Sparse Semiparametric Nonlinear Models with Applications to Chromatographic Fingerprints

Traditional Chinese herbal medications (TCHMs) are comprised of a multitude of compounds and the identification of their active composition is an important area of research. Chromatography provides a visual representation of a TCHM sample's composition by outputting a curve characterized by spikes corresponding to compounds in the sample. Across different experimental conditions, the location of the spikes can be shifted, preventing direct comparison of curves and forcing compound identification to be possible only within each experiment. In this talk, I will first discuss a sparse semiparametric nonlinear modeling framework for the establishment of a standardized chromatographic fingerprint across different experimental conditions. Data-driven basis expansion is used to model the common shape of the curves while a parametric time warping function registers across individual curves. Penalized weighted least squares method with the adaptive lasso penalty provides a unified criterion for registration, model selection, and estimation. We will then extend this framework to compare fingerprints from different groups of herbal medicine. Two real datasets will be used as illustrations. *This is based on my former student Michael R. Wierzbicki’s dissertation.*

Thursday, November 5, 2015  3:30 PM - 4:30 PM
Blue Cross & Blue Shield Auditorium (0001 MHRC)