STAT 280B-01: Seminars in Statistics on Nov-4th, 2019 (Monday 4pm in Engineering 2, Room 192)

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Title: Spatial Statistics Methods for the Analysis of XANES Stacks Data

Abstract: Arsenic in drinking water, even in trace amounts, can be extremely harmful to human health with prolonged exposure. In many parts of the world where there is not access to filtered, clean drinking water, arsenic poisoning is an extreme danger. It is well known how arsenic should bind in pure systems through chemical formulas, but in the complex and heterogeneous conditions of soil, the proclivities and diversity of its binding mechanisms are not well understood. Current technologies such as synchrotron X-Ray fluorescence microprobe (XRF) and X-Ray absorption near edge structure (XANES) spectroscopy allow for the examination of the sub-micron binding of arsenic and to characterize its variation on an arsenic-treated sand grain. By fitting collected normalized spectra to known standards, scientists draw inferences about chemical species of a given element in a sample. Often, micro-scale spectra are normalized and fit individually using conventional software designed for bulk-sample spectra, and the physical spatial connection between spectra taken on the same sample may not be considered. I present an approach for incorporating spatial dependence in the normalization of the spectra, selecting standard spectra, and finally the fitting to those selected standards of known composition. These methods are applied to draw inference on arsenic fluorescence XANES data collected at the SRX Beamline at NSLS-II at Brookhaven National Laboratory in order to determine spatially contiguous mappings of likely variation in arsenic species across a 10 × 10 micron region on a soil sand grain.