Thermodynamics-informed Symbolic Regression

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Thermodynamic equations of state (EOS) are essential for many industries and in academia. Even when leaving aside the expensive and extensive measurement campaigns required for data acquisition, the development of EOS is still an intensely time-consuming process, often relying heavily on expert knowledge and iterative fine-tuning.

To improve upon and accelerate the EOS development process, we are developing Thermodynamics-informed Symbolic Regression (TiSR), a symbolic regression tool aimed at thermodynamic EOS modeling. TiSR is already a capable symbolic regression tool, used in our previous work (Int. J. Thermophys. 2023, 44, 7). It aims to combine a symbolic regression base with the extensions required to work with often strongly scattered experimental data, to use different residual

pre- and post-processing options, and various additional features required to consider the development of different thermodynamic EOS.

Although TiSR is not ready for end users yet, we report on its current state, showcase the progress, and discuss (distant and not-so-distant) future directions. Furthermore, we will discuss selected use cases and how TiSR was applied. TiSR is open source and available on GitHub at https://github.com/scoop-group/TiSR.