

# Wasserstein-type interpolation for generic mixture models: application to model-order reduction in quantum chemistry

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Optimal transport theory has recently been observed to yield interesting nonlinear model-order reduction approaches for parametric problems with slow decaying Kolmogorov widths. This is the case for transport-dominated problems, but also in quantum electronic structure calculations which is the main motivation of the present work. One possible strategy, which has been studied by different groups with various flavours, is to build reduced solutions as interpolations in a Wasserstein sense, more precisely as barycenters of "snapshots solutions" with respect to the Wasserstein distance. The main drawback of this type of approaches is that the computation of these Wasserstein barycenters may be extremely costly from a numerical point of view for high-dimensional problems. However, a modified Wasserstein-metric has recently been introduced by Julie Delon and Agnès Desolneux defined on the set of Gaussian mixtures which present two main advantages in our context: (i) the computation of barycenters with respect to this modified Wasserstein metric is much easier than the computation of barycenters with respect to the exact Wasserstein metric, especially for high-dimensional problems; (ii) interpolation with respect to this modified Wasserstein metric yield similar results than with the original metric.

The aim of this work is to generalize the work of Julie Delon and Agnès Desolneux in order to define and efficiently compute similar modified Wasserstein distances for generic mixture models. This plays a significant role in particular in electronic structure calculations, where the unknown to interpolate is the electronic wavefunction of the set of electrons within a molecule depending on the location of the nuclei. Preliminary numerical tests will be shown in order to illustrate the efficiency of the approach.