Doubly Spectral Analysis of Functional Time Series and the Molecular Dynamics of DNA

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The Karhunen-Loeve(KL) expansion has evolved into the workhorse of the statistics of functional data: the Fourier representation it affords on the one hand serves as a basis for motivating methodology by analogy to multivariate statistics; and, on the other hand, appears as the natural means of regularization in problems such as regression, testing and prediction, which are ill-posed in the functional case. With the aim of obtaining a similarly canonical representation of dependent functional data, we develop a doubly spectral analysis of a stationary time series of functions, decomposing it into an integral of uncorrelated functional frequency components (Cramer representation), each of which is in turn expanded into a KL series. This Cramer-Karhunen-Loeve representation separates temporal from intrinsic curve variation, and it is seen to yield a harmonic principal component analysis when truncated: a finite dimensional proxy of the time series that optimally captures both within and between curve variation. This work on doubly spectral analysis is motivated by and applied to the study of the molecular dynamics of DNA minicircles; specifically, we consider the problem of studying the effect of small perturbations of the base-pair composition of such strands on their dynamics in solution, based on molecular dynamics simulations. (Based on joint work with S. Tavakoli, EPFL).