Basis set completeness profiles in two dimensions

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In 1995 D. P. Chong [1] introduced a method to give a visual assessment of the quality of the completeness one electron basis sets. The so called *basis set completeness profile* is obtained by plotting $Y(\alpha)$ against $\log(\alpha)$ with $Y(\alpha) = \sum \langle G(\alpha)|\,\Psi_m\,\rangle\langle\,\Psi_m\,|G(\alpha)\rangle \simeq 1$, Ψ being any orthonormal one electron basis set and $G(\alpha)$ being a scanning GTO. In the framework of explicitly correlated methods an analogue two electron completeness surface can be constructed by evaluating :

$$Y(\alpha,\beta) = \sum\sum \langle G(\alpha)G(\beta)|\,\tfrac{1}{r_{12}}\,|\Psi_m\Psi_n\rangle\,\langle\Psi_m\Psi_n|\,r_{12}\,|G(\alpha)G(\beta)\rangle$$

Two dimensional completeness surfaces for different basis sets are presented as well as an investigation with $G(\alpha)$ and $G(\beta)$ placed on different centers. The long therm perspective of this study is the design of auxiliary basis sets to improve the performance of methods using linear r_{12} terms in explicitly correlated wavefunctions.

[1] D. P. Chong, Completeness profiles of one-electron basis sets,Can. J. Chem.,**73**,79,(1995)