HF notes

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March 14, 2019

Here, we will be preforming the Hartree-Fock self consistent field method for a water molecule in the cc-pVDZ method. This method finds mean field solution to the electronic structure Hamiltonian.

1 Load Data

1. Load the convergence criteria: the maximum iterations `data/iteration_max.txt`, convergence of density matrix `data/convergence_DM.txt`, and convergence of the energy `convergence_E.txt`. The Hartree-Fock method is an iterative method and these decide when the method has converged. We'll talk more about these below.

2. Load in the integrals. These integrals are the overlap `data/S.txt`, the kinetic `data/T.txt`, the nuclear attraction `data/V.txt`, and the electron repulsion integrals `data/eri.txt`. These are real-valued integrals over gaussian fucntions.

3. Load in the nuclear repulsion energy `data/E_nuc.txt`, the number of electrons alpha `data/num_elec_alpha.txt`, the number of electrons beta `data/num_elec_beta.txt`, and the number of atomic orbitals `data/num_ao.txt`.

2 Load Data