Sharpened Signal Regression

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Abstract

A wide range of scientific studies often provide data that are obtained in the form of "functional" curves that are observed on a fine grid. The type of problem we consider is one where one wants to predict a scalar response from regressors in the form of digitized curves or spectra. We propose two variations of P-spline signal regression: space-varying penalization signal regression (SPSR) and additive polynomial signal regression (APSR). SPSR uses space-varying roughness penalty according to the estimated coefficients from the partial least-square regression, while APSR expands the linear basis to polynomial bases. SPSR and APSR are motivated in the following two scenarios respectively: (i) some region(s) of the regressor channels contain more useful information for prediction than others; (ii) the relationship between the response and regressor channels is highly nonlinear. In doing so we offer a compromise between signal regression and partial least squares approaches. We also extend the methods to the generalized linear regression setting. As illustration, we apply the methods to two published data sets showing highly competitive performance. This is joint work with Bin Li and Paul Eilers.

Keywords: Multivariate calibration, P-splines, partial least squares.