelaRafael ReisenhoferLeon GerardPhilipp MarquetandPhilipp Grohs	DUPLICATES	163
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	abstract		abstract	Accurate numerical solutions for the Schrödinger equation are of utmost importance in quantum chemistry. However, the computational cost of current high-accuracy methods scales poorly with the number of interacting particles. Combining Monte Carlo methods with unsupervised training of neural networks has recently been proposed as a promising approach to overcome the curse of dimensionality in this setting and to obtain accurate wavefunctions for individual molecules at a moderately scaling computational cost. These methods currently do not exploit the regularity exhibited by wavefunctions with respect to their molecular geometries. Inspired by recent successful applications of deep transfer learning in machine translation and computer vision tasks, we attempt to leverage this regularity by introducing a weight-sharing constraint when optimizing neural network-based models for different molecular geometries. That is, we restrict the optimization process such that up to 95 percent of weights in a neural network model are in fact equal across varying molecular geometries. We find that this technique can accelerate optimization when considering sets of nuclear geometries of the same molecule by an order of magnitude and that it opens a promising route towards pre-trained neural network wavefunctions that yield high accuracy even across different molecules.		
	versions		versions			