Single-Index Signal Regression

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Abstract

We take a novel approach the signal regression (multivariate calibration) problem, in particular where the signal (spectra) regressors have two-dimensional structure. In general linearity is assumed to hold, but this may not be true. Our application considers UV-VIS spectra taken over several temperatures used to predict components of a ternary mixture. Through simultaneous estimation, we parse out and estimate two separate modeling components: (1) a single *smooth regression coefficient surface* associated with the two-dimensional signal, and (2) an unknown, possibly nonlinear, *link function*. Although the first component is linear, the second component explicitly models the nonlinearity, while enhancing insight into the measurement process. Linking the response to the linear predictor is in the spirit of single-index models. Using (tensor product) P-splines for each component, we will see that their combination can lead to a systematic and tractable statistical modeling approach, while having improved external prediction performance when compared to standard signal regression approaches and partial least squares. Optimal tuning will be discussed. We close with other applications that demonstrate simplifications to 1D signals and extensions to binary response.

Keywords: Multivariate calibration; P-splines; signal regression; single-index; spectra; tensor product; ternary mixtures.

*Joint work with Bin Li and Paul Eilers
Reference: Chemometrics and Intelligent Lab Systems, 2011, **109**