School of Computer Science and Engineering
Presentation

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Bayesian Networks Resource for Meta-analysis: Cellular Toxicity of Quantum Dots

Title:

Nanotechnology is being used increasingly in the manufacturing of various nano-enabled products that we use every day. Engineered Nanomaterials (ENMs) of dimension in the size range of 1 - 100 nm with incredibly complex and emergent properties are making breakthroughs, but concerns are also rising about their safety. Due to data scarcity and highly complex and heterogeneous configurations of ENMs, their environmental and health impact assessment is challenging. It is therefore imperative to utilize data driven and machine learning/artificial intelligence (ML/AI) approaches for informed decision making and policies around the regulation of ENMs. In this talk, I will present the meta-analysis of the cellular toxicity of cadmium containing Quantum Dots (QDs) that I developed in collaboration with the US Naval Research Laboratory(NRL). The study extracted pertinent knowledge from the largest available body of evidence in Nanotechnology (517 peer reviewed publications) via ML approaches (Bayesian Networks (BNs) and association rule mining) to identify the most significant QD attributes and the experimental conditions that largely influence their cytotoxicity. I will first discuss the statistical methods used to quantify the correlations of QD properties with their cytotoxicity. I will then present BNs, developed for QD *cell viability* (%) and *IC50*as online tools, which can: (a) serve as an intelligent query (IQ) system for exploring the compiled dataset,(b) identify the quantitative and qualitative attributes most relevant to these QD cytotoxicity metrics via parameter sensitivity analysis, and (c) identify causal relationships of the QD cytotoxicity with QD attributes as well as reported experimental conditions. Using these models, we identified the most relevant attributes for correlating *IC50* as: QD diameter, exposure time, QD surface ligand, shell, assay type, surface modification, and surface charge, with the addition of QD concentration for the cell viability analysis. I will discuss the applicability of such meta-analysis to any given nanomaterial as an online decision support tool to establish a roadmap for interrogating wide-ranging toxicity data and streamlining safer by design principles for Nanomaterials. Finally, I'll highlight other potential areas of interest where the proposed AI based approaches are best suited for discovery and advances.