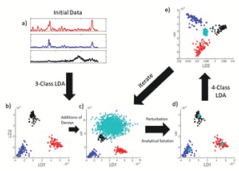
# GENERATIVE ADVERSARIAL LINEAR DISCRIMINANT ANALYSIS FOR DISTINGUISHING API POLYMORPHS BY RAMAN SPECTROSCOPY

ZIYI CAO, CASEY J SMITH, YOULIN LIU, ALEX M SHERMAN, GARTH SIMPSON, *Department of Chemistry, Purdue University, West Lafayette, IN, USA*.




Raman Spectroscopy is a great way to distinguish different kinds of API polymorphs.[a]However,adversarial attacks on spectral classifiers were shown to enable identification of potential vulnerabilities in common dimension reduction analyses of Raman spectra. We tackled this susceptibility with the Generative Adversarial Linear Discriminant Analysis (GALDA) approach. GALDA is analogous to Generative Adversarial Nets (GAN) in the machine learning context. Conceptually in a typical GAN, two models were simultaneously trained, a generative model G that attempts to estimate the sample distribution and a discriminative model D that classifies the output of G.These two models seek to achieve Nash equilibrium during the iterative adversarial training process.[b] We herein incorporated this concept into spectral classification. Spectral classification in the spectroscopic context seems to lag albeit the mass development in the computer science area. As such, the analyzation methods' robustness and susceptibility to malicious attack is considered even less. Therefore, GALDA aims to test against the robustness of LDA classifiers and provide a new framework for considerations for classification strategies less susceptible to spurious misclassification.

[a] Shijie Zhang, et al. Dynamic Sparse Sampling for Confocal Raman Microscopy, Analytical Chemistry 2018

[b] Goodfellow, Ian, et al. Generative adversarial nets, Advances in neural information processing systems. 2014