entropy 2021

sciforum

Abstract

Conformational and Translational-Rotational Entropy from Molecular Ensembles †

Federico Fogolari

University of Udine, Udine, Italy

† Presented at the Entropy 2021: The Scientific Tool of the 21st Century, 5–7 May 2021; Available online: https://sciforum.net/conference/Entropy2021/.

Published: 5 May 2021

Entropy calculation is an important step in the postprocessing of molecular dynamics trajectories or predictive models. In recent years the nearest neighbor method proposed by Demchuk and coworkers [1] has emerged as a powerful method to deal in a flexible way with the dimensionality of the problem. Applications to most important biomolecular processes have been presented [2,3] and a specific development has concerned the computation of rotational-translational entropy which required in turn the definition of a metric in rotation-translation space [4]. Two programs have been developed to compute conformational and rotational-translational entropies from biomolecular ensembles [5]. Possible estensions of the method will be presented.

References

1. Singh, H.; Misra, N.; Hnizdo, V.; Fedorowicz, A.; Demchuk, E. Nearest neighbor estimates of entropy. *Am. J. Math. Manag. Sci.* **2003**, *23*, 301–321.
2. Fogolari, F.; Corazza, A.; Esposito, G. Free energy, enthalpy and entropy from implicit solvent end-point simulations. *Front. Mol. Biosci.* **2018**, *5*, 11.
3. Fogolari, F.; Corazza, A.; Fortuna, S.; Soler, M.A.; VanSchouwen, B.; Brancolini, G.; Corni, S.; Melacini, G.; Esposito, G. Distance-based configurational entropy of proteins from molecular dynamics simulations. *PLoS ONE* **2015**, *10*, e0132356.
4. Fogolari, F.; Foumthuim, C.J.D.; Fortuna, S.; Soler, M.A.; Corazza, A.; Esposito, G. Accurate Estimation of the Entropy of Rotation-Translation Probability Distributions. *J. Chem. Theory Comput.* **2016**, *12*, 1–8.
5. Fogolari, F.; Maloku, O.; Foumthuim, C.J.D.; Corazza, A.; Esposito, G. PDB2ENTROPY and PDB2TRENT: Conformational and Translational-Rotational Entropy from Molecular Ensembles. *J. Chem. Inf. Model.* **2018**, *58*, 1319–1324.