UNIVERSIDADE DA CORUÑA

gmodes DPTO. DE MATEMÁTICAS

CONFERENCIA

"Using BAGIDIS for investigating functional data with sharp local features, with applications to spectroscopy"

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Abstract

The talk presents a new methodology in the context of nonparametric functional statistics. It aims to tackle some common but challenging issues in H-NMR spectroscopic studies: investigating differences between groups of spectra in a dataset, determining a statistical model for the prediction of a measured quantity or a group membership associated to a spectrum, and identifying the zones of the spectra that carry significant information for the discrimination. Statistically, this requires the study of curves with sharp local features, those features being the peaks associated to given resonance frequencies in the spectra, and of which the intensity reflects the concentration of given chemical compounds. A challenge in this problem is to define an efficient measure of the dissimilarity between the spectra. Indeed, a given peak in a set of spectra might be affected by vertical amplifications, horizontal shifts or both simultaneously, the source of those variations possibly being a significant chemical difference or resulting from noise. However, commonly used dissimilarity measures do not return coherent results as soon as there is a horizontal component of variation from one spectrum to another. I propose therefore a new dissimilarity measure which has the ability to capture both horizontal and vertical variations of the peaks in datasets of spectra, in a unified framework. This dissimilarity measure has been called BAGIDIS for BAses GIving DIStances. BAGIDIS is data-driven and highly adaptive to the features of the spectra. Moreover, the scope of application of the method is not restricted to the analysis of H-NMR data, but enlarges to any functional dataset with sharp local features that might possibly be misaligned. An extension is also provided for image data. The method has a sound theoretical background as it fully takes into account three cutting-edge statistical concepts: the nature of functional data, the nonparametric functional regression technique and unbalanced Haar wavelets. As a result, practitioners are provided with a highly flexible tool that can be advantageously used in association with or in addition to state-of-the-art methods for H-NMR spectroscopic data analysis.

Lugar: Aula de Grados Víctor Gulías (Facultad de informática, UDC)

Fecha: 29 de noviembre de 2012

Hora: 10:30