

Approaching the atomic radii from in a data-oriented way: how can we benefit from a set of 'useless' structural properties?

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We report utilization of a collection of interatomic distances, obtained from 28 710 molecules after optimizing their geometries with quantum-chemical methods, to introduce a new set of atomic radii for H, B, C, N, O, F, Si, P, S, Cl, Ge, As, Se, Br elements. This problem is tackled from a perspective which differs significantly from many conventional approaches, like van der Waals radii or the covalent ones, which typically focus on introducing the atomic radii as the descriptors tailored for modeling specific sort of atomic contacts or bonded states found in diatomic fragments respectively. In contrast to that, we study the possibility of finding the atomic radii as parameters of a linear machine-learned binary classifier, trained to distinguish between bonded and non-bonded pairs of atoms [1]. We demonstrate, that although the distances between non-bonded atomic pairs play an essential role in training this classifier, the obtained radii still exhibit considerable similarities to the conventional covalent ones [2]. We thereby provide an example for how a proper data-oriented treatment can turn seemingly useless data into the useful one. Additional details on the procedure [3] used to create a dataset of interatomic distances in fully automated, yet chemically sound manner, are discussed.

References

- [1] T.Y. Nikolaienko and L.A. Bulavin, *Comput. Theor. Chem.* (2021), 1204: 113389.
- [2] T.Y. Nikolaienko, V.S. Chuiko and L.A. Bulavin, *Mol. Phys.* (2020), **118**: e1742937.
- [3] T.Y. Nikolaienko, V.S. Chuiko and L.A. Bulavin, *Comput. Theor. Chem.* (2019), **1163**: 112508.

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