BALL STATE UNIVERSITY

The Mathematical Laws of Morphology and Biomechanics

PURDUE FORT WAYNE

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Virtual Presentation: https://purdue.webex.com/meet/aselvite

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Statistical Challenges in Shape Prediction of Biomolecules

The three-dimensional /higher-order structure of biomolecules determines its functionality. While assessing their primary structure is fairly easily accessible, reconstruction of the higher order structure is costly. It often requires elaborate correction of atomic clashes, frequently not fully successful. Using RNA data, we describe a purely statistical method, learning error correction, drawing power from a two-scale approach: Our microscopic scale describes single suites by dihedral angles of individual atom bonds. Here, addressing the challenge of torus principal component analysis (PCA) leads to a fundamentally new approach to PCA. Based on an observed relationship with a mesoscopic scale, landmarks describing several suites, we use Fréchet means for angular shape and size-and-shape, correcting within-suite-backbone-to-backbone clashes. We validate this method by comparison to reconstructions obtained from simulations approximating biophysical chemistry and illustrate its power by the cutting-edge RNA example of SARS-CoV-2. This is joint work with Benjamin Eltzner, Kanti V. Mardia and Henrik Wiechers.

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