The Structural Information Content of Chemical Networks

Matthias Dehmer\textsuperscript{a} and Frank Emmert-Streib\textsuperscript{b}

\textsuperscript{a} Institute of Discrete Mathematics and Geometry, Vienna University of Technology, Wiedner Hauptstrasse 8–10, A-1040 Vienna, Austria
\textsuperscript{b} Department of Biostatistics, Department of Genome Sciences, University of Washington, 1705 NE Pacific St, Box 355065, Seattle, WA 98195-5065, USA

Reprint requests to M. D.; E-mail: mdehmer@geometrie.tuwien.ac.at


We present an information-theoretic method to measure the structural information content of networks and apply it to chemical graphs. As a result, we find that our entropy measure is more general than classical information indices known in mathematical and computational chemistry. Further, we demonstrate that our measure reflects the essence of molecular branching meaningfully by determining the structural information content of some chemical graphs numerically.

\textit{Key words}: Structural Information Content; Graph Entropy; Information Theory; Chemical Graph Theory.