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Application of deep symbolic regression for approximation problems in statistical mechanics

Alina Popova[1], Rasul Abdusalamov[2], Mikhail Itskov[3]

[1] [1] RWTH Aachen University, Aachen, Germany [2] University of Galway, Galway, Ireland, Germany.
alina99popova@gmail.com
[2] Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany, Germany.
abdusalamov@km.rwth-aachen.de
[3] [1]Department of Continuum Mechanics, RWTH Aachen University, [2]School of Computer Science & Mathematics, Keele University, Germany. itskov@km.rwth-aachen.de

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Abstract

In this study, the Deep Symbolic Optimization (DSO) algorithm is used to derive precise approximations for both the extension-force relationship of the Worm-Like Chain (WLC) model and a non-Gaussian probability distribution function for polymer chain length. The latter one is based on Kuhn and Gruen's non-Gaussian statistical theory [1]. Existing approximation methods in literature frequently yield complex equations that deviate from analytical solutions, thus limiting their practical utility. The objective of this work is to identify a set of simple yet accurate approximations that effectively characterize polymer extension models. The proposed expressions for the WLC extension-force dependency achieve a very small relative error within the relevant variable range, enabling direct application to fit force-extension curves in molecular force spectroscopy experiments. A comparative analysis with recently suggested methods [2] reveals that the DSO-based approach surpasses traditional techniques in accuracy while preserving equation simplicity. Furthermore, we introduce novel approximations for the non-Gaussian probability distribution function of polymer chain length [3], expanding its applicability across a wider spectrum of chain segment numbers. This enhancement allows for more precise modeling of the behavior of polymers. REFERENCES 1. Kuhn, Werner, and Felix Grün. "Beziehungen zwischen elastischen Konstanten und

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