The Gradient Boosting Tree for the prediction of two-electron integrals

Kaoutar EL HALOUI[A] **Nicolas SISOURAT**[B] **Pierre Louis BOURGEOIS**[C] **Nicolas THOME**[D]

A, B, C) Sorbonne Université, CNRS, UMR 7614, Laboratoire de Chimie Physique-Matière et Rayonnement, 75005, Paris, France;
D) Sorbonne Université, CNRS, ISIR, F-75005, Paris, France.

kaoutar.el_haloui@sorbonne-universite.fr

A common bottleneck in most quantum chemistry (QC) techniques is the computation and handling of extremely numerous two-electron integrals. There is thus a continuous search for always faster methods to compute and store these integrals. In this work, we investigate the use of machine learning as a way to by-pass the direct computation of the two-electron integrals of a molecular system and facilitate their storage. We show that a gradient boosting tree Regressor (GBR) model can be trained to predict the values of two-electron integrals when only given a set of features describing each integral. This can be used to drastically reduce the memory cost of QC computations as only the parameters of the GBR are needed to be stored (instead of all the integral values). Those can then be used to compute the integrals on the fly. We also investigate the possibility of using GBR models to predict the two-electron integrals values of different basis sets or of different geometries of a molecule.

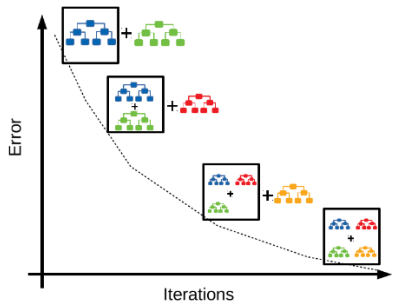

Figure 1. Gradient Boosting Tree illustration

Keywords: Machine Learning, Gradient boosting, Two-electron integrals, OVGF.