

Abstract Submitted  
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**What does a protein network look like? A solution from network inference and the inverse Ising problem**<sup>1</sup> JENNY LIU, Northwestern University — Advances in protein structure determination have created increasing interest in the dynamics of folded proteins and their role in function, further increasing the importance of molecular dynamics simulations. To analyze these large datasets, proteins are often modeled as networks to take advantage of well-developed methods from network science. Protein networks are often constructed from correlative measures. Yet, in the field of network science, it has been demonstrated that solving the inverse problem is required to identify the interactions. Thus, we apply this inverse approach to the dynamics of protein dihedral angles, a system of internal coordinates that avoids the structural alignment issue in hinge-like proteins. Focusing on the adhesion protein, FimH, we show that our method identifies networks that are related to underlying physical interactions and are robust across replicates. We extend our approach to Siglec-8, an immune adhesion protein, and the SARS-CoV-2 spike protein. Due to the differences in the networks constructed by correlation and by solving the inverse problem, there are also downstream differences in network analysis. We apply community detection to identify flexible and rigid regions that regulate collective motion relevant to protein function.

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Jenny Liu  
Northwestern University

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