

USING WRITHE TO PRODUCE REALISTIC PROTEIN STRUCTURE PREDICTIONS FROM BIOSAXS DATA

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ABSTRACT

The writhe is a measure of global self entanglement of a curve. The usual technique for studying entanglement of protein backbones requires artificial or probabilistic closures, thus altering the geometry of the curve. By using the open curve definition of the writhe we can study the geometry of protein curves in a more natural way. In particular, I will present bounds on the amount of global entanglement as measured by both the writhe and absolute writhe. With these bounds, we can produce realistically folded structures from BioSAXS data^[1] with a much higher chance of success when passed into an MD simulation. These bounds, inspired by work in the magnetic helicity community^[2], give rise to interesting classifications of proteins for further study. By studying the writhe of subsections of the protein's backbone, we are also able to highlight sites of interest such as highly flexible sections allowing large scale conformational changes or areas of maximal entanglement.

This is joint work with Chris Prior.

- [1] Prior, C., Davies, O.R., Bruce, D. and Pohl, E. 2020 Obtaining tertiary protein structures by the ab initio interpretation of small angle X-ray scattering data. *J. Chem. Theory and Computation* **16**, 1985–2001.
- [2] Cantarella, J., DeTurck, D. and Gluck, H. 2001. Upper bounds for the writhing of knots and the helicity of vector fields. *AMS IP Studies in Advanced Mathematics* **24**, 1–22.