FUNCTIONAL PRINCIPAL COMPONENT ANALYSIS VIA REGULARIZED BASIS EXPANSIONS AND ITS APPLICATION TO PROTEIN STRUCTURAL DATA

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Recently, functional data analysis (FDA) has received considerable attention in various fields such as meteorology, criminology, chemometrics, and a number of successful applications have been reported (see, e.g., Ramsay and Silverman, 2005). The basic idea behind FDA is the expression of discrete observations in the form of a function and the drawing of information from a collection of functional data by applying concepts from multivariate data analysis. Moreover, there are some reports discussed a principal component analysis for functional data. We introduce the *regularized functional principal component analysis* for multivariate functional data set, using Gaussian radial basis functions. An advantage of our regularized Gaussian radial basis function network approach to functional data analysis is that it creates a much more flexible instrument for transforming each individual's observation into a functional form. The use of the proposed method is illustrated through the analysis of the three-dimensional (3D) protein structural data by converting the 3D protein data to the 3-variate functional data set. As a result, the visual inspection showed that the PC plot mostly coincided with the biological classification.