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Optimal Transport distances for classifying electronic excitations

In chemistry, electronic excitations may be seen as an electron moving from one energy level to another. They are heuristically divided into three groups based on certain characteristics of the involved energy levels. Knowing which group an excitation belongs to can be useful, because calculated excitation energies can vary greatly in accuracy depending on which group the excitation belongs to. On the quest to finding a systematic classification, we introduce a diagnostic based on the Sinkhorn divergence from Optimal Transport and compare it to an existing one which uses the overlap. We then apply both to a selected set of molecules and study the quality of the resulting classifiers.