



भारतीय प्रबंध संस्थान बेंगलूर
INDIAN INSTITUTE OF MANAGEMENT
BANGALORE

The Decision Sciences Area at IIM Bangalore welcomes you to a webinar, titled:

A Statistical Model for Helices with Applications

by

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Date: 10th December, 2021

Time: 3:00 p.m. to 4:00 p.m.

Abstract:

Motivated by a cutting edge problem related to the shape of alpha-helices in proteins, we formulate a parametric statistical model, which incorporates the cylindrical nature of the helix. Our focus is to detect a “kink,” which is a drastic change in the axial direction of the helix. We propose a statistical model for the straight α -helix and derive the maximum likelihood estimation procedure. The cylinder is an accepted geometric model for alpha-helices, but our statistical formulation, for the first time, quantifies the uncertainty in atom positions around the cylinder. We propose a change point technique “Kink-Detector” to detect a kink location along the helix. Unlike classical change point problems, the change in direction of a helix depends on a simultaneous shift of multiple data points rather than a single data point, and is less straightforward. Our biological building block is crowdsourced data on straight and kinked helices; which has set a gold standard. We use this data to identify salient features to construct Kink-detector, test its performance and gain some insights. We find the performance of Kink-detector comparable to its computational competitor called “Kink-Finder.” We highlight that identification of kinks by visual assessment can have limitations and Kink-detector may help in such cases. Further, an analysis of crowdsourced curved alpha-helices finds that Kink-detector is also effective in detecting moderate changes in axial directions.