Nonlinear reduced basis using mixture Wasserstein barycenters: application to an eigenvalue problem

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We are interested in the computation of the ground state of a given molecular system composed of M nuclei characterized by their positions $r_1, \dots, r_M$ in space and their electric charges $z_1, \dots, z_M$. The ground state of this system is an eigenfunction with lowest corresponding eigenvalue (called energy) of an operator, called Hamiltonian. Ground states are generally computed using linear approximations such as Galerkin methods, but such methods rely heavily on the heuristic of a good choice for the basis. Moreover, determining the ground state is in general very costly, especially when it needs to be computed for a lot of different geometries, as in geometry optimization and molecular dynamics.

In this poster, I will focus on a one-dimensional Hamiltonian, with Dirac delta potentials placed at atomic positions $r_1, \dots, r_M$, for which ground states are fully described in [4]. In [3], a method based on optimal transport was proposed for different problems, where solutions were approximated as Wasserstein barycenters between solutions for different parameters. However, this method is not expected to scale with the dimension due to the high-computational cost of Wasserstein barycenters.

In this work, we propose a new approach based on a decomposition of the ground state as a mixture of Slater functions, for which modified Wasserstein barycenters can be computed efficiently [1, 2]. In this method, we select a few representative solutions using a greedy algorithm in a first phase, called offline phase, which serves the purpose of reducing computational time for solution computations and can be done only once. Solutions are then computed on-the-fly in an online phase, as barycenters of the previously selected solutions. Some numerical results will illustrate our approach.

References

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