Data Sciences: Bridging Mathematics, Physics and Biology

Tutorial on Geometry and Shape Analysis in Biological Sciences

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Tutorial 1: Overview: Geometry and Topology in Biology

Structural information on biological shapes can be obtained via a number of experimental techniques, including X-ray crystallography, NMR, and cryo-electron microscopy tomography for molecular systems, multiple microscopy and scanning techniques for larger biological shapes, and scanners for even larger shapes, to name only a few. However, it is the geometric and topological modeling that interprets and translates the data generated by those techniques into a meaningful model of the structure-function relationship for those systems, allowing the geometric information to be integrated into physical models that shed new light on the mechanisms of life. In this tutorial, we will introduce the different techniques for collecting data on biological objects, and describe geometric and topological problems that arise in attempting to analyze those data. We will focus on the geometric description of biomolecules, introducing the concepts of implicit solvent models and their use for predicting protein-drug interactions, and on bones and their use in 3D morphometrics.

Tutorial 2: How to describe a shape: Biological shape descriptors

The problem of describing, measuring and comparing shapes arises in image processing when searching for or recognizing objects in an image or a video. This problem is now surfacing in many more disciplines that are generating increase amounts of quantitative and visual information. Biology occupies a central place among these fields of applications. In cellular biology, the measurements of cell morphology and dynamics by imaging techniques such as light or fluorescent microscopy yield large numbers of 2D and 3D images that need to be segmented and quantified. In molecular biology the common assumption that the structure (or shape) of a protein is a major determinant of its function has stimulated the development of many methods for representing, measuring and comparing protein structures. The description of a shape increases in complexity as the object departs from regularity. The objective of most scientists is not necessarily to describe such shapes completely but to identify a small set of attributes of the shape that are information-rich with respect to the problem at hand. We will explore different options for defining such attributes.

Tutorial 3: Comparing biological shapes (1)

In a chapter titled “The Comparison of Related Forms”, D’Arcy Thompson explored how differences in the forms of related animals can be described by means of simple mathematical transformations This inspired the development of several shape comparison techniques, with the goal of defining a map, or correspondence, between two shapes that can be used to measure their similarity. This is a challenging problem, as the space of all possible maps is extremely large and difficult to characterize mathematically. In this tutorial and its follow-up, we will cover this problem, focusing first on the discrete representation of shapes in biology, and later on the theory of conformal mapping and its applications to study biological shapes. While three-dimensional (3D) data representing a shape come in many forms, we concentrate on the important case where the surface of the shape is available and described with a discrete triangular mesh. Mathematically, these objects are 2-dimensional Riemannian manifolds in the smooth case, and piecewise-flat surfaces in the discrete setting.

Tutorial 4: Comparing biological shapes (2)

Now that we have described discrete surfaces and the concept of conformal mapping, we will study in more detail the problem of defining a standard correspondence, or map, between two surfaces, sometimes called a parameterization. Such a map allows a mesh, or triangulation representing one of the surfaces to be transported to the second surface. We will describe approaches to this problem through circle packing and Ricci flow. The methods described so far for comparing two shapes focus on the differences in the geometry of a pair of shapes. An alternative approach ~~is to~~ attempts to capture the cost of deforming one shape into the other. We will describe one implementation of this approach, based on the idea of a variational distance that generalizes the concept of Euclidean distance.