Topological Data Analysis in quantum chemistry - the electron density of Au complexes case study.

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We demonstrate the use of the Topological Data Analysis (TDA) for the electron density (ED) of Au complexes evaluated at different levels of accuracy. TDA tracks the evolution of critical points of data, hence if applied to ED, it has a direct connection to the Quantum Theory of Atoms in Molecules (QTAIM). Our study contributes to the discussion of the use of QTAIM for the non-covalent interactions, especially in relativistic regime, and proposes to consider TDA as a modern complement to QTAIM.