MLtool++ package for machine learning and its applications to materials data

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Abstract

We are developing Mltool++ package of software programs for machine learning (ML). Given the MLtool Python code, we create a faster C++ code with the potential for parallelization. We have extracted materials data from the literature. One dataset contains melting temperatures of stoichiometric 1:1 metallic compounds XZ, composed by elements X={Al, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W} and Z={Co, Ni, Cu, Rh, Pd, Ag, Ir, Pt, Au}, and another contains solid-solid symmetry-breaking phase transition temperatures. We studied dependences of temperatures on composition, found several correlations, and parametrized them by analytical functions. Mltool++ package is generic and applicable to any tabulated numeric data.

Mltool++ software implementation

MLtool++ reads two text files, containing data and input parameters. The data is fitted by the selected analytical model; choices include polynomials, rational functions, gaussians, plane waves, or arbitrary user-defined functions. MLtool Python code cross-validates all models, returns a ranked list, and points at the best predictive models; MLtool++ package will be faster, parallel, with a similar functionality. MLtool++ package is object-oriented and multithreaded; there are plans for its further parallelization and optimization.

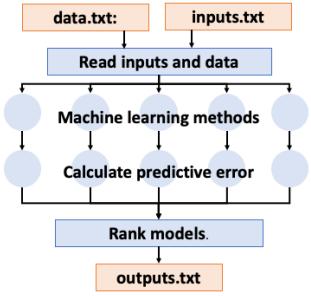

Figure 1: Flowchart of MLtool++ package.

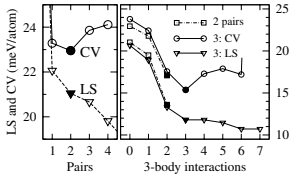

Figure 2: Cross-validation (CV) predictive and least-squares (LS) fit errors versus number of parameters, see Fig. 2 in [10].

Applications to materials data

Data sets were extracted from ASM phase diagrams database. Over 90 binary X-Z phase diagrams were considered with chemical elements X={Al, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W} and Z={Co, Ni, Cu, Rh, Pd, Ag, Ir, Pt, Au}.

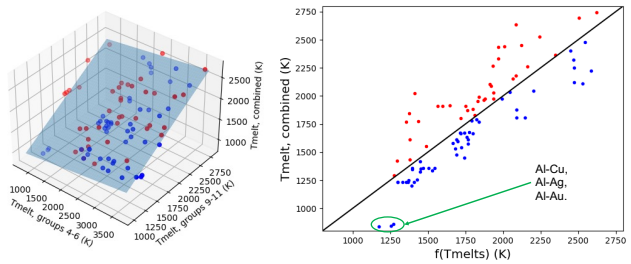

Figure 3: Melting temperatures T_{melt}[K] of 90 XZ stoichiometric 1:1 compounds versus T_{melt} of 10 X (group 4-6) and 9 Z (9-11) elemental metals, fitted by the linear function $T_{melt}(XZ) = \boldsymbol{a} \cdot \vec{T}_{melt}$, where $\boldsymbol{a} = [106\ [K]\ \ 0.0992\ \ 0.791]$ and $\vec{T}^{T}_{melt} = [1\ \ T_{melt}(X)\ \ T_{melt}(Z)]$.

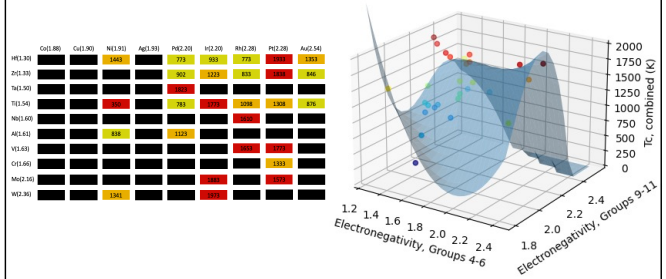

Figure 4: Solid-solid transition temperatures T_c[K] of 31 stoichiometric 1:1 compounds versus electronegativity of 10 X (group 4-6) and 9 Z (group 9-11) metals.

Considering solid-solid symmetry-breaking phase transition temperatures T_c[K] of stoichiometric 1:1 compounds XZ versus properties of elemental metals X and Z, we found a moderate correlation and approximated it by a third-degree polynomial:

$$T_c\,[K] = \boldsymbol{a} \cdot \overrightarrow{en}\,;$$

$$\boldsymbol{a} = [57.5\ \ -23.4\ \ -63.4\ \ 2.77\ \ 17.5\ \ 23.2\ \ -0.0398\ \ -1.17\ \ -3.13\ \ -2.84] * 10^4\ \text{K},$$

$$\overrightarrow{en}^{T} = [1\ \ en_X\ \ en_Z\ \ en_X^2\ \ en_X en_Z\ \ en_Z^2\ \ en_X^3\ \ en_X^2 en_Z\ \ en_X en_Z^2\ \ en_Z^3]$$

Conclusion

We started implementing components of MLtool++ software package, considered 90 ASM phase diagrams, performed data mining, and extracted relevant data sets. We applied our software to our data, found correlations and parametrized them by analytical equations.

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Provided a versatile fitting tool for any tabulated numeric data

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