Detecting and Localizing Differences in Functional Time Series Dynamics: A Case Study in Molecular Biophysics

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Abstract

Motivated by the problem of inferring the molecular dynamics of DNA in solution, and linking them with its base-pair composition, we consider the problem of comparing the dynamics of functional time series, and of localising any inferred differences in frequency and space. The approach we take a frequency domain one, where the complete second-order structure of the functional time series is encoded by its spectral density operator, indexed by frequency and curvelength. The comparison is broken down to a hierarchy of stages: at a global level, we compare the spectral density operators of the two functional time series, across frequencies and curvelength, based on a Hilbert-Schmidt criterion; then, we localise any differences to specific frequencies; and, finally, we further localise any differences along the length of the random curves. A hierarchical multiple testing approach guarantees control of the averaged false discovery rate over the selected frequencies. In this sense, we are able to attribute any differences to distinct dynamic (frequency) and spatial (curvelength) contributions. Our approach is presented and illustrated by means of a case study in molecular biophysics: how can one use molecular dynamics simulations of short strands of DNA in order to infer their temporal dynamics, and probe whether these depend on the sequence encoded in these strands?

Keywords: *DNA minicircles; linear contrast; multiple testing; spectral density operator; two-sample test.*