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# REAL SPACE MODELING OF SOLUTION-STATE SAXS USING INFORMATION THEORY

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**Small angle X-ray scattering measurements of dilute, homogenous particles in solution are resolution limited measurements of the thermodynamic ensemble. Similar to X-ray crystallography and electron microscopy, SAXS observations made at higher resolutions imply a greater detail in the structural measurement. Here, I present a new approach to understanding bioSAXS data using two fundamental properties of Information Theory (namely, the Shannon Sampling and Noisy-Coding Channel theorems). These theorems allow for the error-free recovery of the SAXS signal, in the form of a real-space, cross-validated pair-distance, P(r), distribution function. The P(r)-distribution contains the structural assessment of the thermodynamic ensemble. I will show that the Information theory framework can be used to develop structural modeling algorithms for shape determination and docking. Specifically, I will demonstrate an adaptive simulated-annealing, density modeling algorithm that targets the P(r)-distribution using the Kullback-Liebler divergence, an Information Theory difference metric. The algorithm scales with resolution. Using a SAXS dataset of a 25 base-pair, double-stranded DNA, the volumetric model illustrates features of the major and minor groove as the resolution of the SAXS dataset increases. Further tests on SAXS of the P4-P6 group I intron RNA domain reveal the large solvent channels observed in the X-ray crystal structure. Furthermore, I will show the Information Theory approach can be used in antibody-antigen studies to uniquely determine the structure of the complex in the solution state. Our approach shows that modeling can be made more reliable by exploiting theorems from Information Theory.**

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